ATOMIC-SCALE THEORY OF RADIATION-INDUCED PHENOMENA

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Leonidas Tsetseris

Blair Tuttle

Oscar Restrepo

Kalman Varga

In collaboration with the rest of the MURI team,

especially Ron Schrimpf and Dan Fleetwood

AFOSR/MURI REVIEW 2009

THEORY OBJECTIVES

- DISPLACEMENT DAMAGE
  - Defects, charging
  - Leakage currents
- ROLE OF HYDROGEN, OXYGEN VACANCIES
- ALTERNATIVE DIELECTRICS, CHANNELS
  - Interface structure, interface defects, NBTI,…
- CARRIER MOBILITIES

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
  - Quantum “molecular dynamics”
- CURRENTS

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Leonidas Tsetseris

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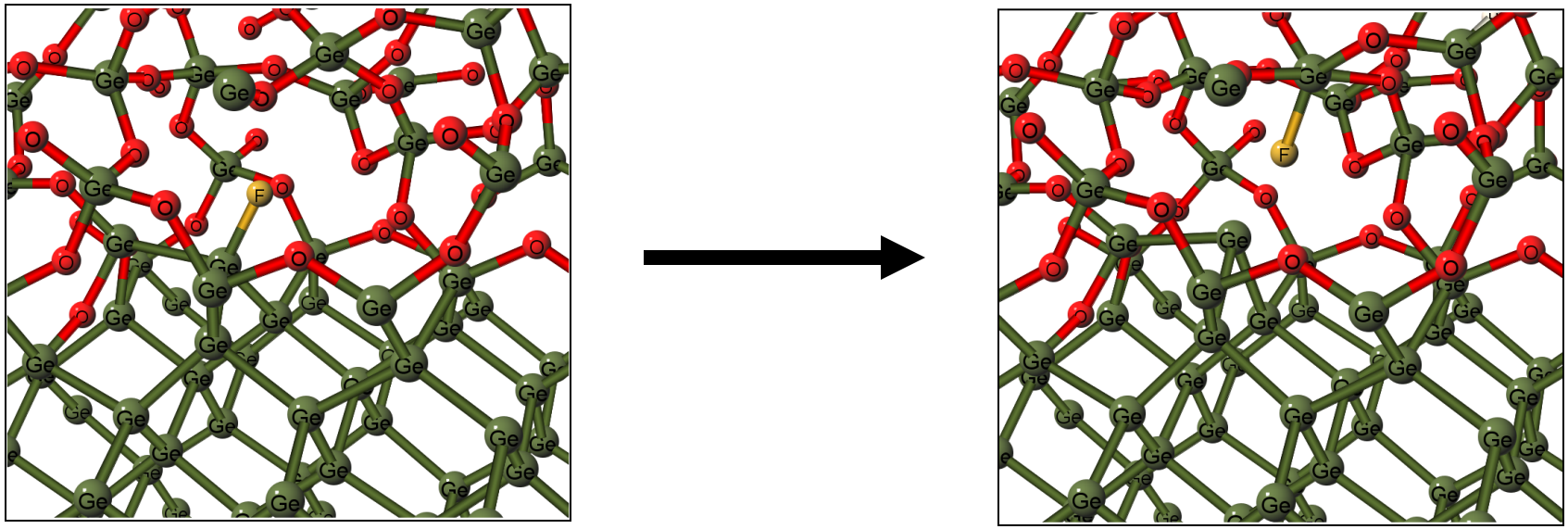
GERMANIUM CHANNELS

$Ge/GeO_2/HfO_2$ structures

PASSIVATION OF INTERFACIAL DANGLING BONDS BY H



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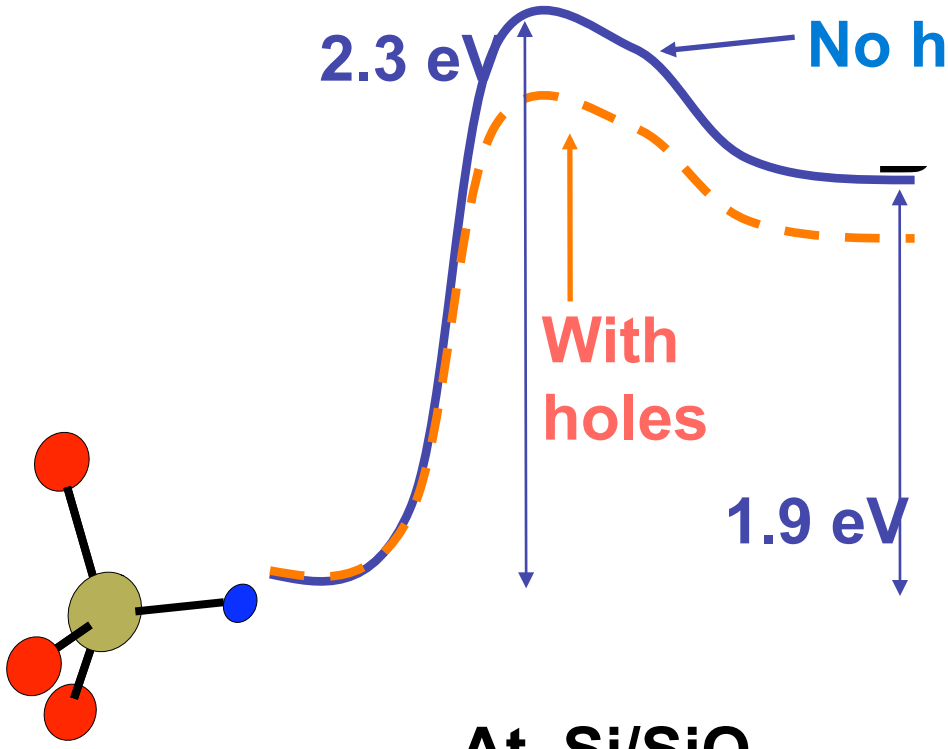
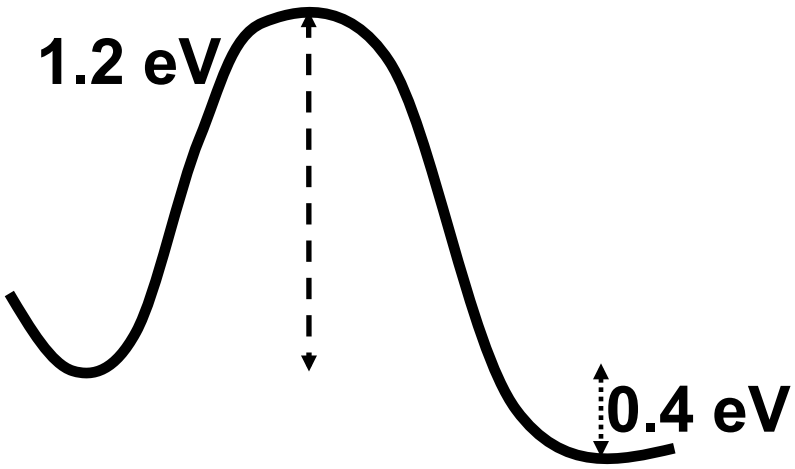


At Si/SiO_2

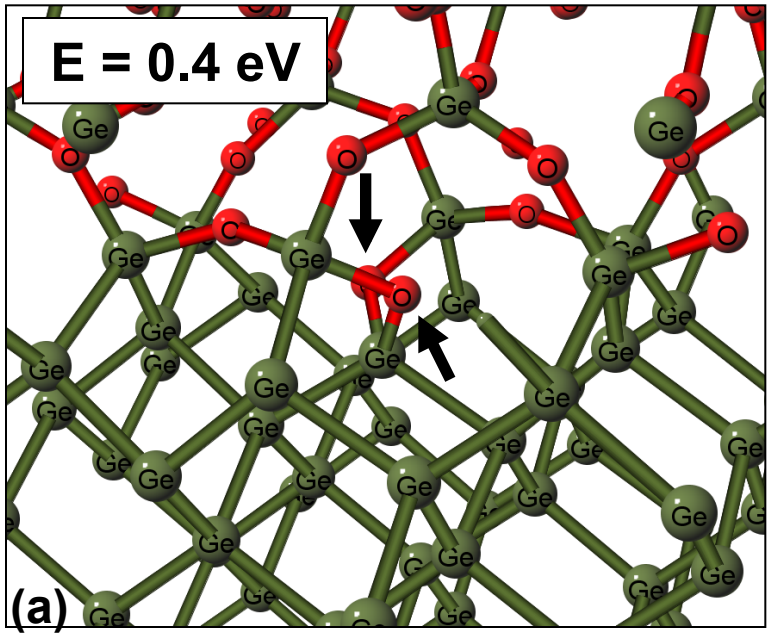


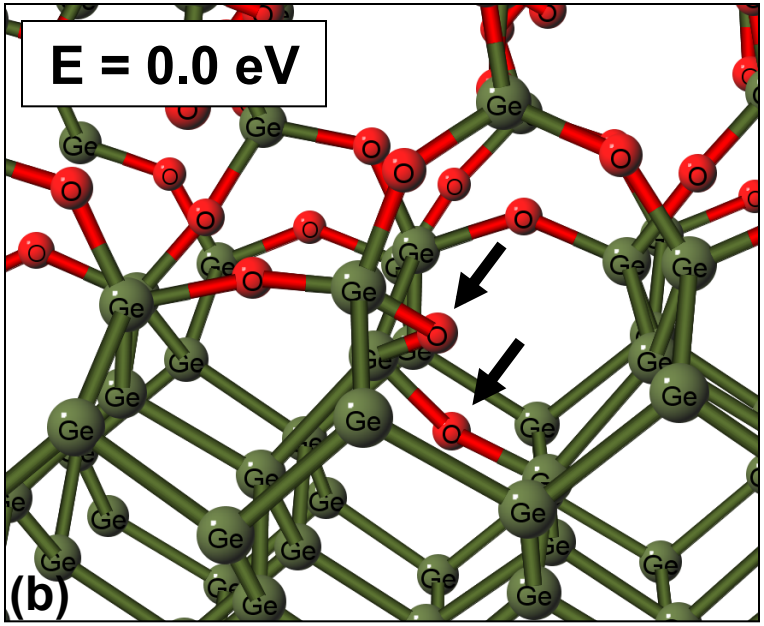
At Ge/GeO_2

F?

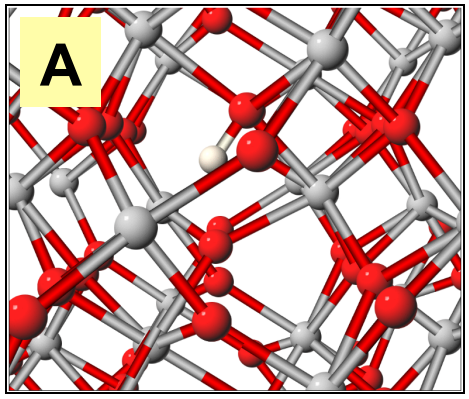
Ge-GeO_2 interface: protrusions

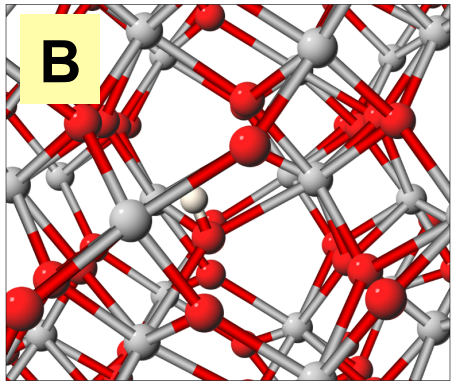
Unlike Si-SiO_2 case, formation of protrusions is favored at the Ge-GeO_2 interface

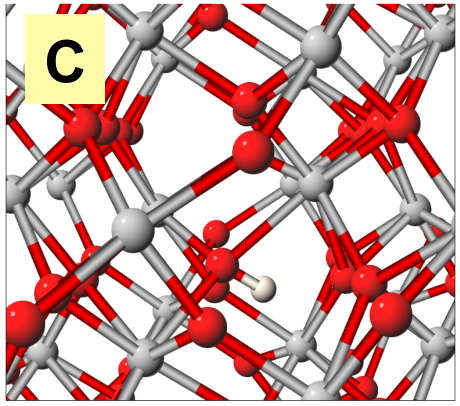




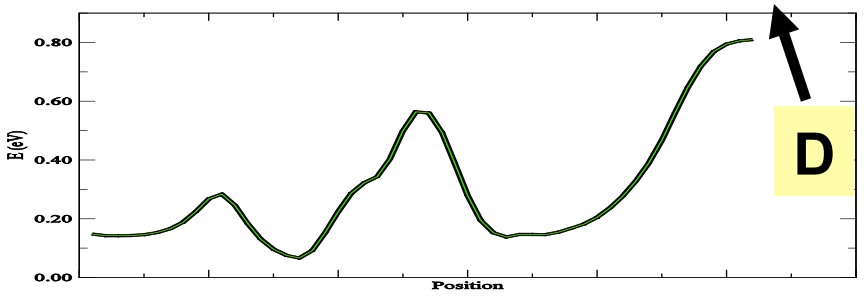
Hydrogen diffusion in monoclinic HfO_2

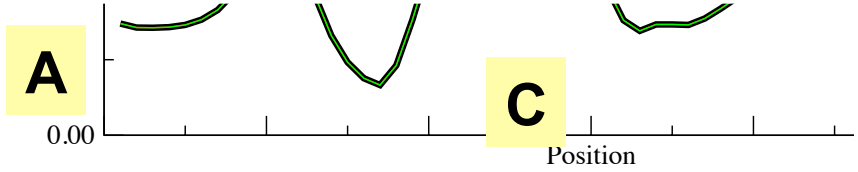






4-fold O

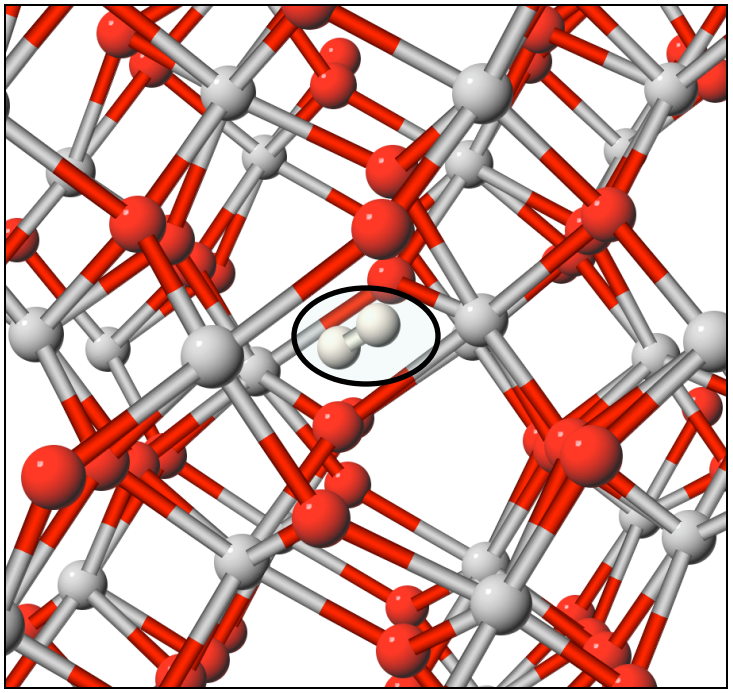




B

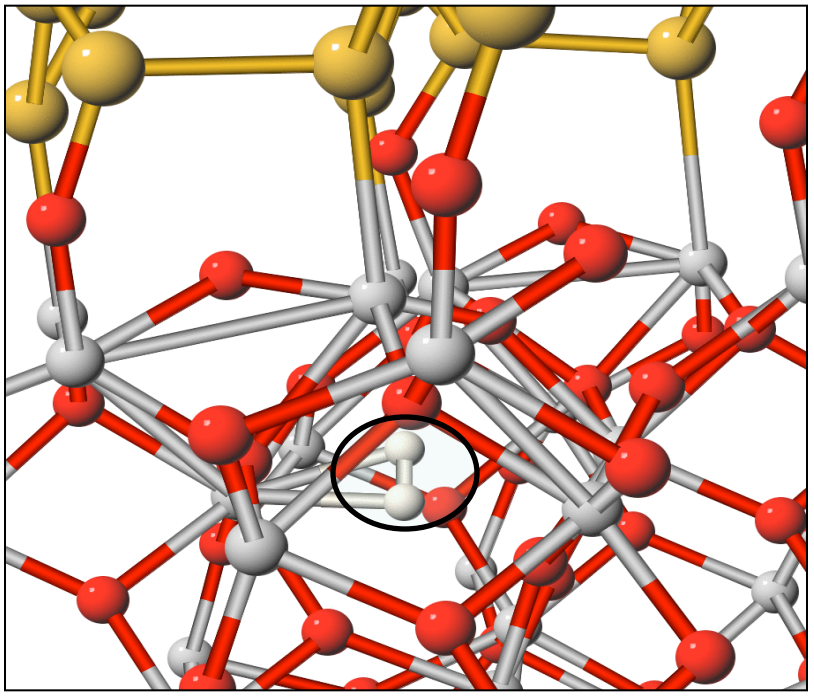
Migration barriers ~ 0.4-0.5 eV

H_2 in HfO_2 and at Si-HfO_2 interface



Monoclinic HfO_2

E_i = 1.82 eV



Model Si-HfO_2 interface

E_i = 0.94 eV

Insertion energy E_i

Compare with 0.7-1.2 eV in a-SiO_2

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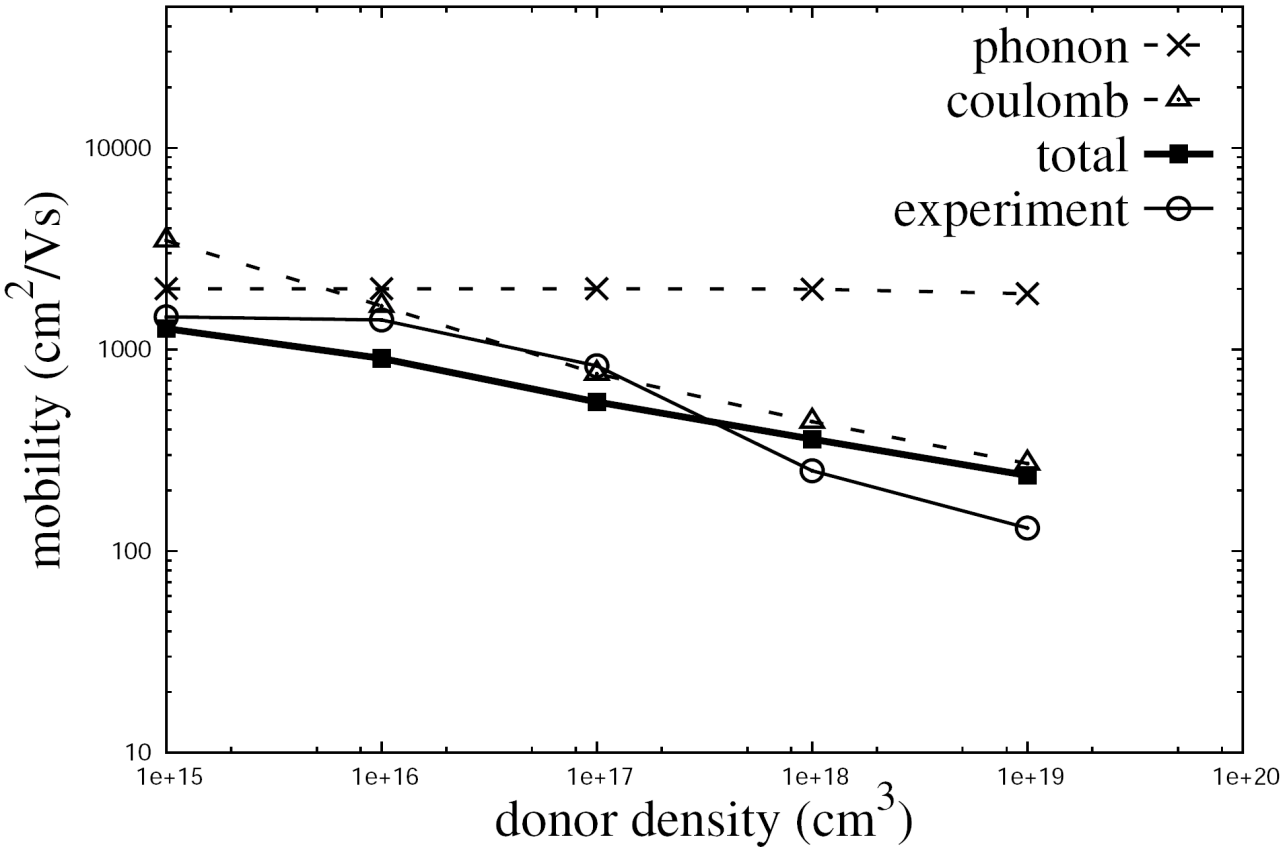
Coulomb and phonon scattering in bulk Si



Restrepo, Varga, and Pantelides, APL in press

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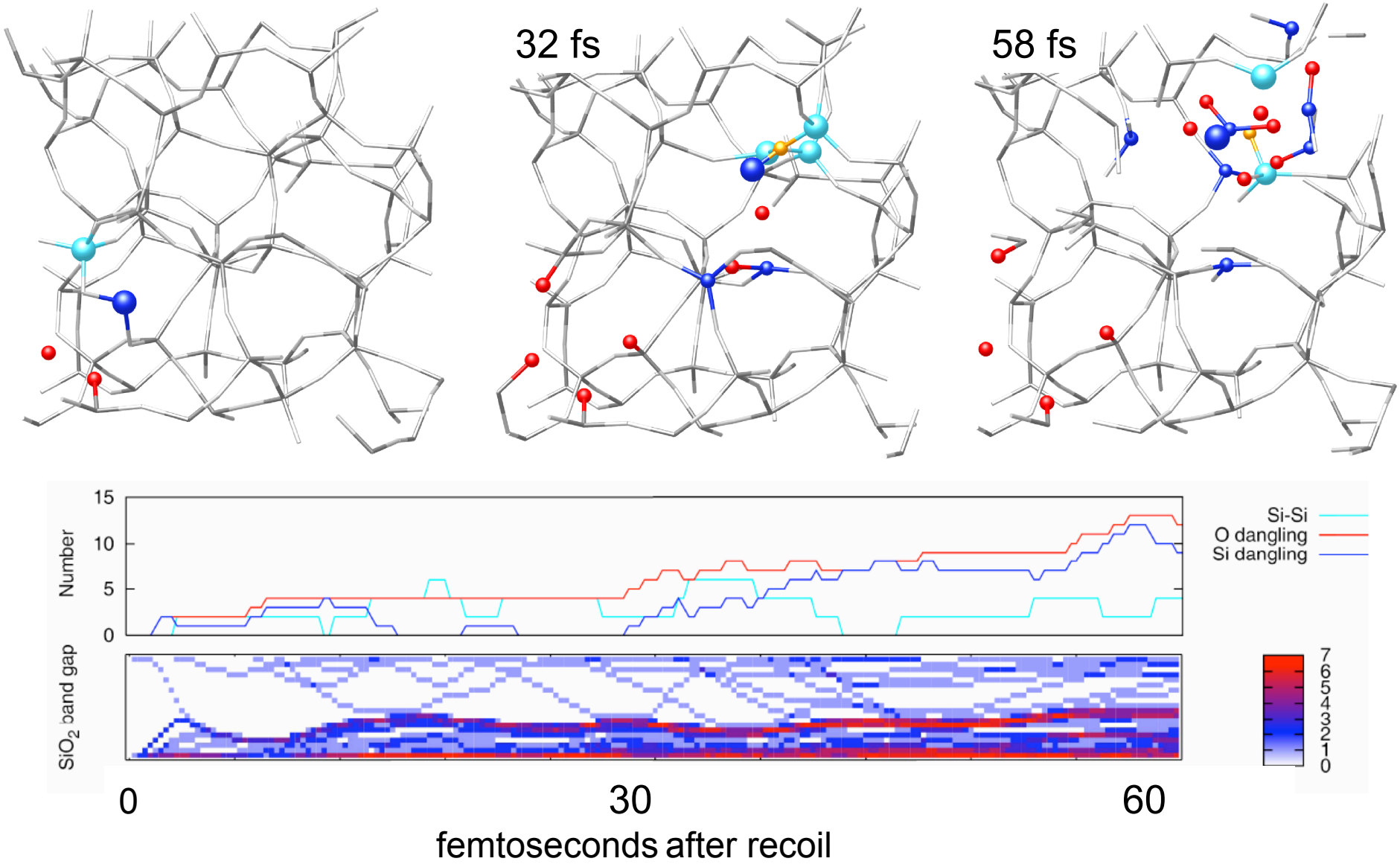
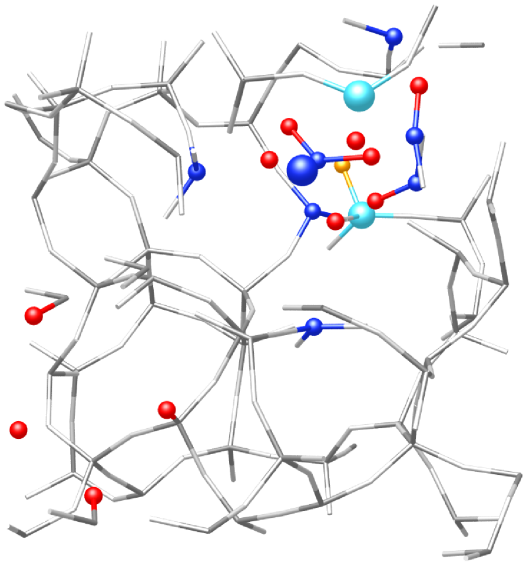
Low-energy recoil dynamics in amorphous SiO_2

100 eV Si recoil



Multi-scale calculation

From QM transport to I-V device characteristics



Mott's defect-defect tunneling