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ESSCIRC ESSDERC 2015

DEFECTS RESPONSIBLE FOR BTI IN CMOS DEVICES: MORDRED PERSPECTIVE

Atomistic picture

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EC FP7 PROJECT MORDRED

Modelling of the reliability and degradation of next generation nanoelectronic devices

- Funded by EC within FP7
- Duration 04/2011 – 03/2015
- Overall funding 4.5 M€
- Consortium of
  - 3 companies
  - 5 research institutes/universities

This project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no 318458.

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OUTLINE

1. Introduction
2. Carrier capture/emission by oxide defects
3. Computational models
4. Defect parameter extraction from experimental data
5. Establishing defect models
6. Defect reactions
7. Summary and Outlook

MORDRED Grand Design

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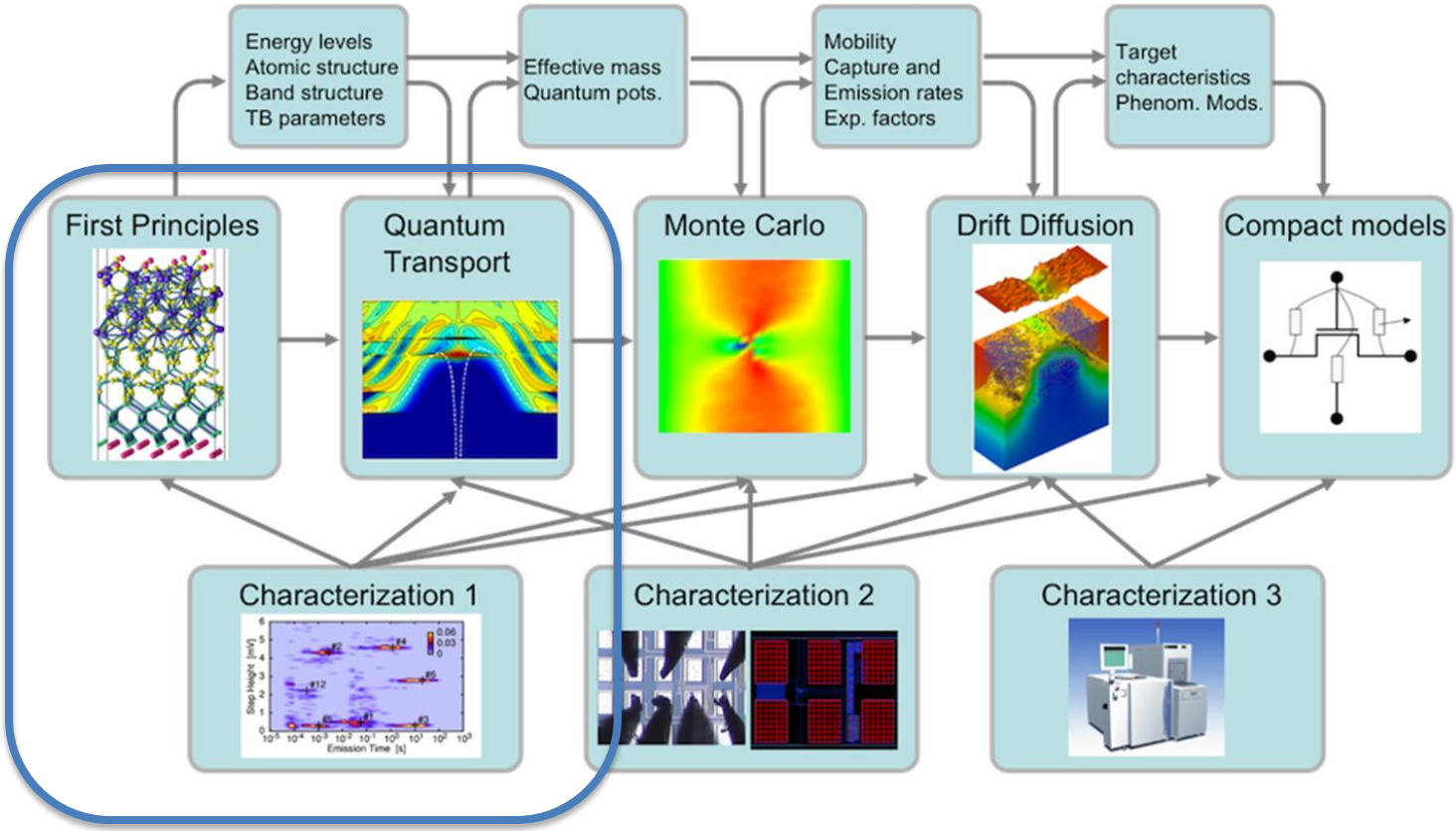

To develop multi-scale modelling technology, supported by comprehensive experimental characterization techniques, to study the degradation and reliability of next generation CMOS devices

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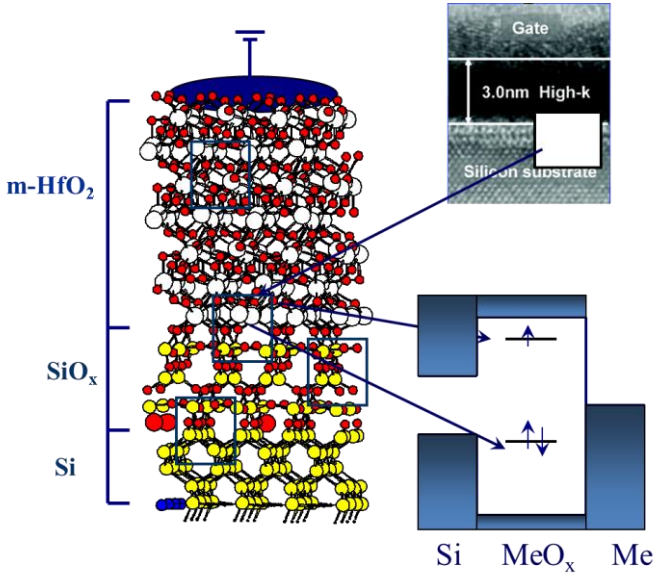
Electronic devices are complex systems of *interfaces*

- Generic atomistic models for interfaces
- Relation between defects structure and interface morphology
- Electronic structure of the electron and hole traps



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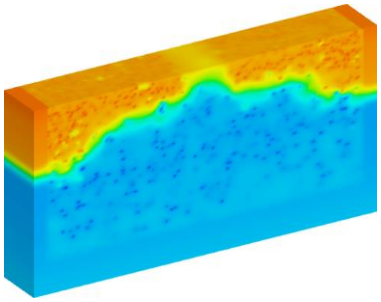
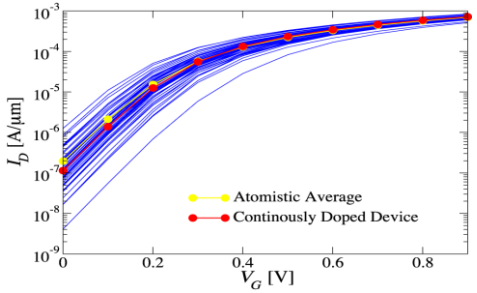
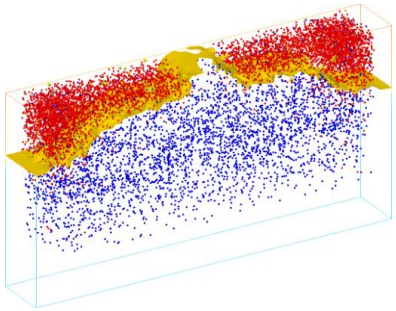
Goal: Linking atomistic and device modelling

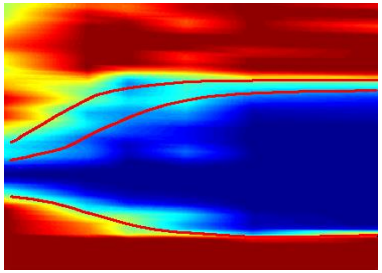




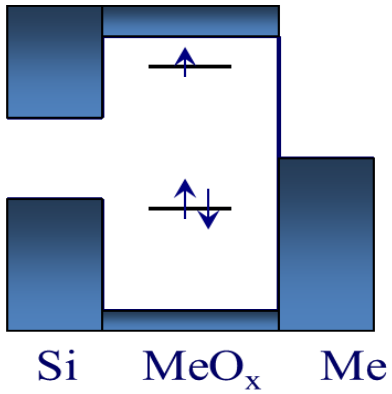


- Three dimensional
- Statistical
- Quantum corrections

Input from atomistic modeling



- Dielectric constant variations.
- Band gap variations.
- Interface states.
- Defect states in the dielectric.
- *e* scattering potentials
- Granularity models



Collaboration with GU and TU Wien

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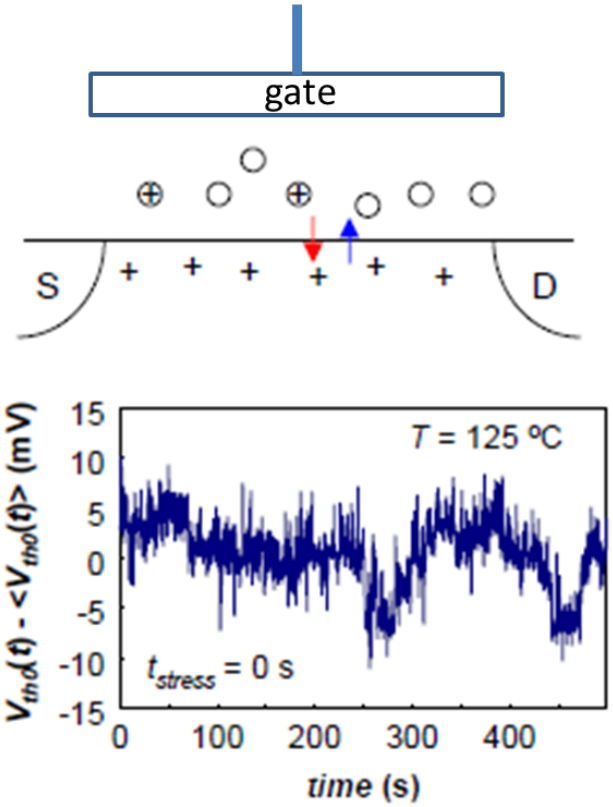
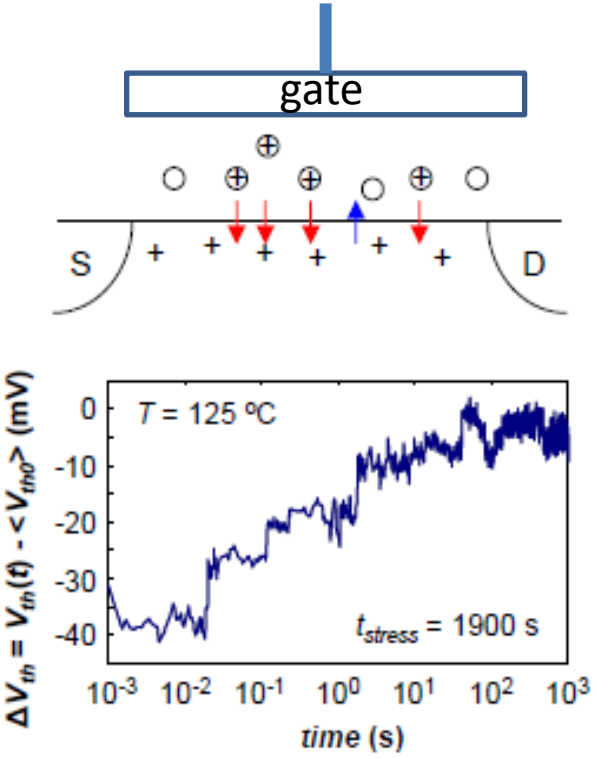
RANDOM TELEGRAPH NOISE



B. Kaczer et al. IRPS10

- At **constant bias** conditions, oxide defects are charged by channel carriers and subsequently discharged back into the channel
- A **wide range of time constants** is controlled by a nonradiative **multiphonon emission process**
- The system is in ***dynamic* equilibrium**, manifested by low-frequency noise or Random Telegraph Noise (RTN) in small devices

(NEGATIVE) BIAS TEMPERATURE INSTABILITY

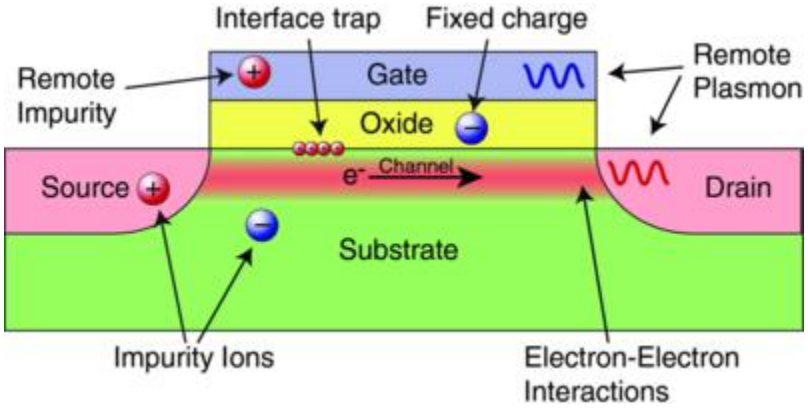


B. Kaczer et al. IRPS10

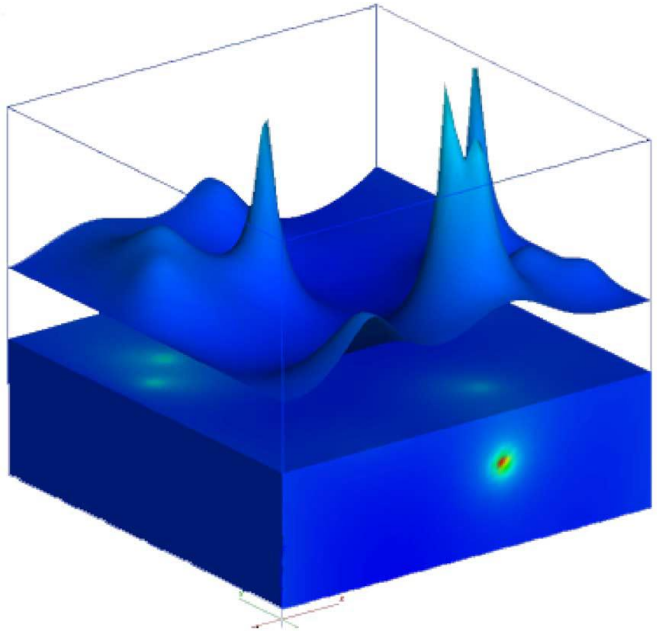
- Following the perturbation by NBTI stress, excess **charged oxide defects gradually discharge** and the system is returning to the dynamic equilibrium of (a), resulting in long NBTI transients

- NBTI in downscaled devices can be treated as a **stochastic ensemble of individual defects**, Poisson-distributed in number per device, with each defect described by its impact on the channel conduction characterized by its **capture and emission times**

PERCOLATION PATH



Carrier scattering centres in CMOS devices



Potential distribution in a 3-D volume with random discrete dopants. The carriers are scattered by Coulombic potential of the dopants.

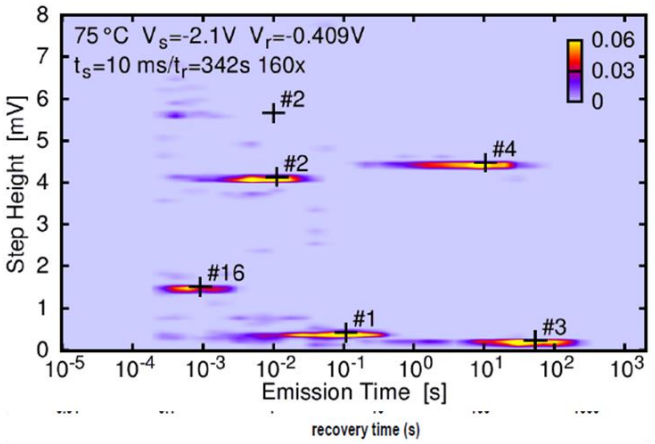
E. A. Towie et al. Semicond. Sci. Techn. 26, 055008 (2011)

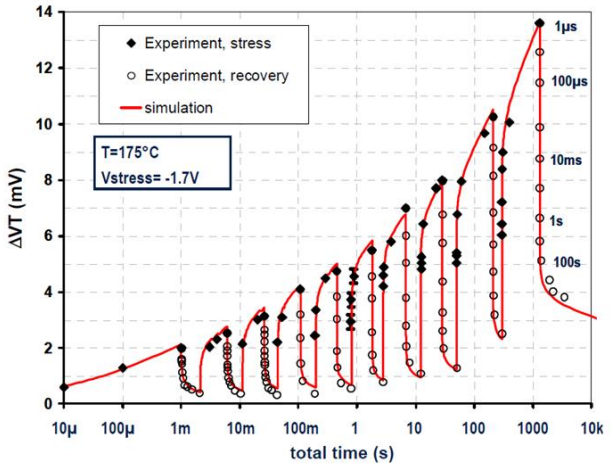
C. Alexander et al., Sol. St El. 49, 733 (2005)

TIME-DEPENDENT DEFECT SPECTROSCOPY

Negative Bias Temperature Instability

- Time dependent defect spectroscopy: Small area devices in which recovery after stress proceeds in discrete steps
- Each discrete step due to emission of **single** trapped charge carrier
- **Individual defects** characterized by step height





REVERSE-ENGINEERING DEFECT MODELS

- Model extraction
- Candidate selection
- Candidate evaluation
- Rate calculation

Defect elimination

Computational details

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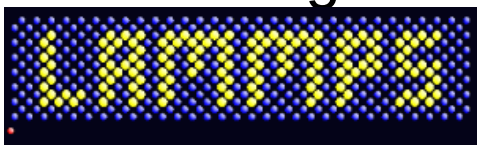
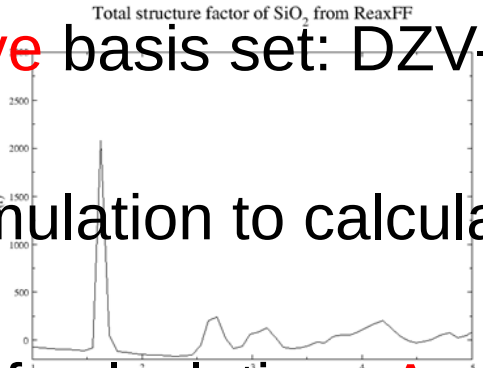
Calculations performed on > 300 models of amorphous silica with cells containing 216 atoms

Amorphous silica generated using empirical force-field (ReaxFF) and molecular dynamics to simulate heating and

$$E(q_1,\ldots,q_N)=\sum_i^N\left(E_{i0}+\chi_i^o q_i+\frac{1}{2}J_{ii}^o q_i^2\right)+\sum_{i<j}^N q_i q_j J_{ij}$$

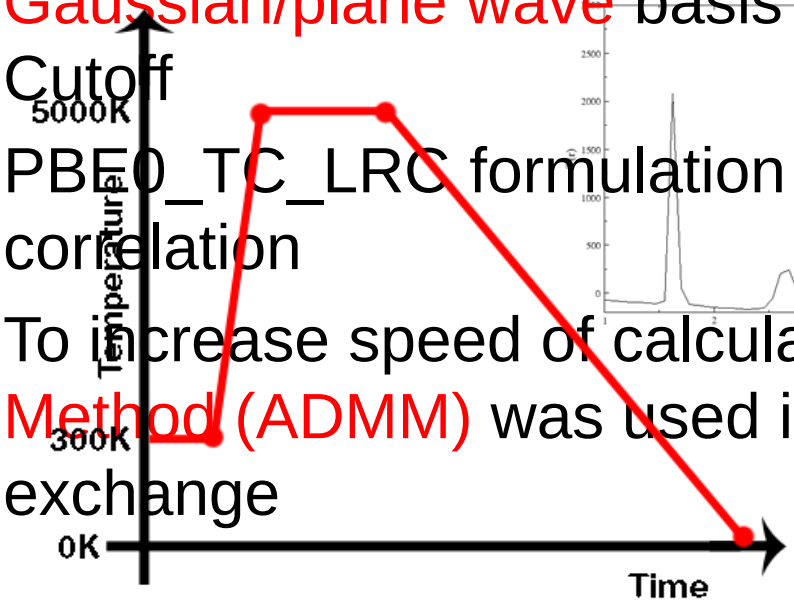


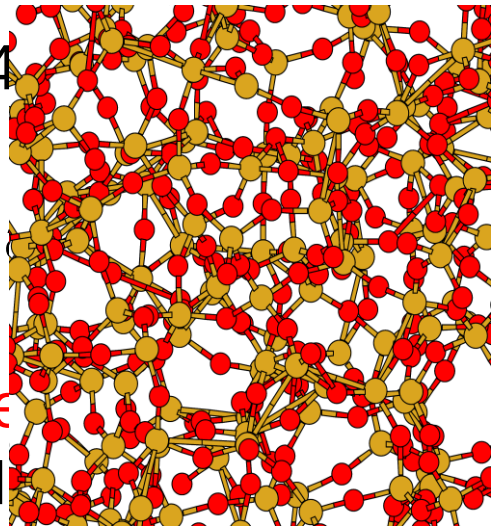
Gaussian/plane wave basis set: DZV-Basis, 4
Cutoff



PBE0_TC_LRC formulation to calculate exch
correlation

To increase speed of calculations Auxiliary De
Method (ADMM) was used in calculation of H
exchange





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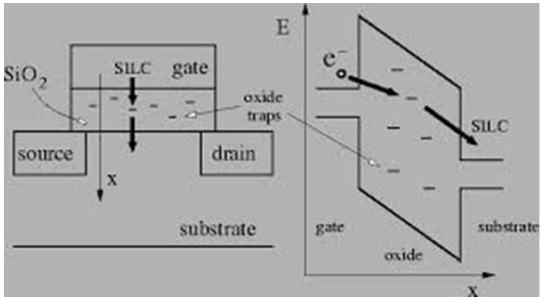
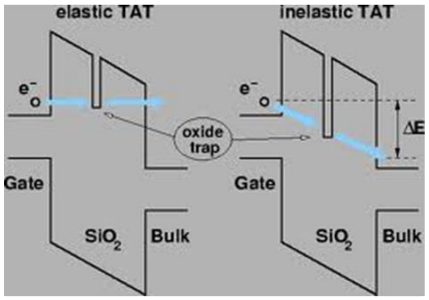
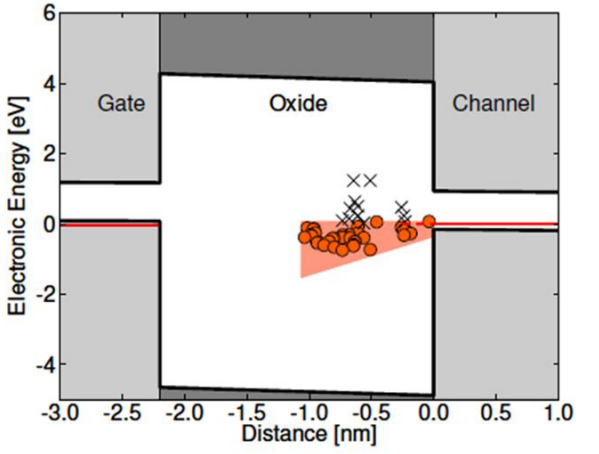
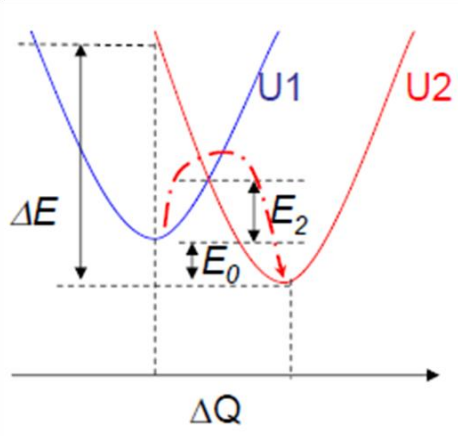
TRAP ASSISTED TUNNELLING







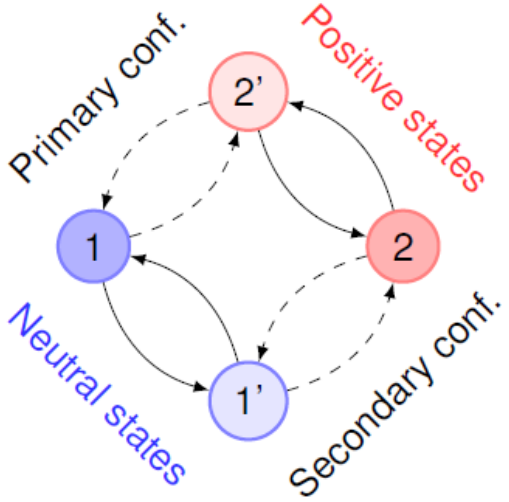
Experimental window



Configuration diagram

MODEL EXTRACTION

Identifying atomistic oxide trap responsible for NBTI:



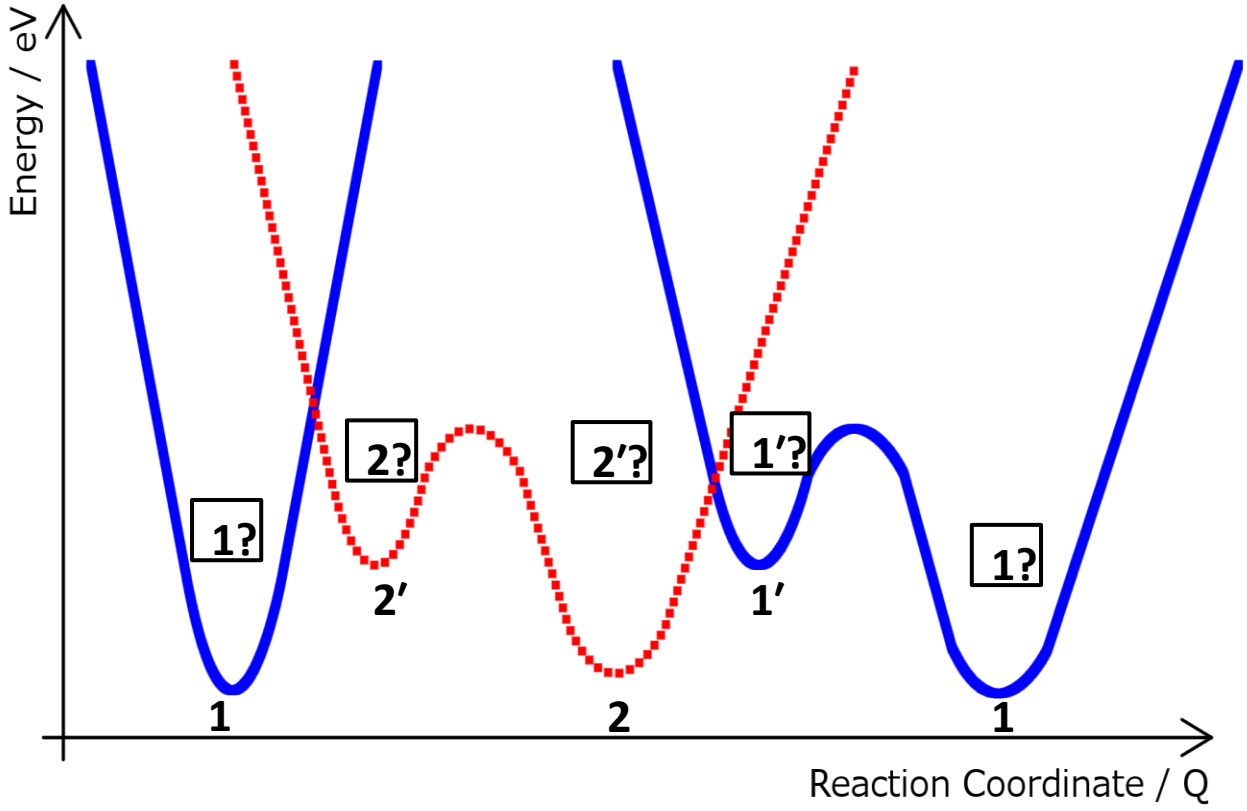
- Multi-state Multi-phonon model
- $\tau_c = \tau_{12'} + \tau_{2'2}(1+ \tau_{12'} / \tau_{2'1})$
- $\tau_e^{-1} = \tau_{e1}^{-1} + \tau_{e2}^{-1}$
- $\tau_{e1} = \tau_{22'} + \tau_{2'1}(1+ \tau_{22'} / \tau_{2'2})$
- $\tau_{e2} = \tau_{21'} + \tau_{1'1}(1+ \tau_{21'} / \tau_{1'2})$

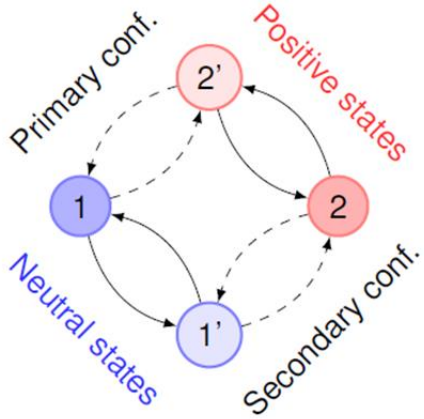
- Barrier-hopping transitions: $\tau_{\alpha\beta} = \nu^{-1} \exp[E_{\alpha\beta}/K_B T]$

- Vibronic transitions: $\tau_{if} = 2\pi/\hbar \, |\langle\Phi_f|V'|\Phi_i\rangle|^2 \, |\langle\eta_{f\beta}|\eta_{i\alpha}\rangle|^2 \, \delta(E_{f\beta}-E_{i\alpha})$
  - Summing over all vibrational states: Lineshape function
  - $fv^{(0/+)} = \text{avg} \, \Sigma \, |\langle\langle +F|0I\rangle\rangle|^2 \, \delta(E_{0I} - E_{+F} - E_{v0} - E)$

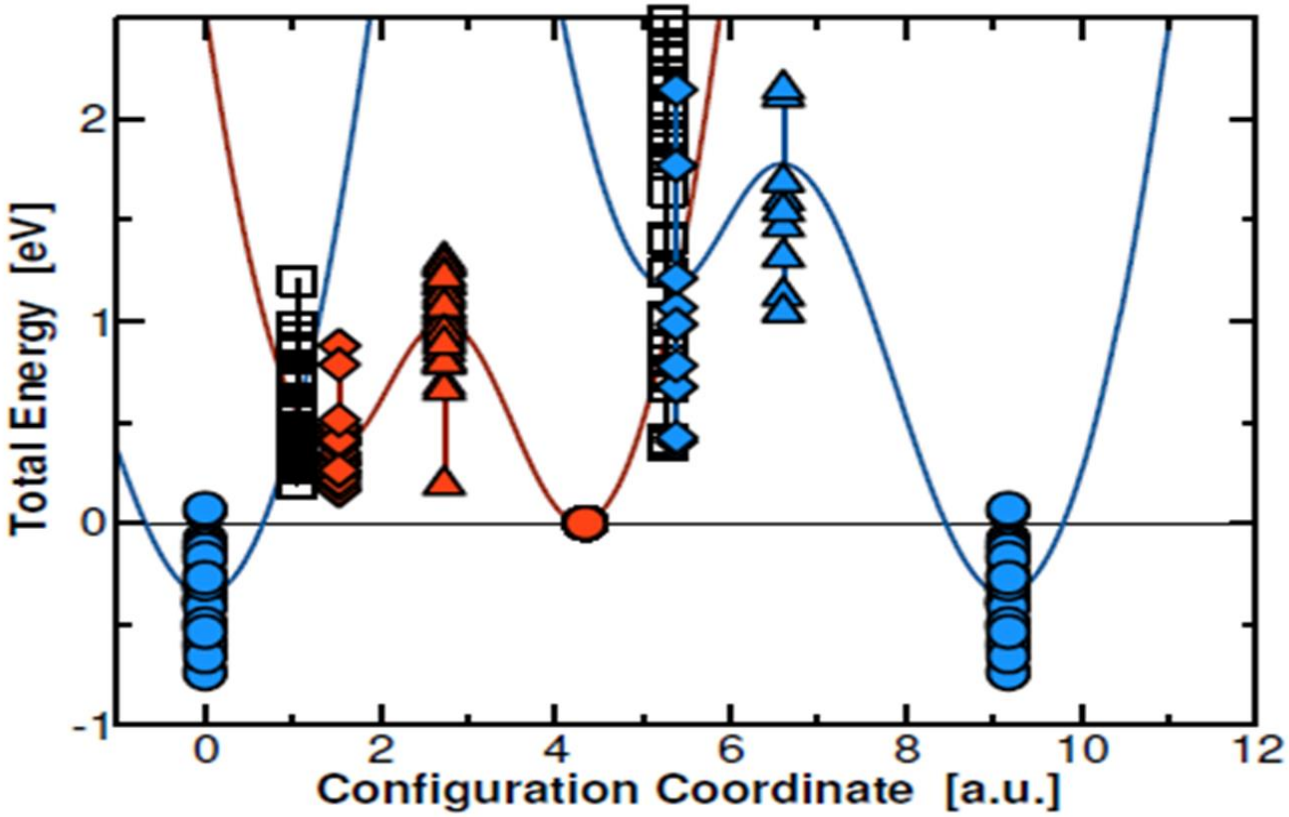
T. Grasser et al., IEEE TRANSACTIONS ON ELECTRON DEVICES 2011

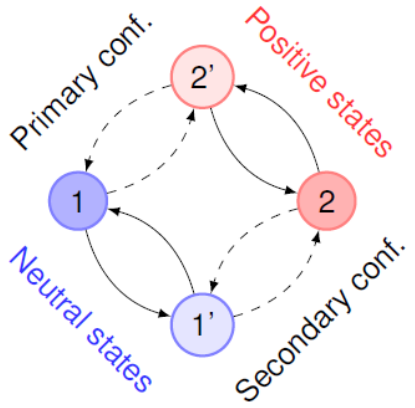
ENERGY LANDSCAPE: HYPOTHETICAL



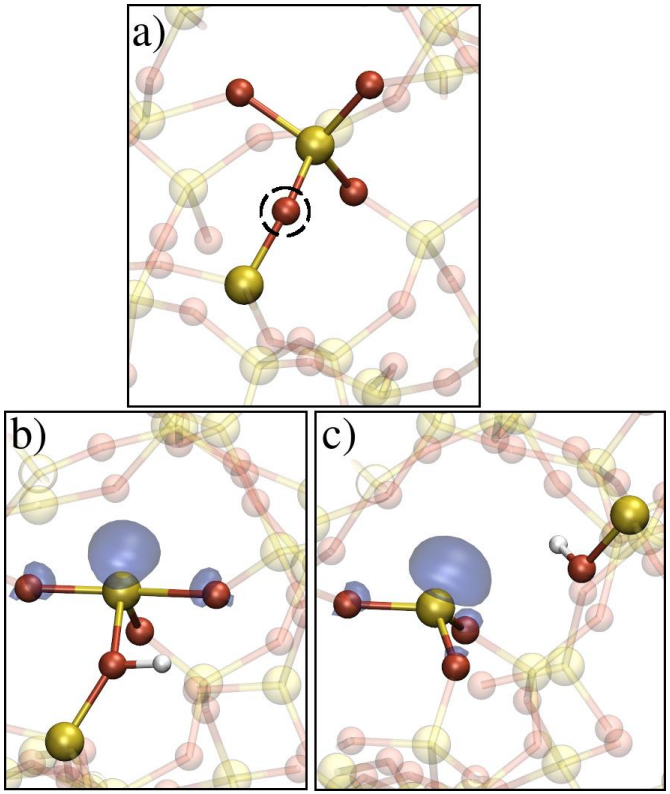


ENERGY LANDSCAPE: EXTRACTED





DEFECT MODELS



Atomic configuration and spin density of the two hydrogen induced defect configurations and their precursor:

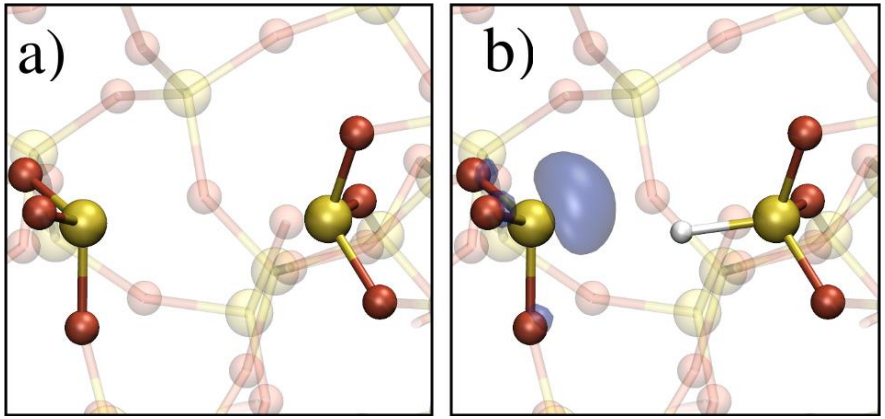
a) An unperturbed SiO_4 tetrahedron;

b) The **$[SiO_4/H]^0$ center**

c) The **hydroxyl E´ center**

A-M. El Sayed et al. Phys. Rev. B. 92, 014107 (2015)

DEFECT MODELS

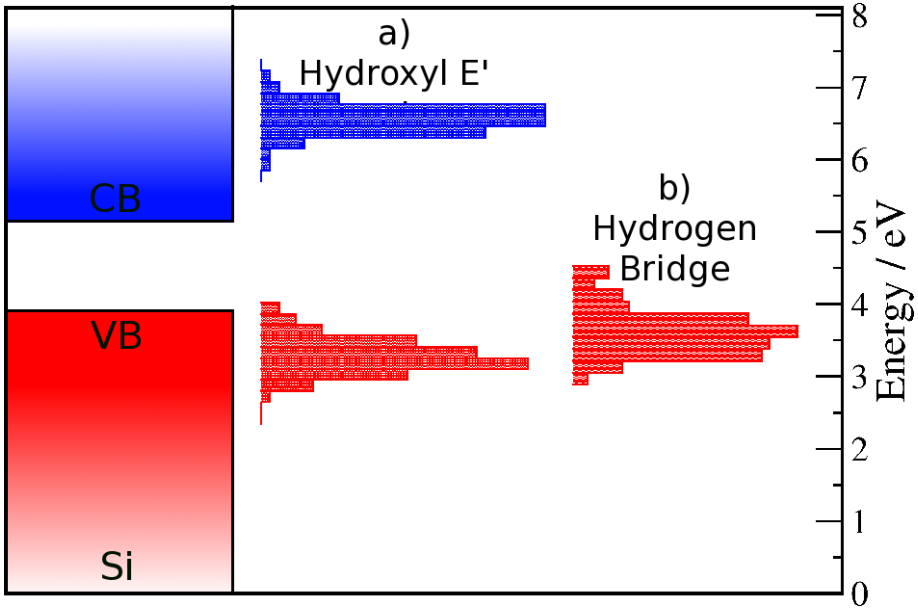


a) Atomic structure of the **oxygen vacancy** which is the precursor to the hydrogen bridge

b) Atomic structure and spin density of the **hydrogen bridge**

A-M. El Sayed et al. Phys. Rev. B. 92, 014107 (2015)

DISTRIBUTION OF DEFECT LEVELS

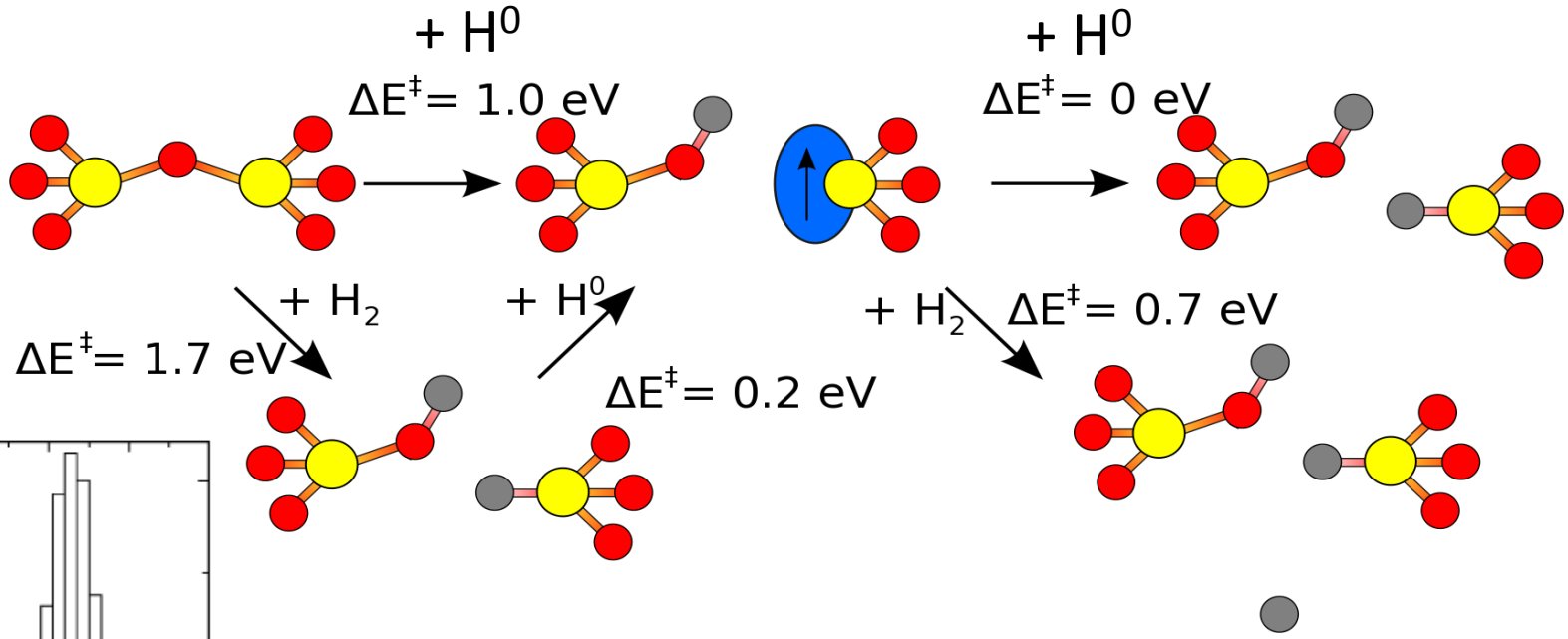


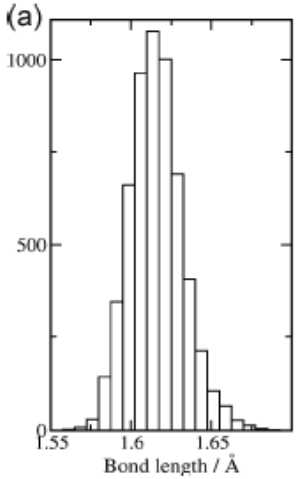
Histogram of the one-electron levels of defect configurations of:
a) the hydroxyl E´ center,
b) the hydrogen bridge defect

The area in the histograms colored dark red show occupied states while the area of the histograms colored blue show the unoccupied states.

A-M. El Sayed et al. Phys. Rev. B. 92, 014107 (2015)

HYDROGEN REACTIONS

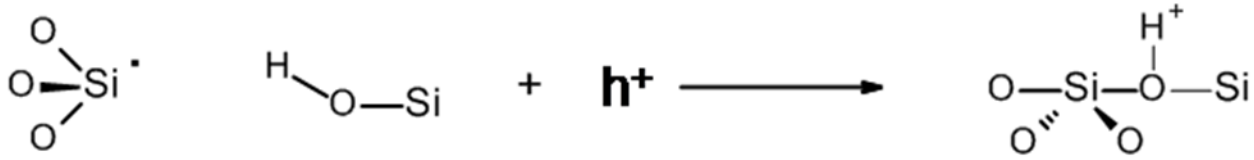




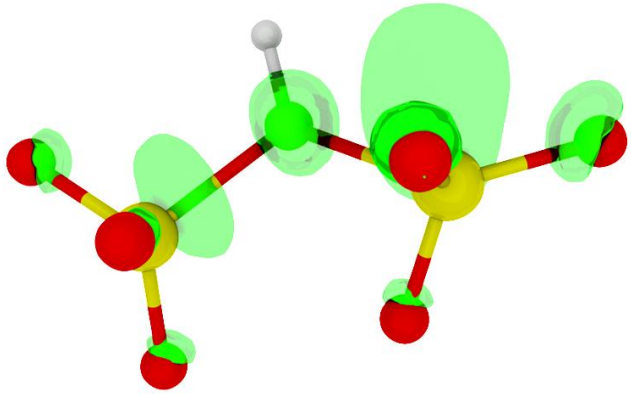
H^0 can break strained Si – O bonds

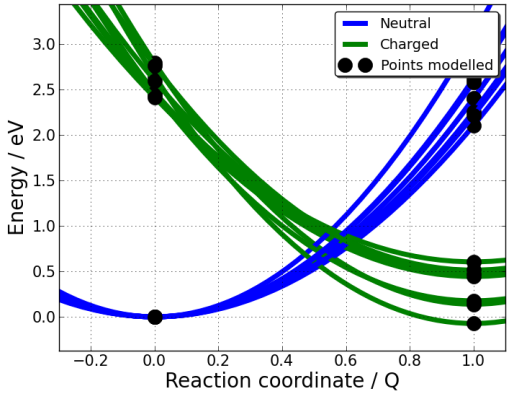
Hydroxyl E' centre is formed at sites where Si – O bond is > 1.65 Å

HOLE TRAPPING AFTER DEFECT ACTIVATION



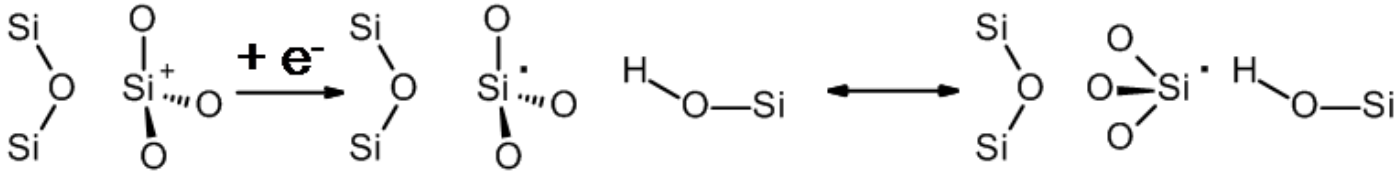
- **Hole** can be trapped on the defect state ~ 3.5 eV above SiO_2 VB
- **Two** configurations are possible. Si-O bond can reform and proton is bound to bridging O

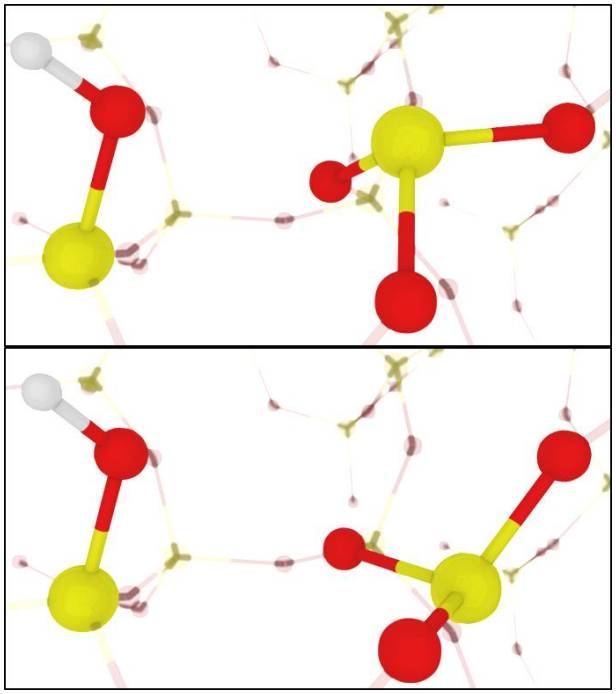




A-M. El-Sayed et al. Microel. Eng. 147, 141 (2015)

ELECTRON RE-TRAPPING





- A metastable state in the neutral charge state for the puckered configurations where an electron is trapped on a back-projected O_3Si
- The barrier from the back-projected configuration to the ground state is <1.1 eV> (0.3 – 1.6 eV) while the back-projected configuration is higher in energy by <0.7 eV> (0.2 – 1.6 eV)

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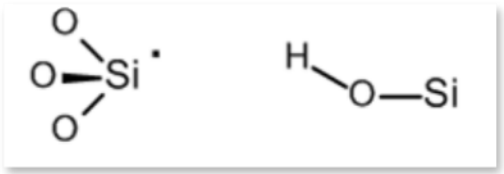
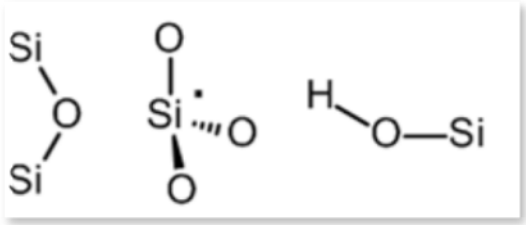
HYDROXYL E´ CENTRE: SUMMARY

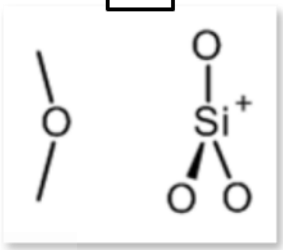
1



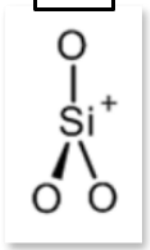
1′

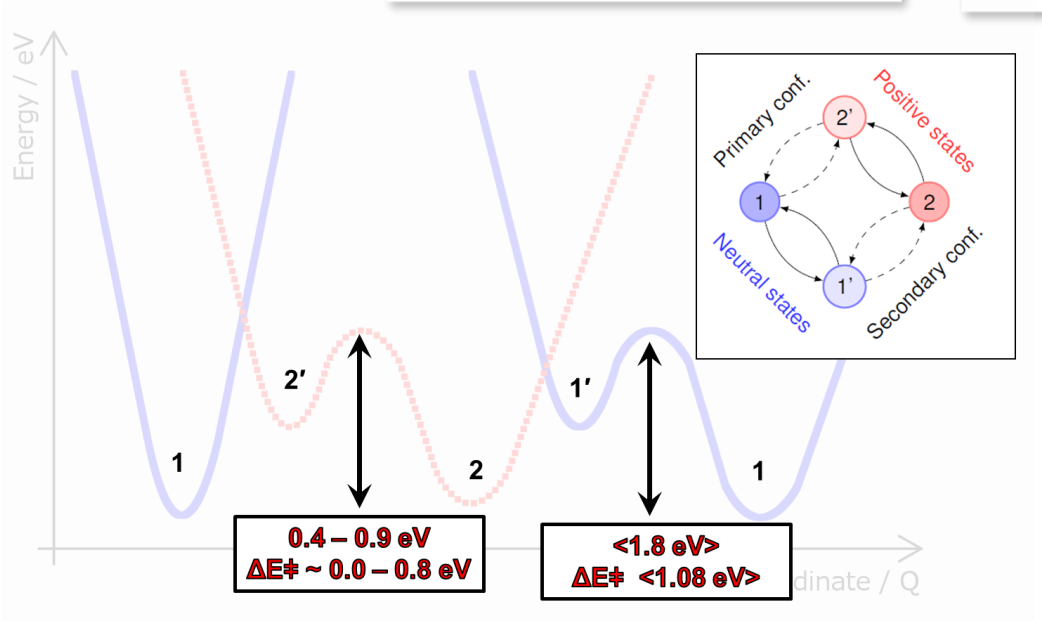


2



2′





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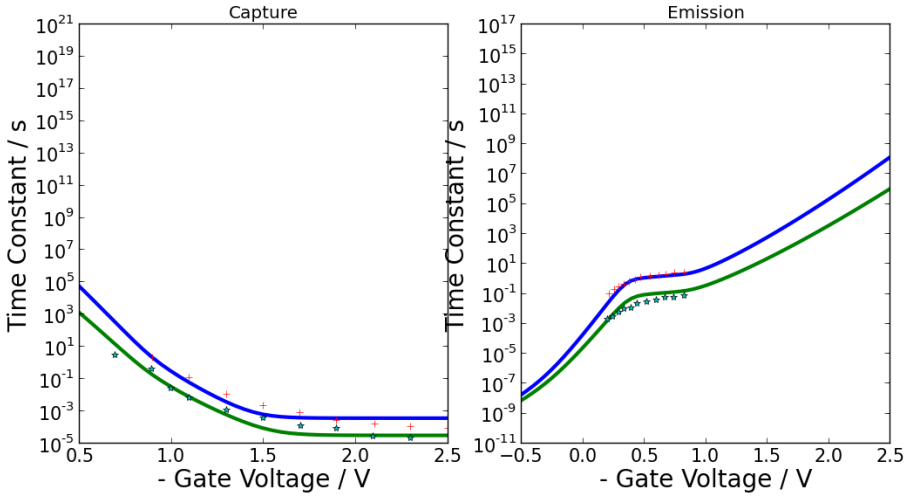
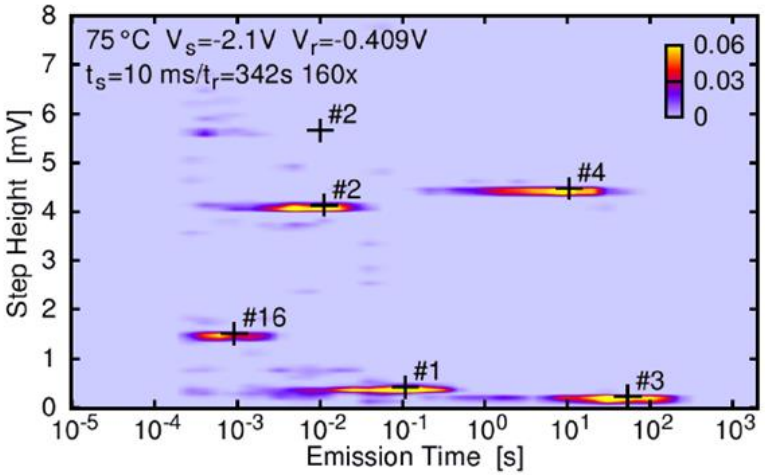
HYDROXYL E´ CENTRE: RATES





Calculated defect parameters give good agreement with the capture and emission rate dependence on voltage and temperature

SUMMARY AND OUTLOOK

- Developed a multi-scale methodology for determining defects in the gate oxide and interface layer responsible for fixed charge and BTI
- Multi-state Multi-phonon model is used to calculate capture and emission events in Si/SiO_2 devices linked to ab initio calculations
- H generates defect states in a-SiO_2 which are resonant with Si CB
- H used in device manufacturing processes to passivate electrically active defects can also activate defects
- Similar processes explain reliability issues in high-k stacks