ATOMIC-SCALE THEORY OF RADIATION-INDUCED PHENOMENA

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In collaboration with the rest of the MURI team

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THEORY OBJECTIVES

- DISPLACEMENT DAMAGE
  - Defects, charging
  - electrons
- ROLE OF HYDROGEN, OXYGEN VACANCIES
- ALTERNATE DIELECTRICS
  - Interface structure, interface defects, NBTI,…
- CARRIER MOBILITIES, LEAKAGE CURRENTS

FROM ATOMIC-SCALE PHYSICS TO ENGINEERING MODELS

Atomic-scale physics:

DENSITY FUNCTIONAL THEORY

- PSEUDOPOTENTIALS, SUPERCELLS
- TOTAL ENERGY, FORCES ON ATOMS
  - Stable defect configurations
  - Bulk, interface
  - Reaction energies, activation barriers
- EVOLUTION OF SYSTEM

  electrons in instantaneous ground state vs

  electrons allowed to evolve freely

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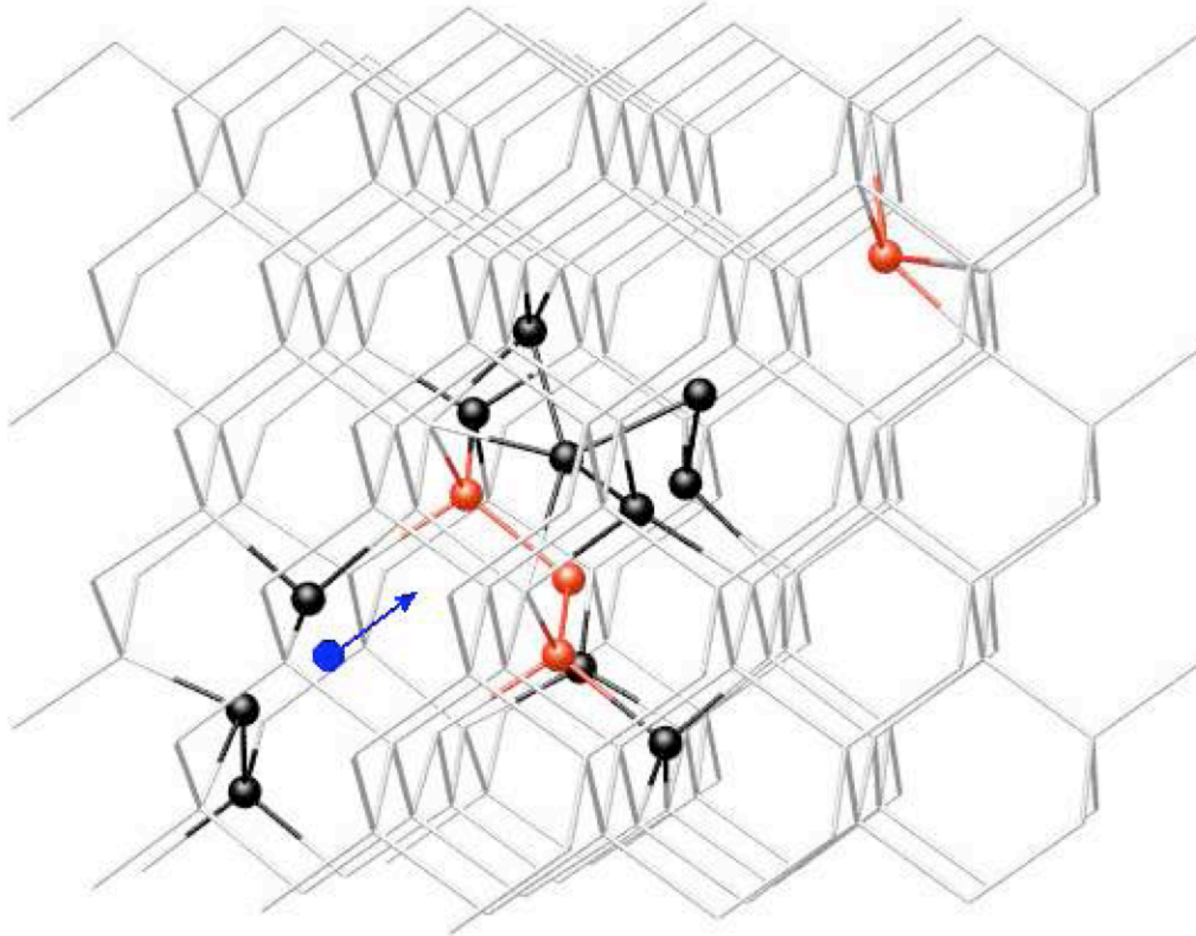
FROM ATOMIC-SCALE PHYSICS TO ENGINEERING MODELS

LAST YEAR: Displacement damage in silicon



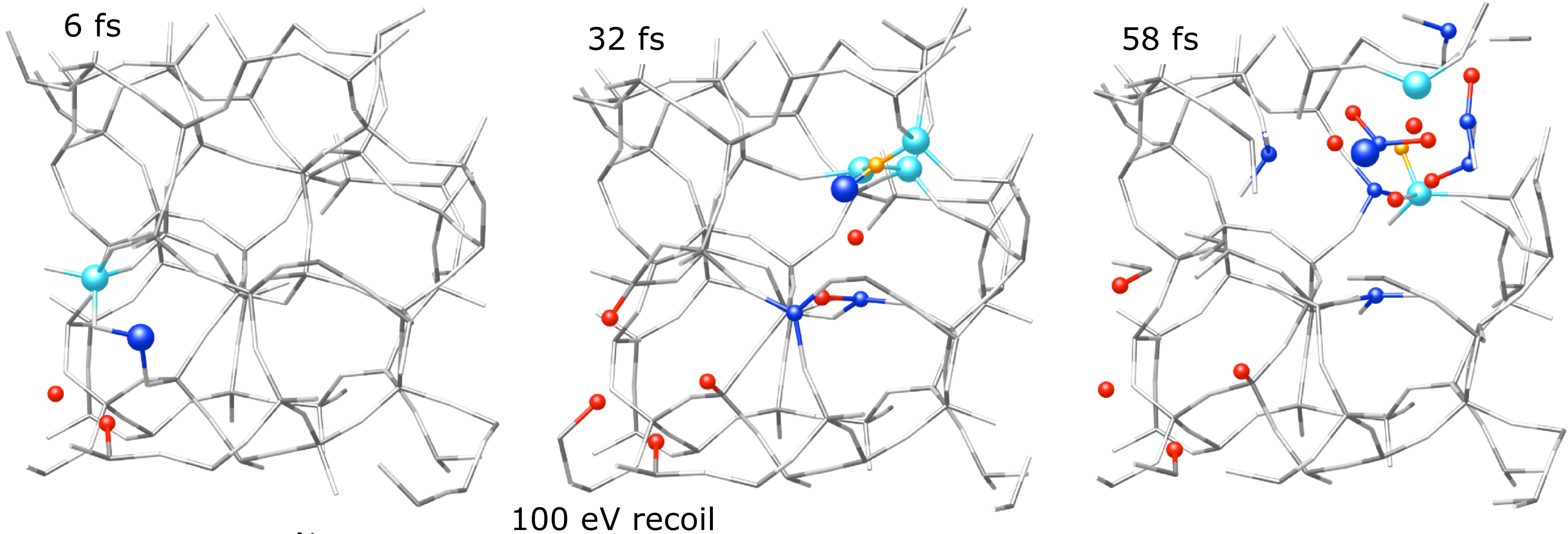
25 eV kick

Snapshot after 100 fs

Red (hot) atoms: KE > 0.22 eV

Black atoms: displaced > 0.2 Å

LOW-ENERGY RECOIL DYNAMICS IN AMORPHOUS SiO_2



Defect	Atom: Silicon	Atom: Oxygen
Dangling Bond	●	●
Extra Bond	●	●
"Self Bond"	Big Ball	

Damage in amorphous material: Network defects

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  TALK BY BATYREV
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FROM ATOMIC-SCALE PHYSICS TO ENGINEERING MODELS

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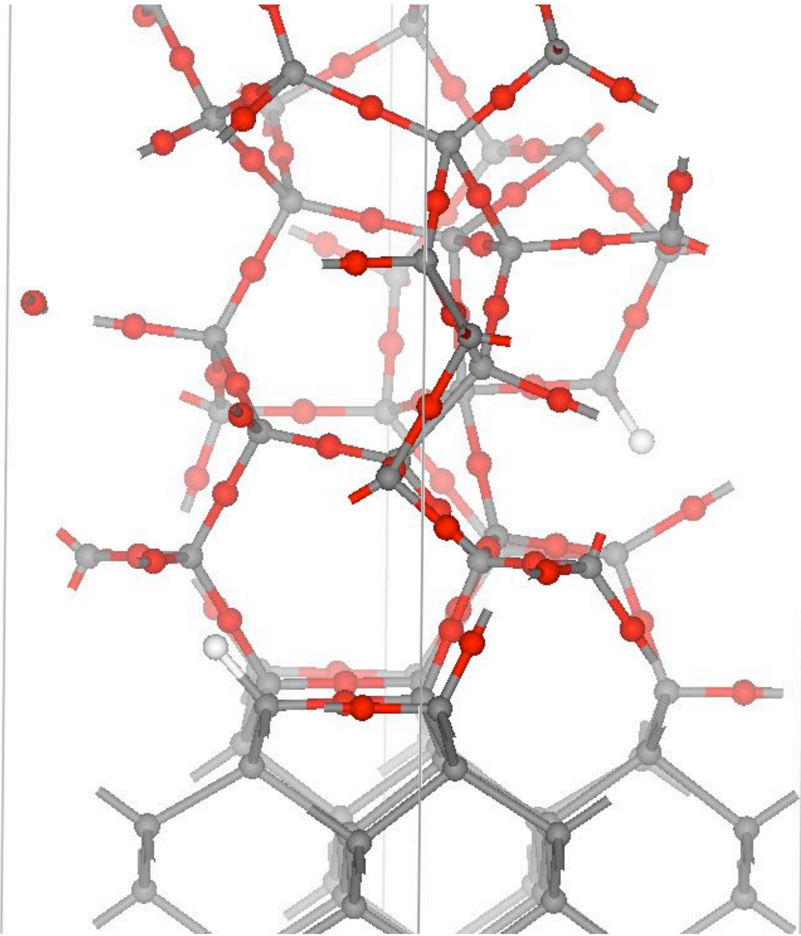
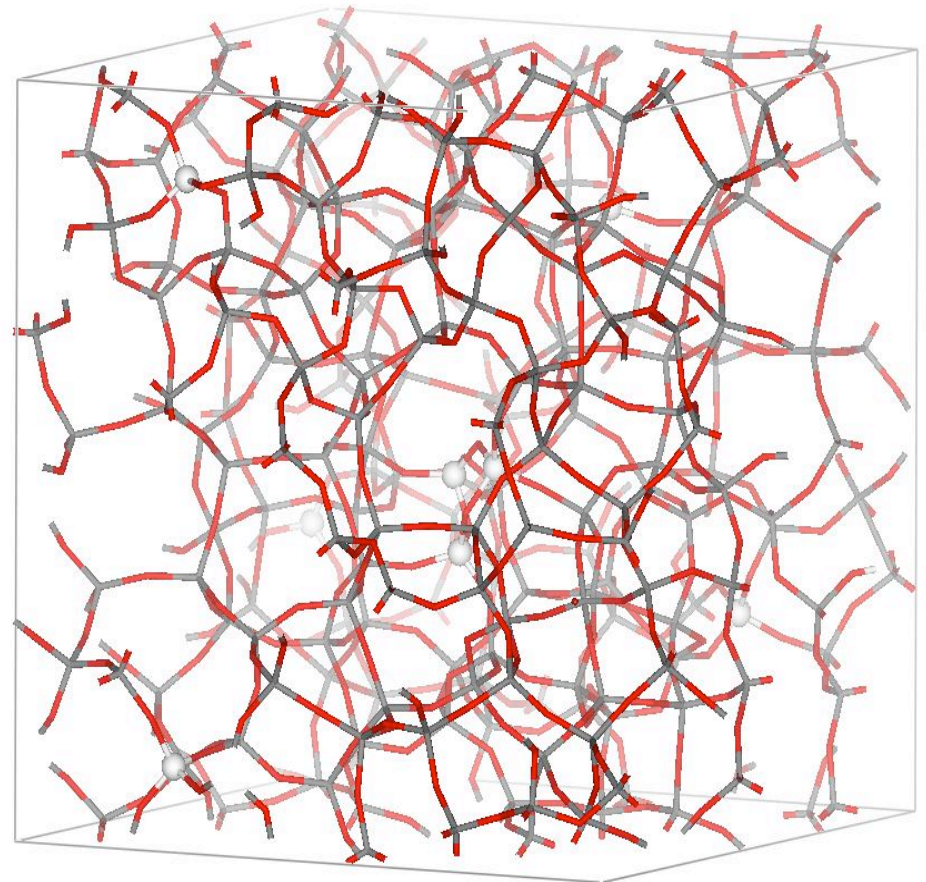
FROM ATOMIC-SCALE PHYSICS TO ENGINEERING MODELS

Amorphous Modeling

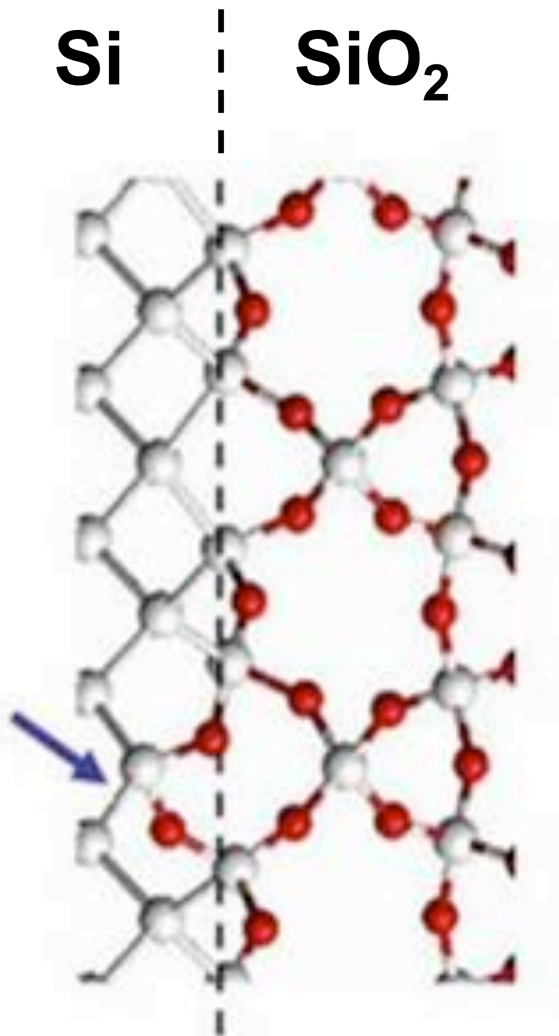


Si-SiO_2 with Si-H bonds

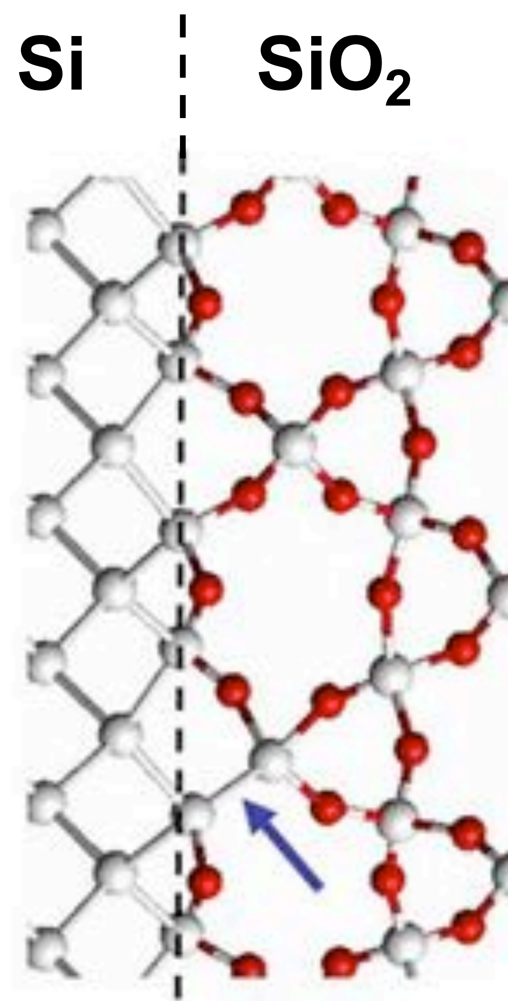


216-atom amorphous SiO_2

ATOMIC-SCALE ROUGHNESS

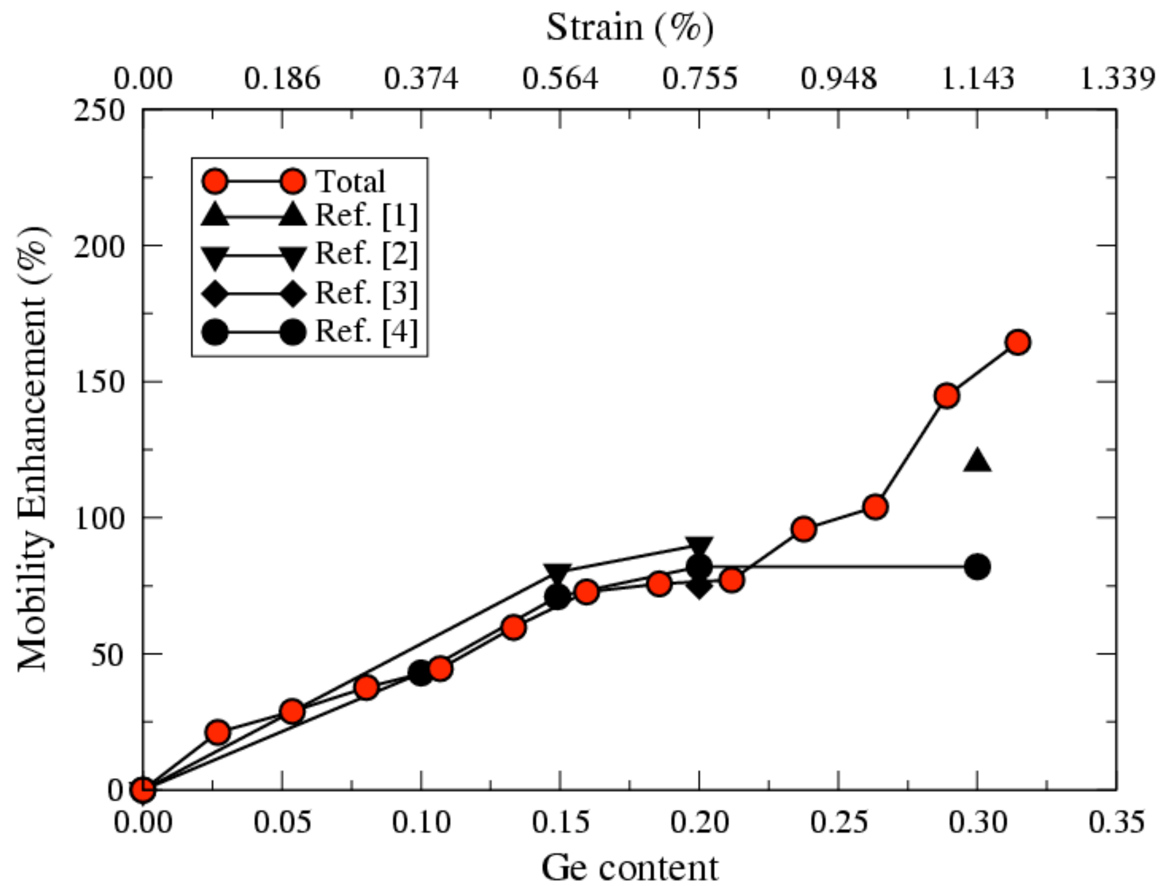


OXYGEN PROTRUSION

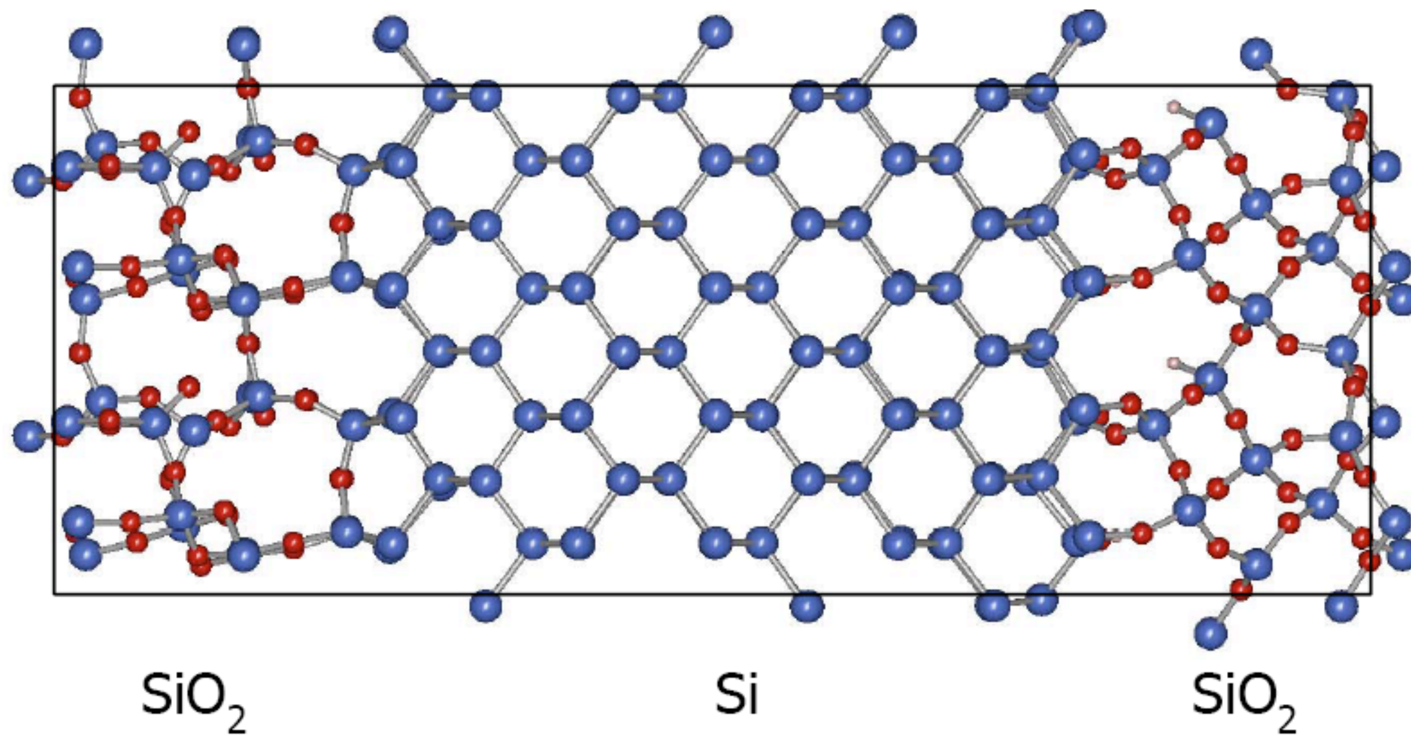


SUBOXIDE BOND

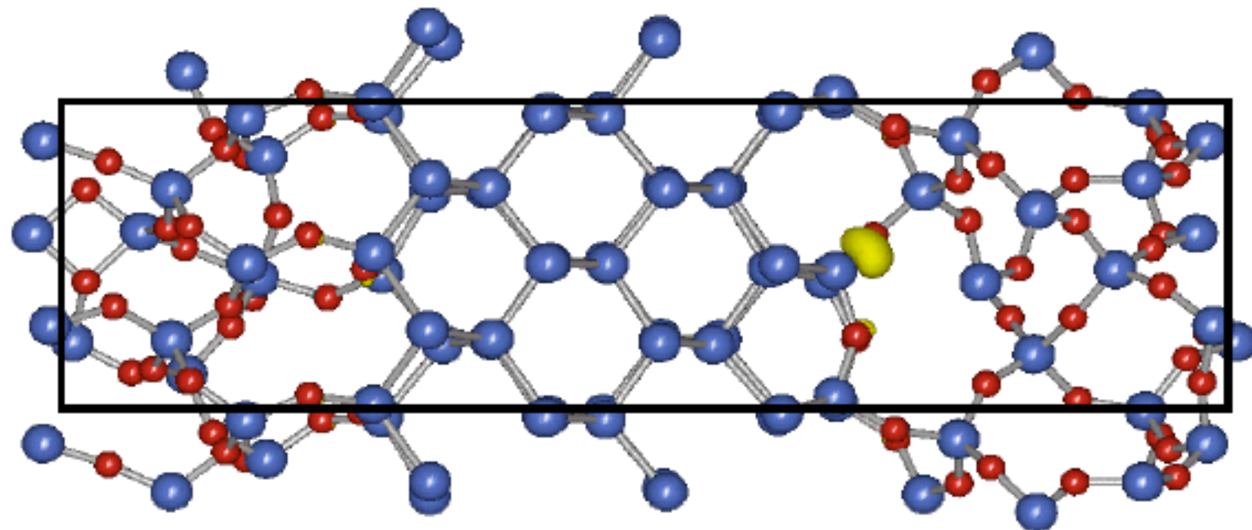
Mobility Enhancement

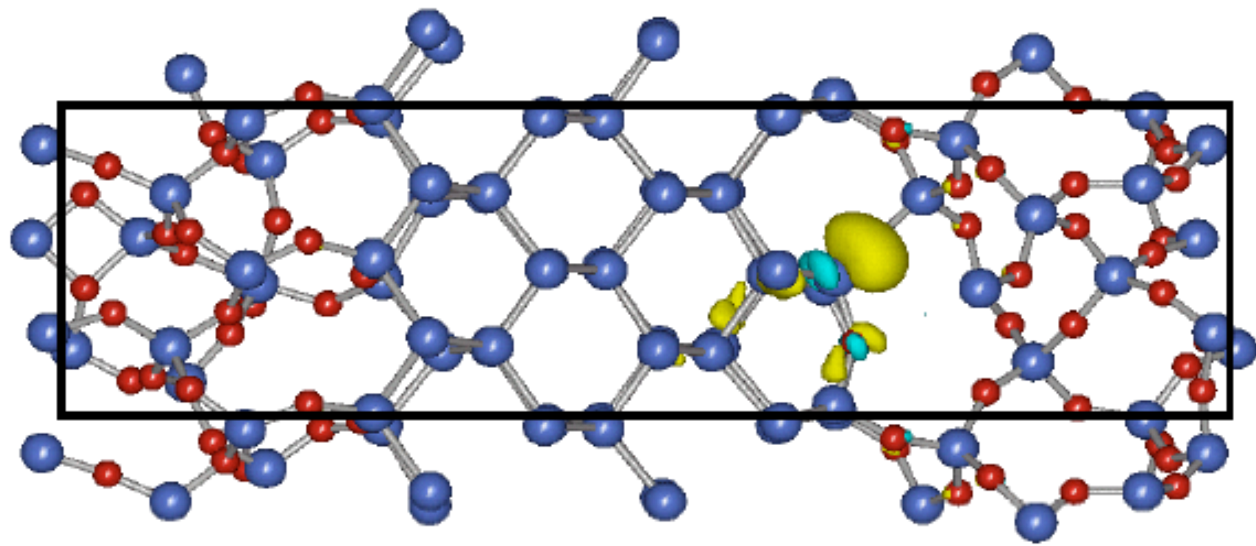


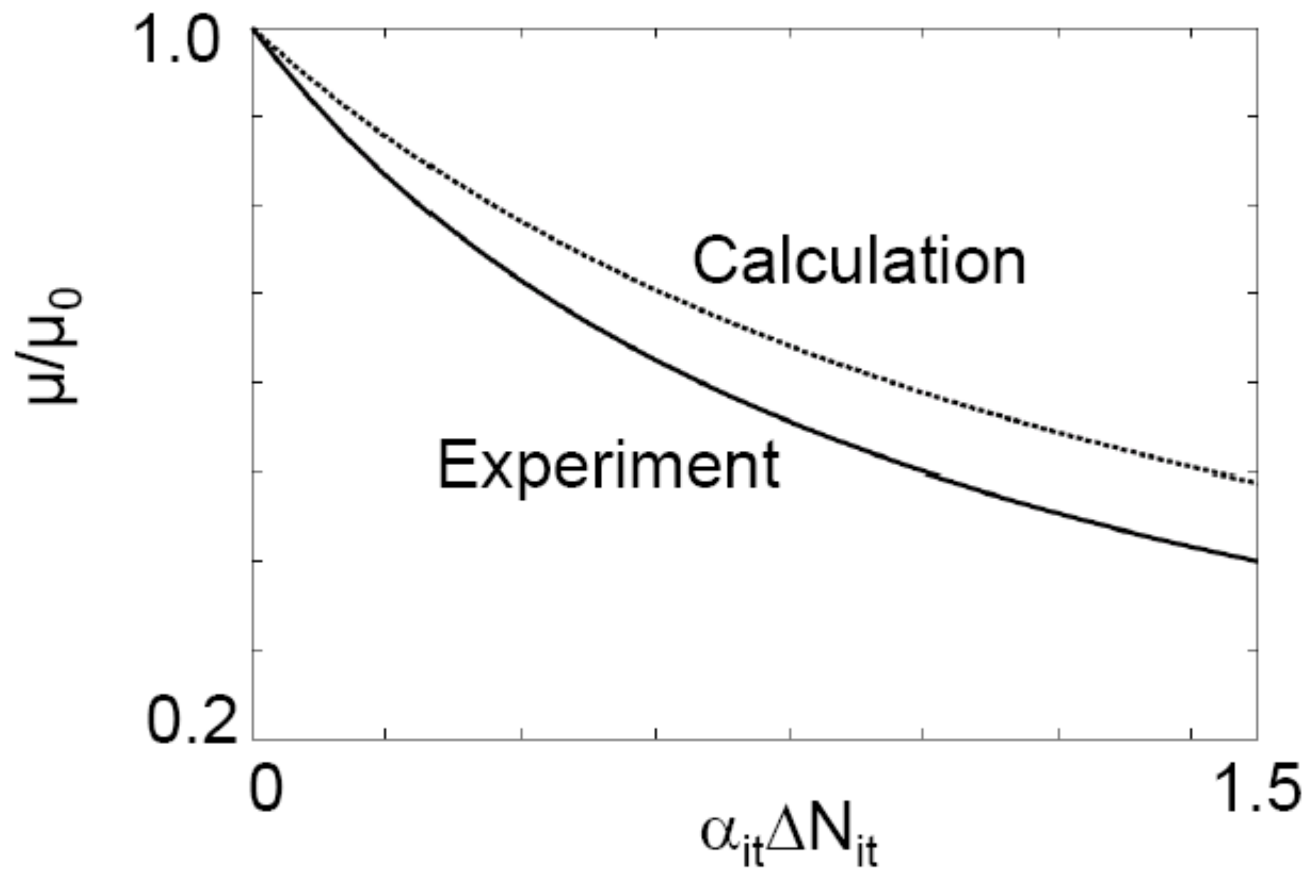
Data from bulk MOSFETs or SOI MOSFETs with t>5 nm



SiO_2
Si
SiO_2

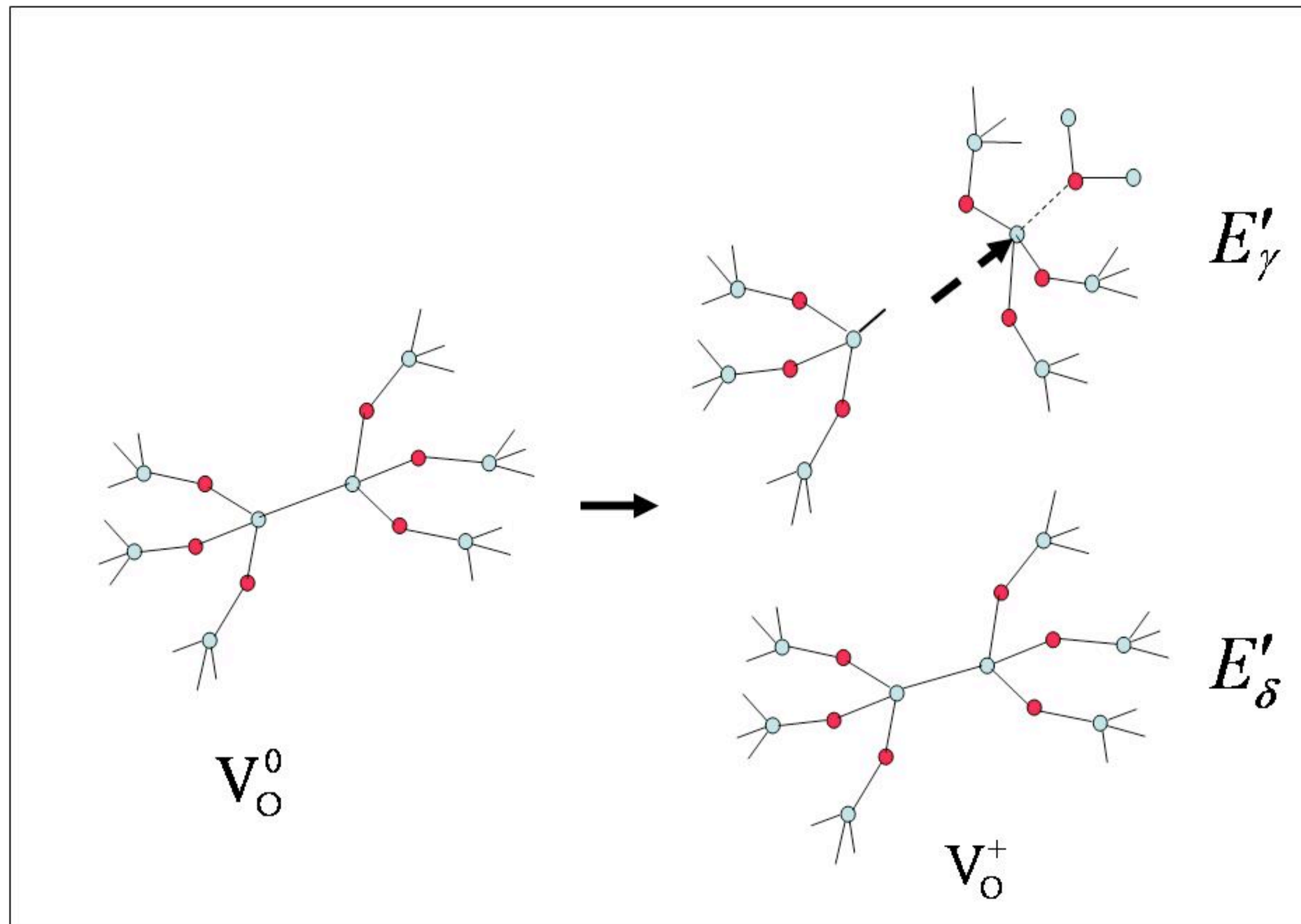


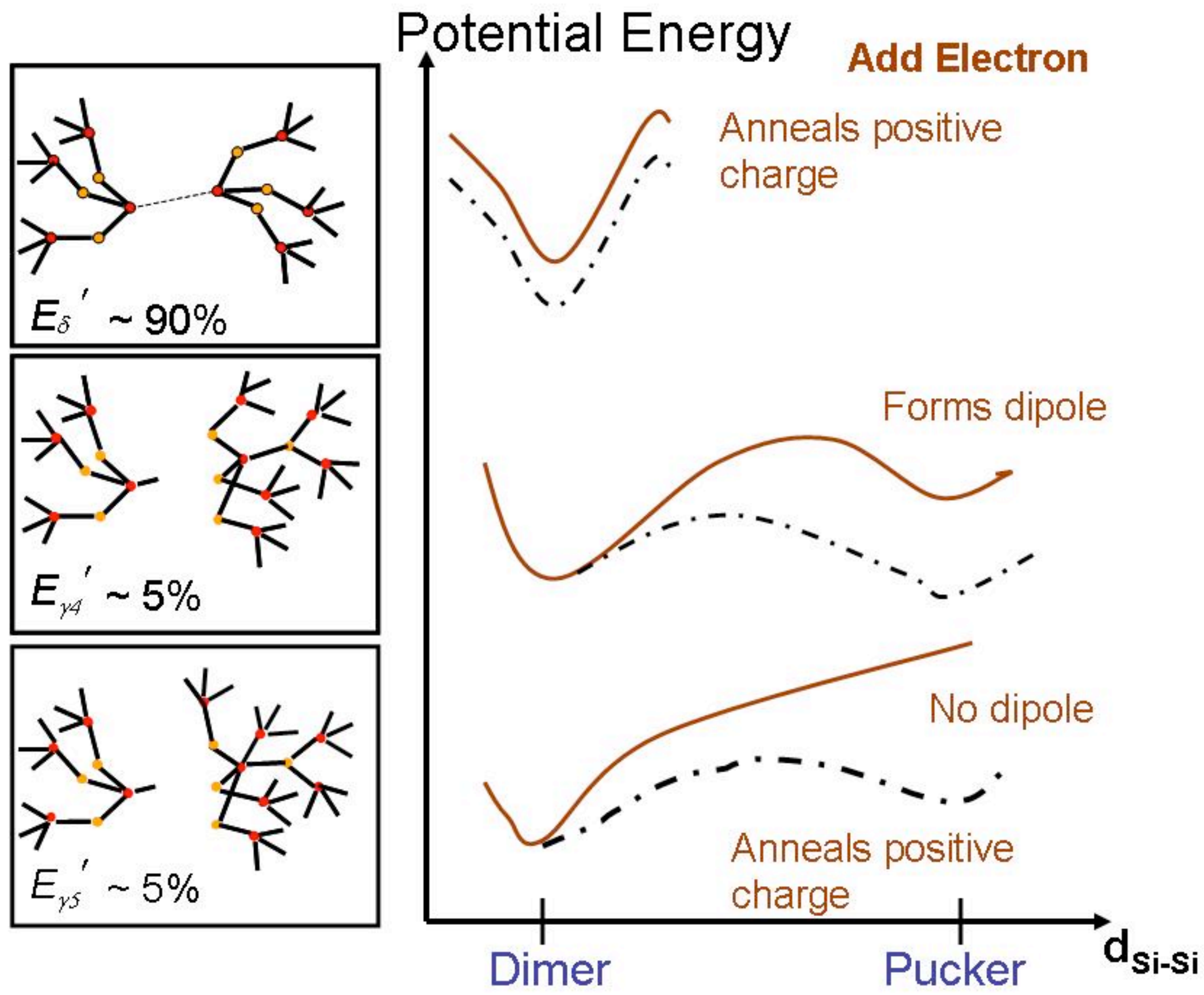




Experiment: Zupac, Galloway, and Schrimpf, 1992

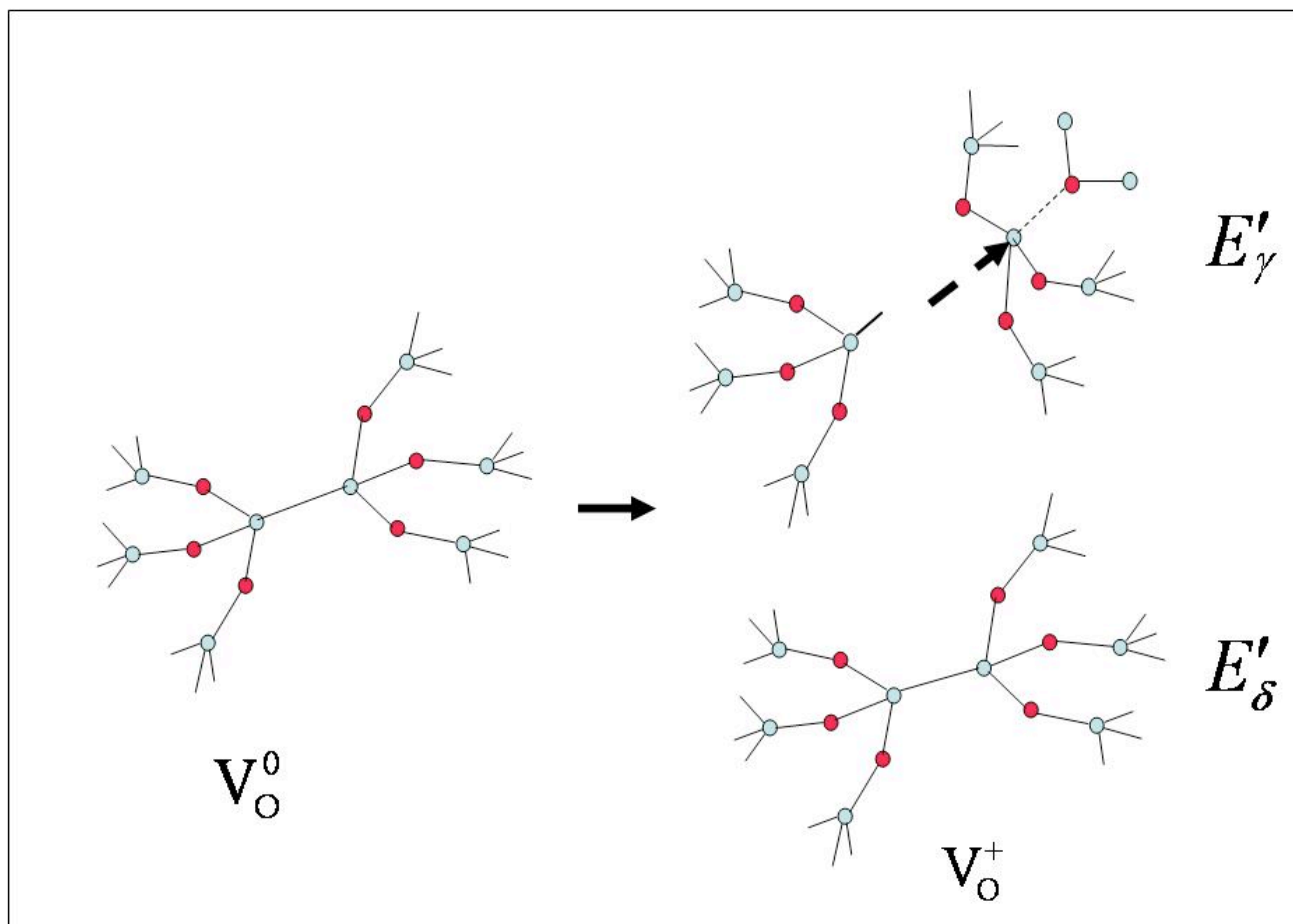
Oxygen vacancies in SiO_2





Lu, Nicklaw, Fleetwood, Schrimpf, and Pantelides, 2002

Revisit oxygen vacancies in SiO_2



EPR

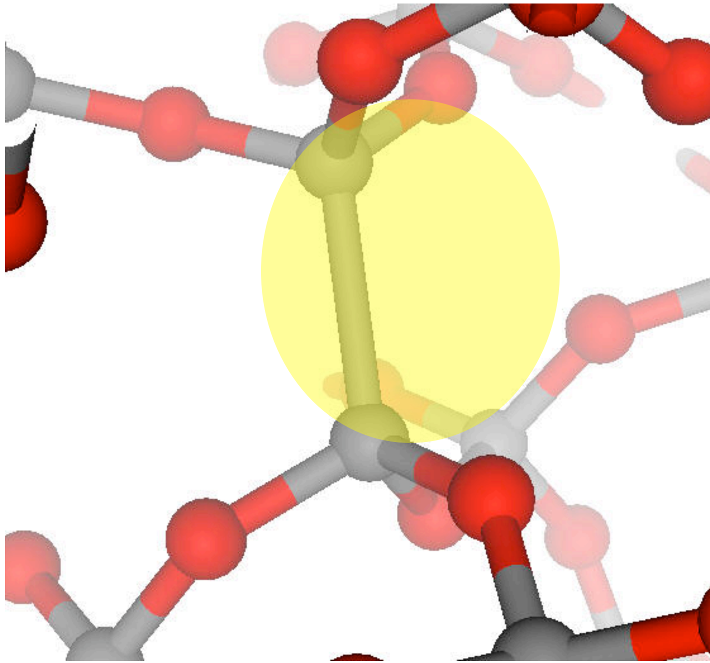
Anisotropic,

HF = 42 mT

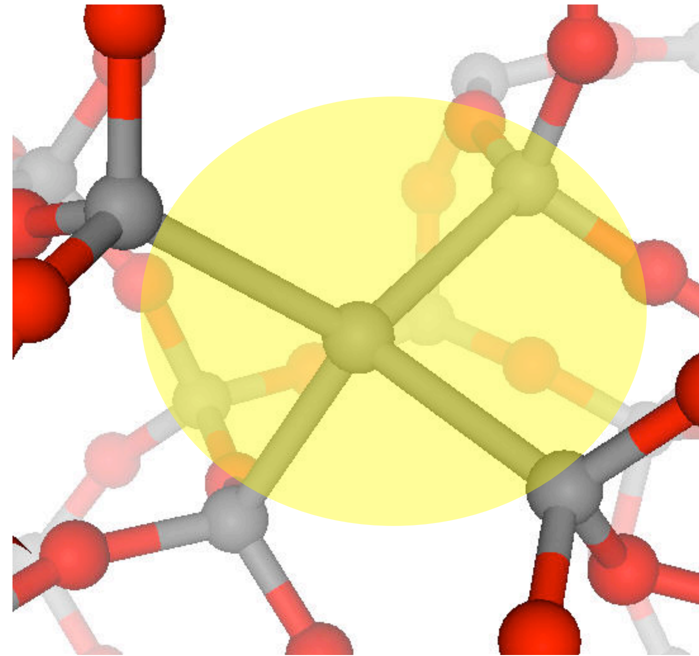
Isotropic,

HF = 10 mT

ALTERNATIVE MODELS FOR E'_{δ}

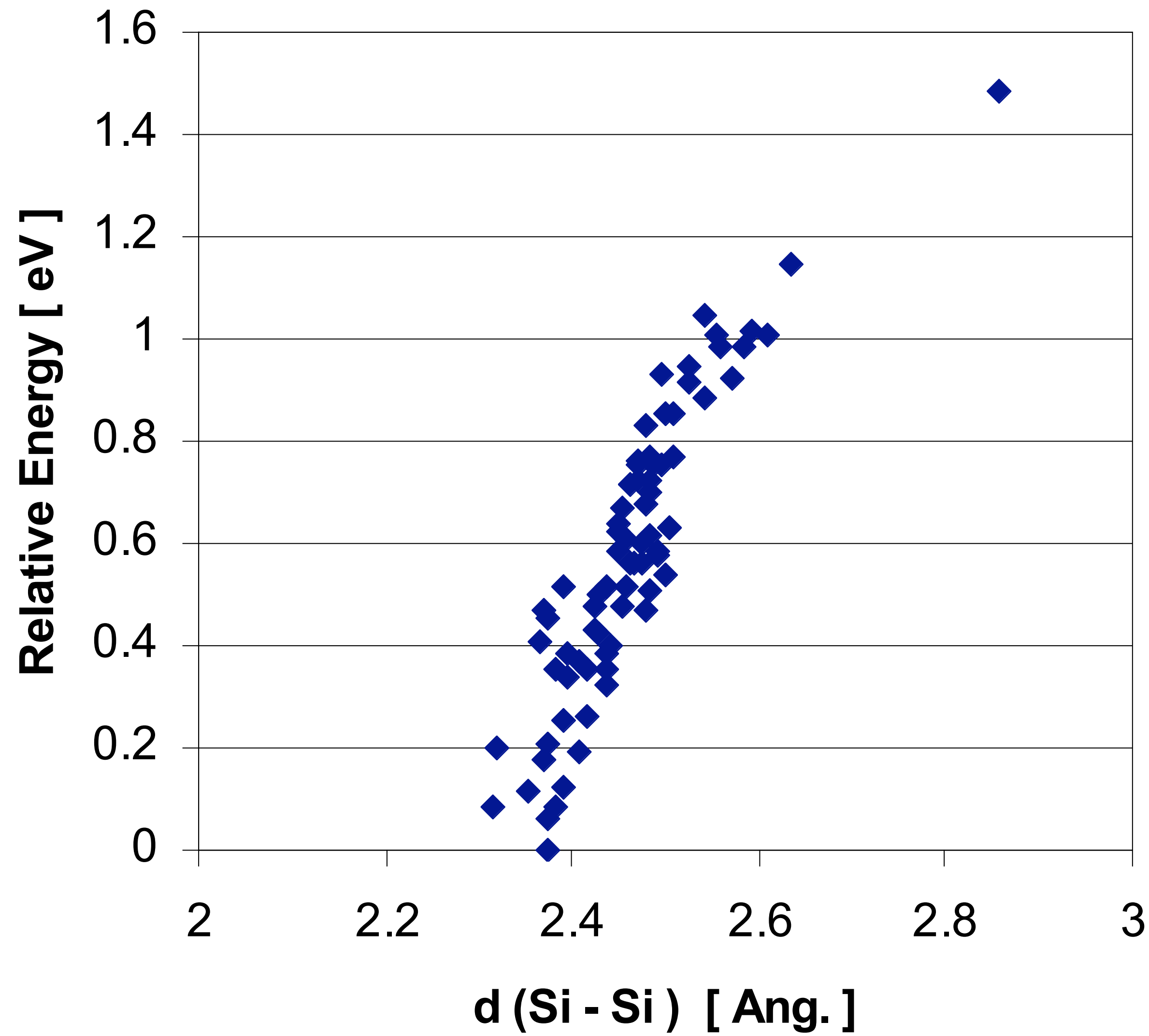


Si_2 defect

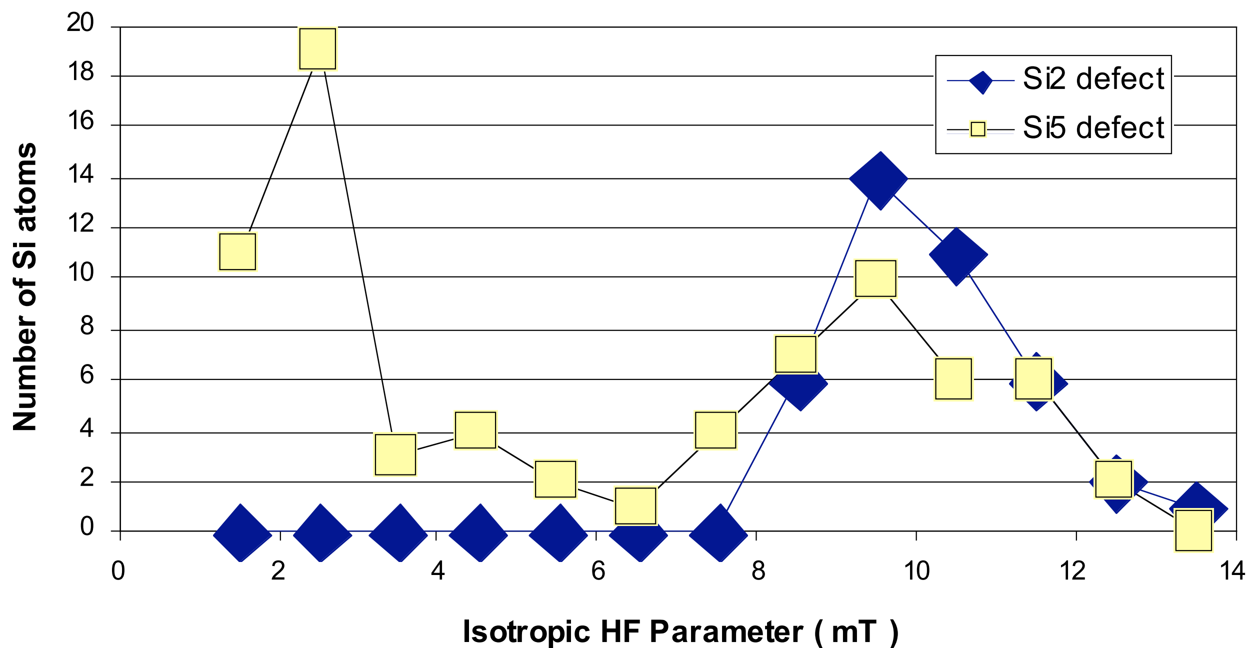


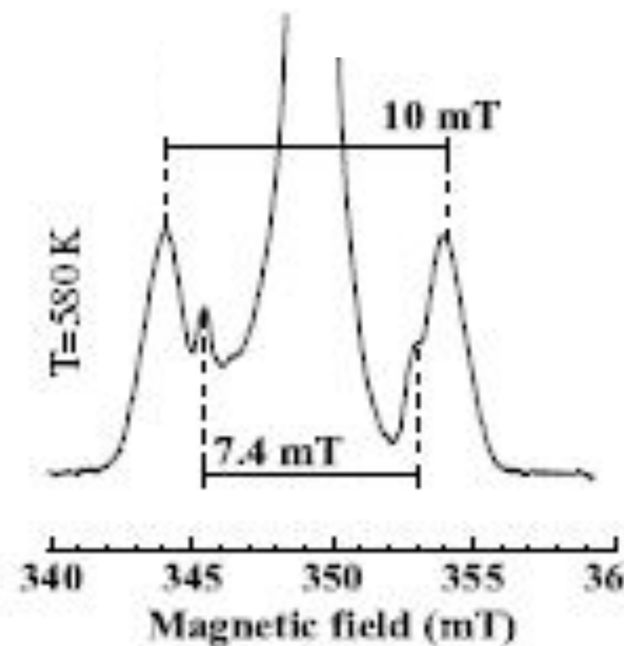
Si_5 defect

Buscarino et al. 2005, 2006


Energy vs [SiSi] bond length
Relative Energy [eV]
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
2
2.2
2.4
2.6
2.8
3
d (Si - Si) [Ang.]

Isotropic Hyperfine Results

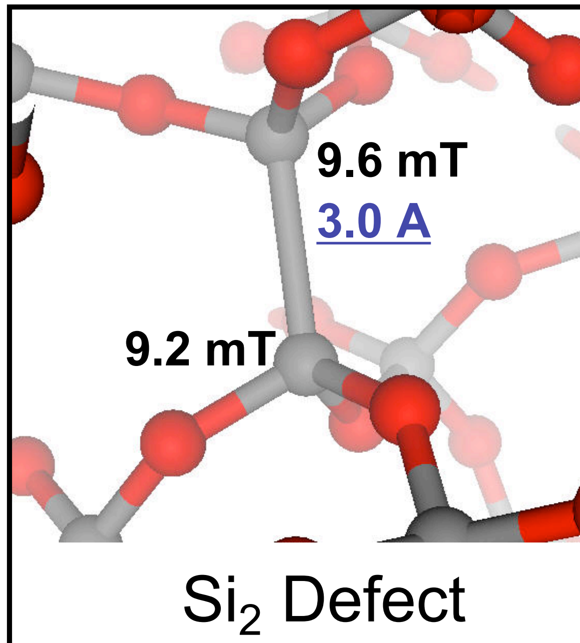




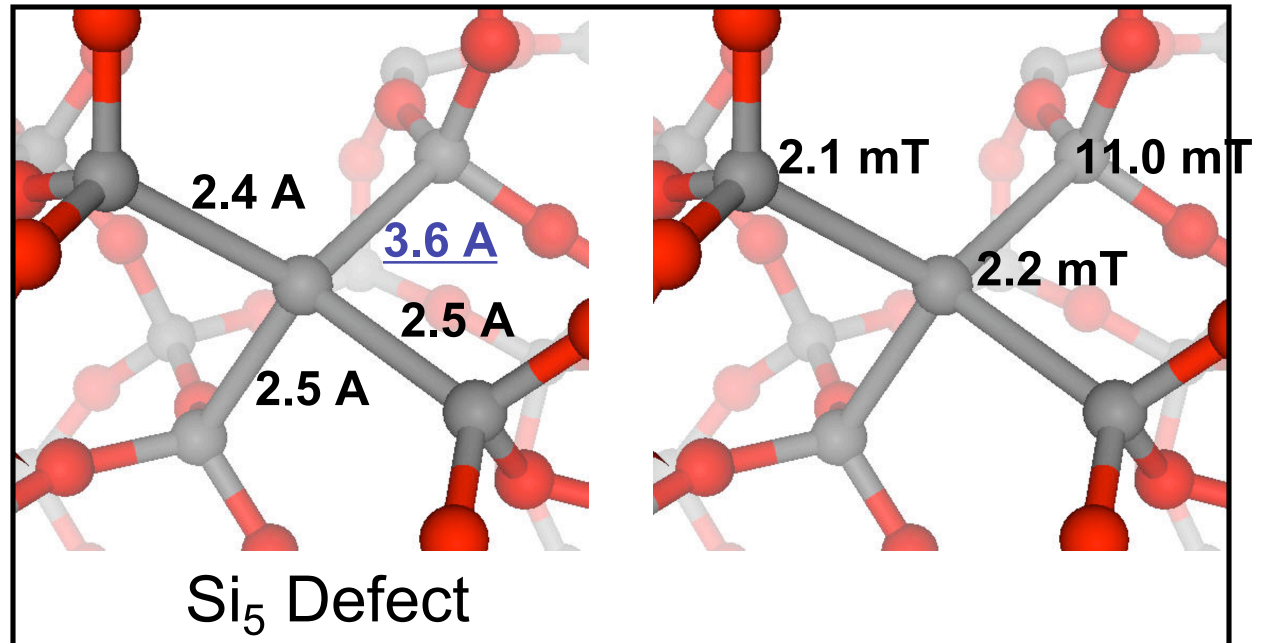
* Both Si_2 & Si_5 defects consistent with HF data

* Si_5 Defect has extra peak at 2 mT buried in central region

Atomic Structure



Si_2 Defect



Si_5 Defect

- Si_5 defect has one main HF active atom !
- Barrier for switching <0.6 eV

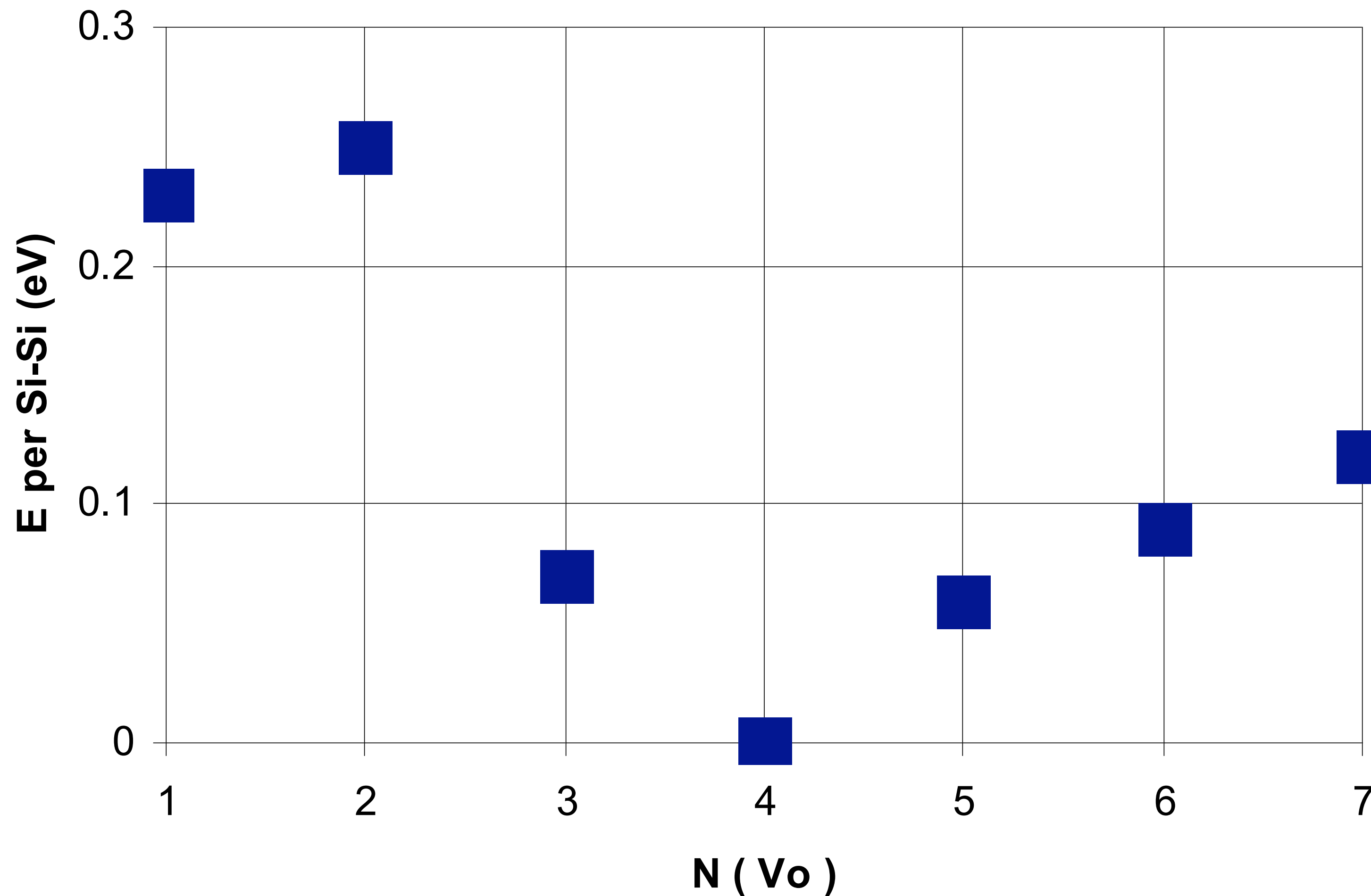
PREDICTION TO TEST: EPR AT LOW TEMPERATURE

Energy Cost/Gain to form O vacancy Clusters

- Quartz Results:
  - $E(4V_o) = 4E(V_o) + 0.05$ eV / V_o
- Amorphous Silica Average Results:
  - $E(4V_o) = 4E(V_o) - 0.07$ eV / V_o
- Amorphous Silica Minimum Results:
  - $E(4V_o,Min) = 4E(V_o,ave) – 0.32$ eV / V_o

Energy Cost of Sub-Oxidation

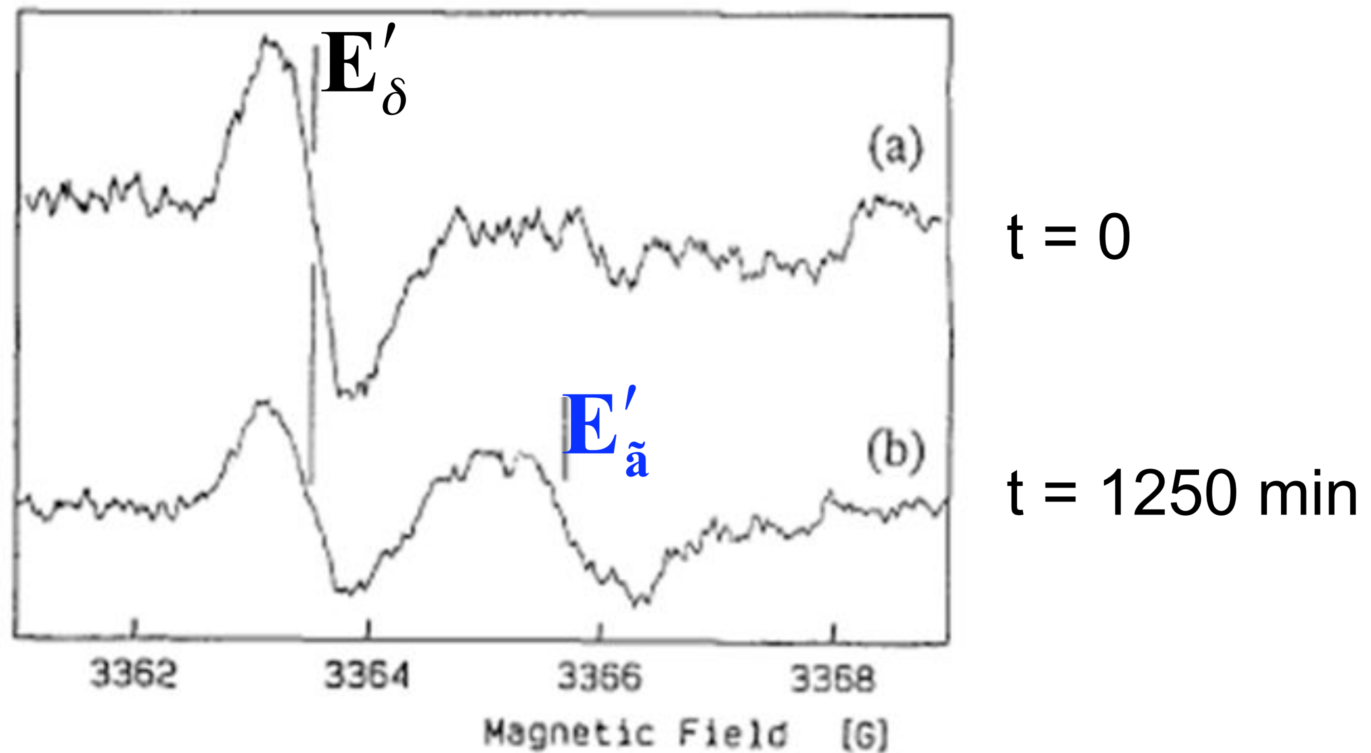
A. Bongiorno and A. Pasquarello, Phys. Rev. B (2000).
D. R. Hamann, Phys. Rev. B (2000).



ENERGY LEVELS OF Si_2: 0.3-0.4 eV

ENERGY LEVELS OF Si_5: 1-2 eV

ENERGY LEVELS OF $E'_{\tilde{a}}$: 3-4 eV



Warren et al. 1994

CONCLUSIONS ABOUT O VACANCIES

- Si_5 MODEL VIABLE FOR $E'_{ä}$,

BUT MUST BE TESTED FURTHER

- LOW-TEMPERATURE EPR
- ENERGY LEVEL MEASUREMENTS