# Ion-Induced Leakage Currents II: Quantum Transport

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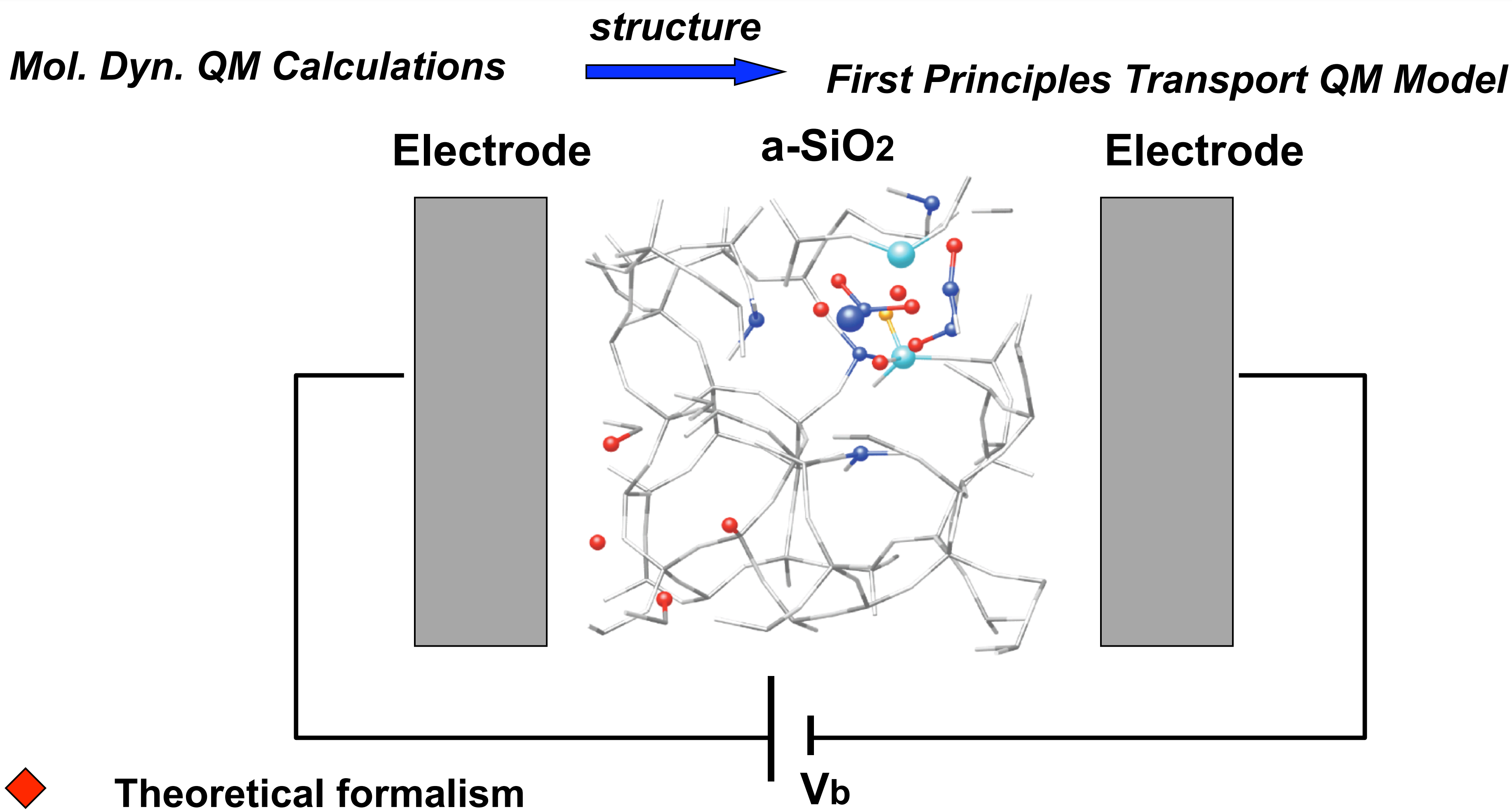


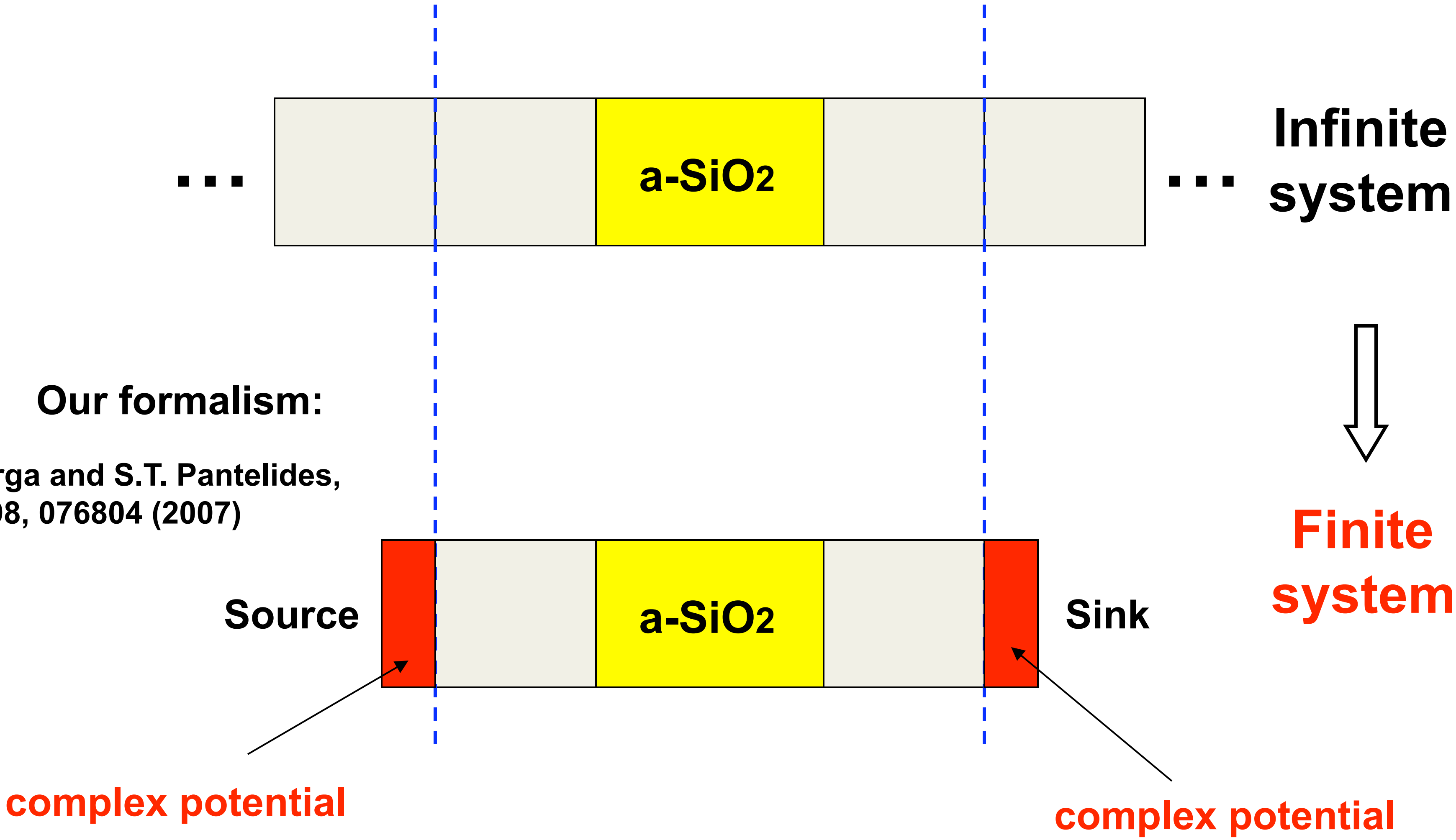

- Theoretical formalism
- Tuning the model: crystalline $SiO_2$ system
- Leakage currents in thin amorphous $SiO_2$

# Density Functional Theory + "Source and sink" method

- **Conventional transport methods:**
  scattering theory, open infinite system

- **Our formalism:**

**K. Varga and S.T. Pantelides, PRL 98, 076804 (2007)**



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**Solve diagonalization problem:**

$W = W_{source} + W_{sink}$

$$(H + iW)\Psi_i = E_i\Psi_i$$

↓

**Compute Green's functions:**

$$G_{\nu\mu} = \sum_k \frac{c_{\nu k} c_{\mu k}}{E - E_k}$$

↓

**Calculate charge density:**

$$\rho(\mathbf{r}) = -\frac{1}{\pi}\oint_C \mathrm{Im}\{G(\mathbf{r},\mathbf{r},E)\}dE$$

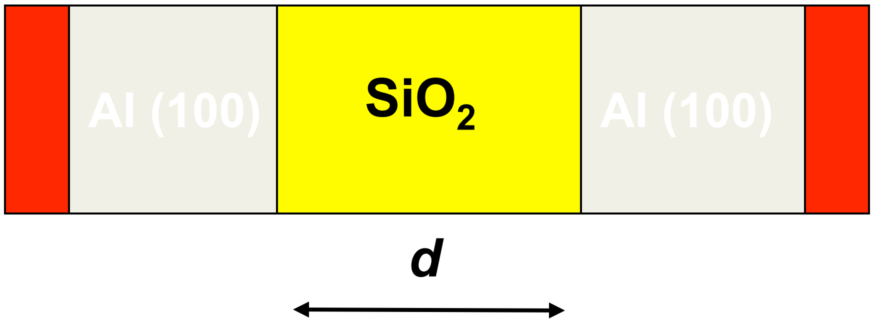
↓

**Compute leakage current:**

$$I(V_b) = \int_{-V_b/2}^{+V_b/2} T(E)dE$$

# Initial model calculations

***Crystalline SiO2*** – computationally fast

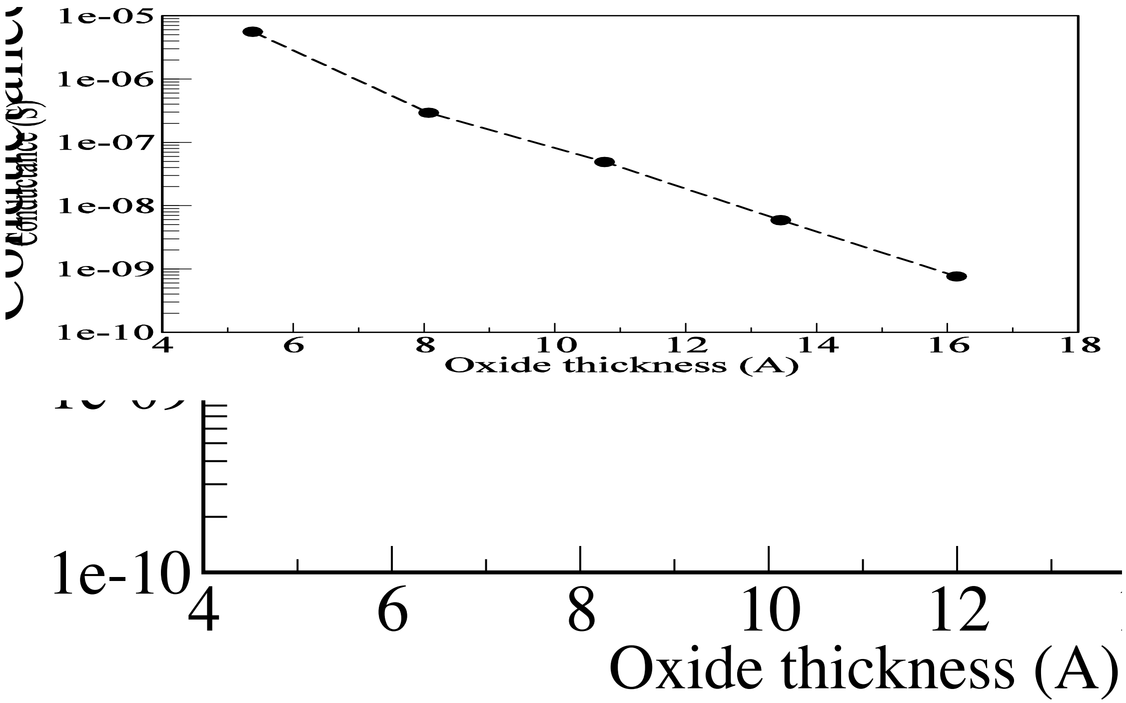



**Can we compute device related property ?**

- **How does conductance of $SiO_2$ depend on oxide thickness *d* ?**

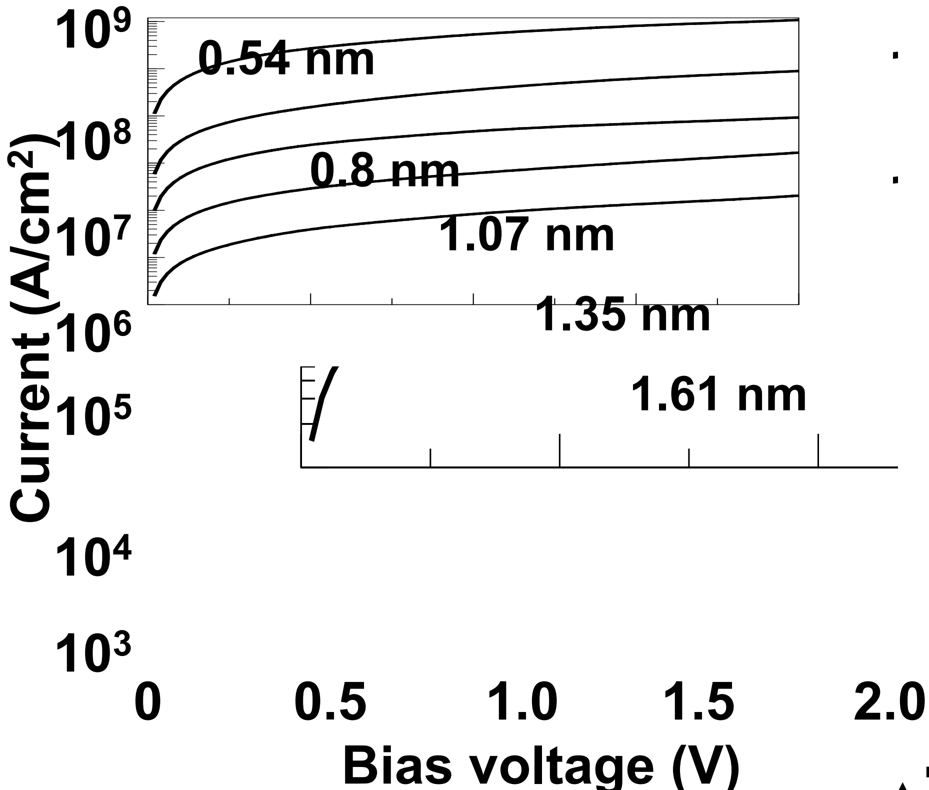
# Conductance vs thickness of $SiO_2$

Not defected structure yet!

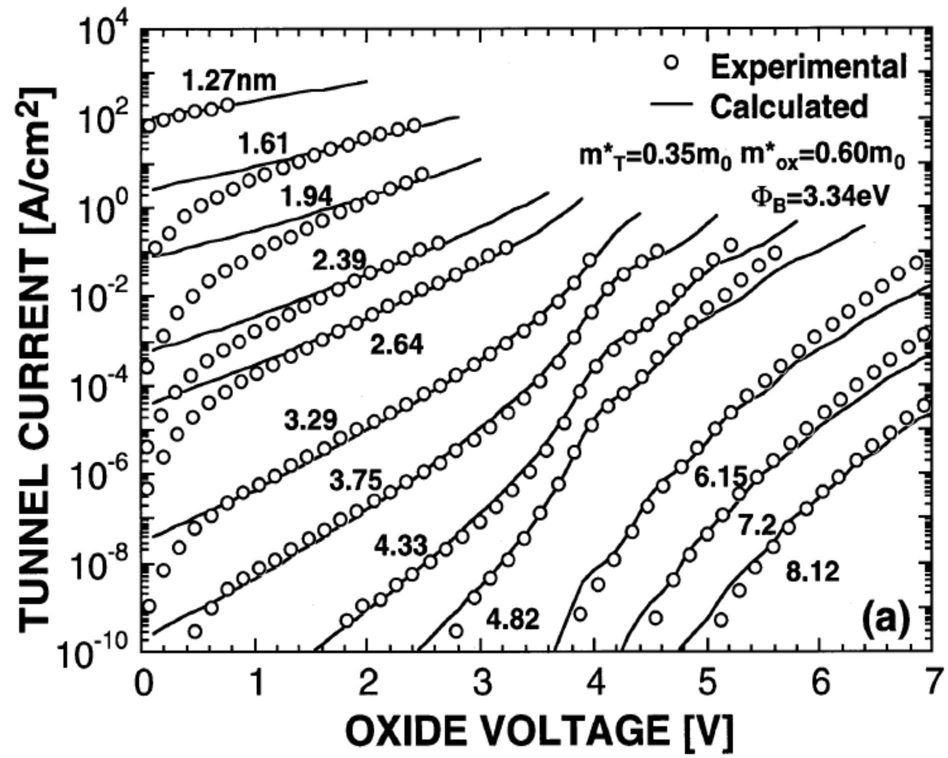



**Conductance: exponential dependence as expected from tunneling**

## Calculations

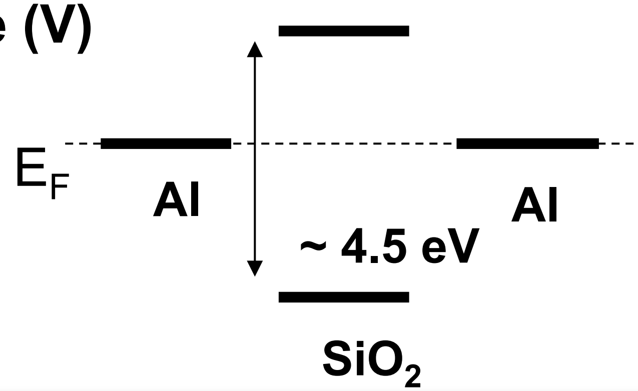



## Experiment




M. Fukuda et al,
Jpn. J. Appl. Phys. (1998)

**We used standard Hamiltonian**



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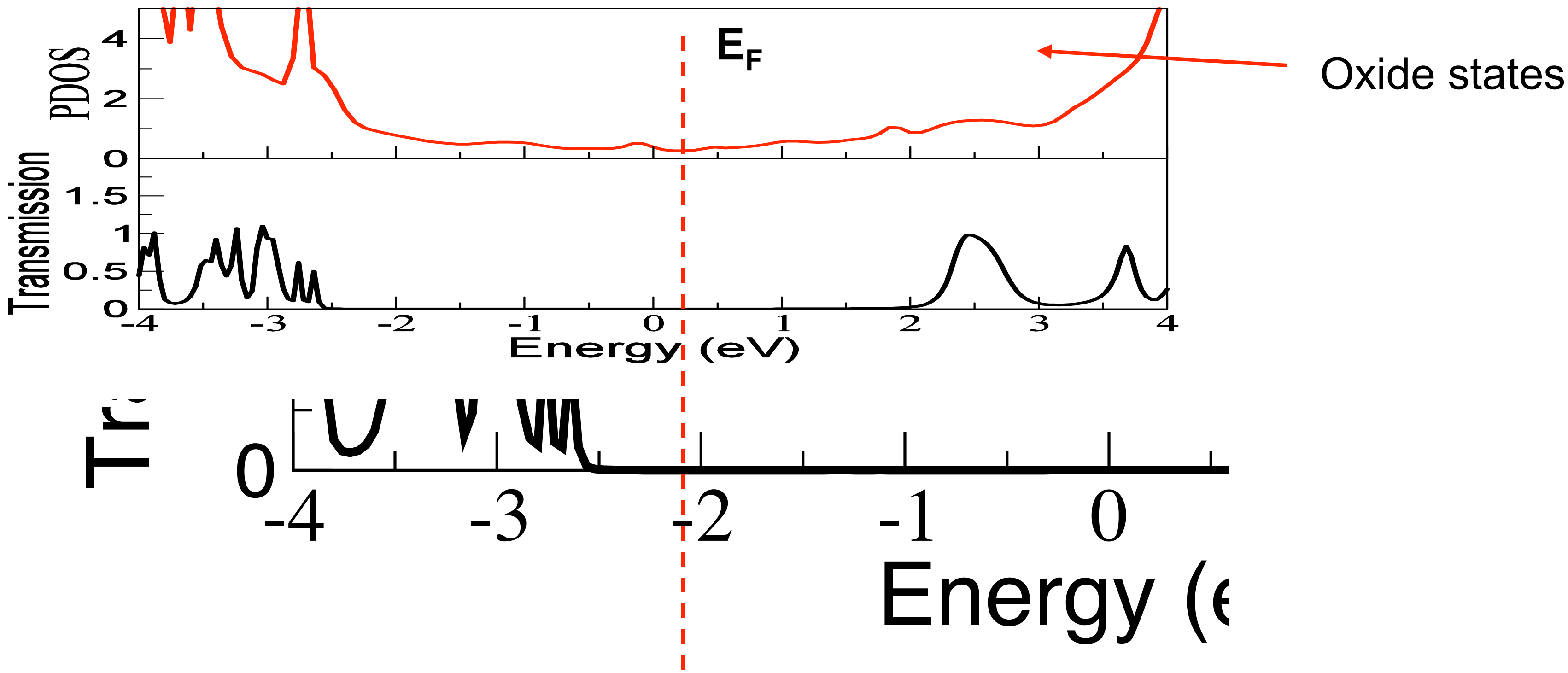
## Our formalism allows:

--- not only to compute current and conductance

--- but also to analyze the transport mechanism




**PDOS** – density of states amplitude is projected on the oxide
**Transmission** – spatial and energy degrees of freedom

# How is the leakage current affected by the defects?

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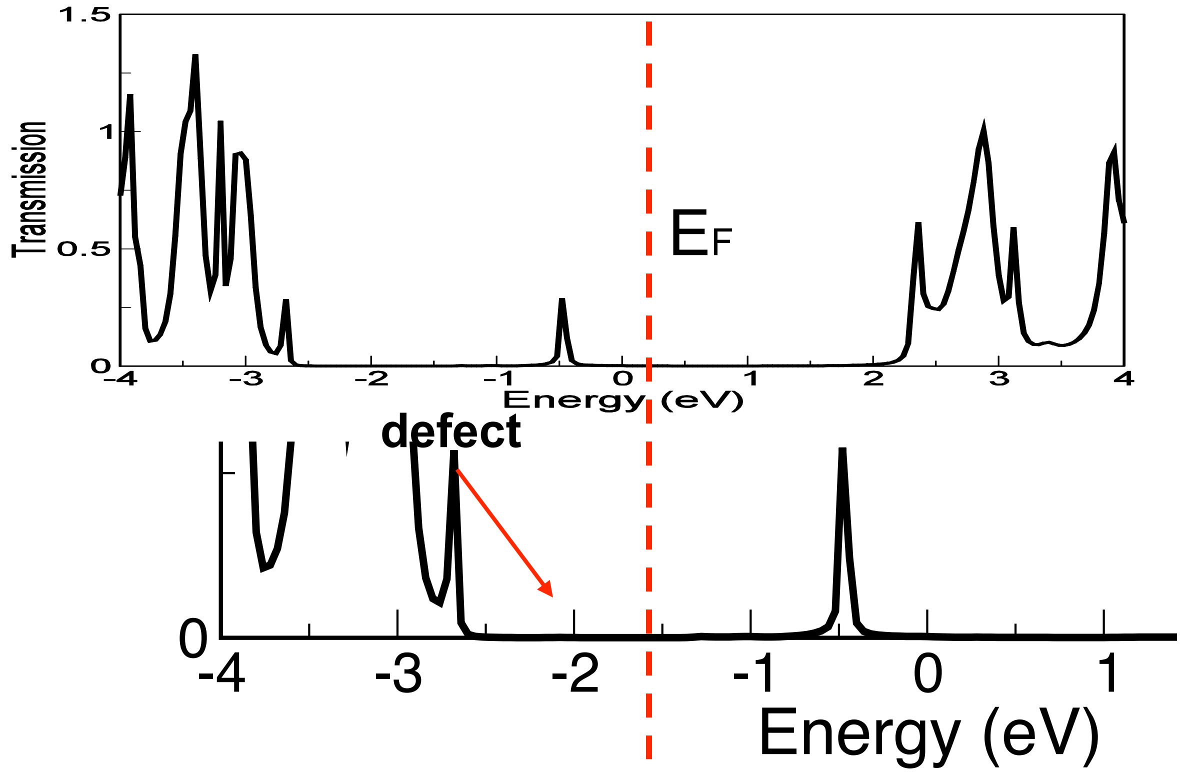
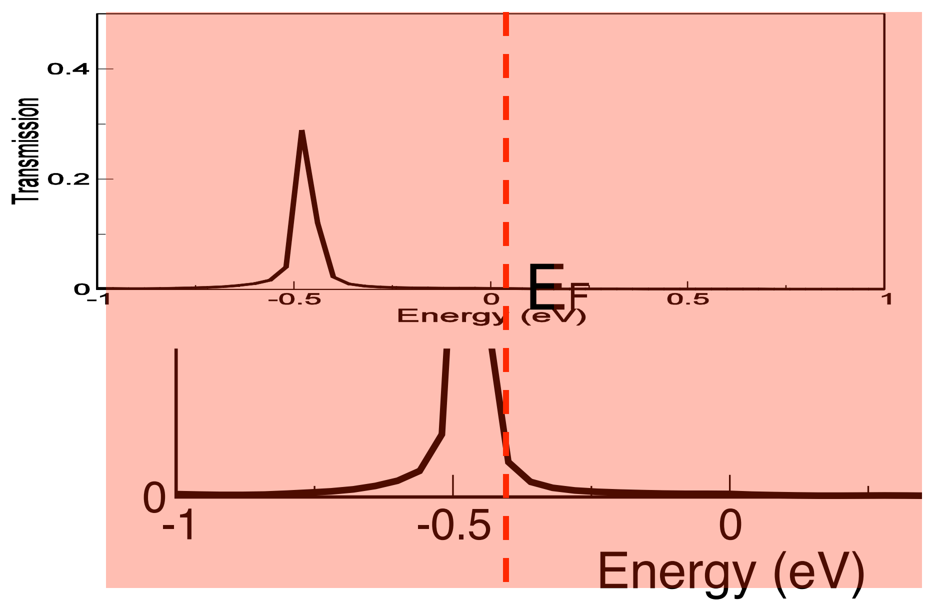
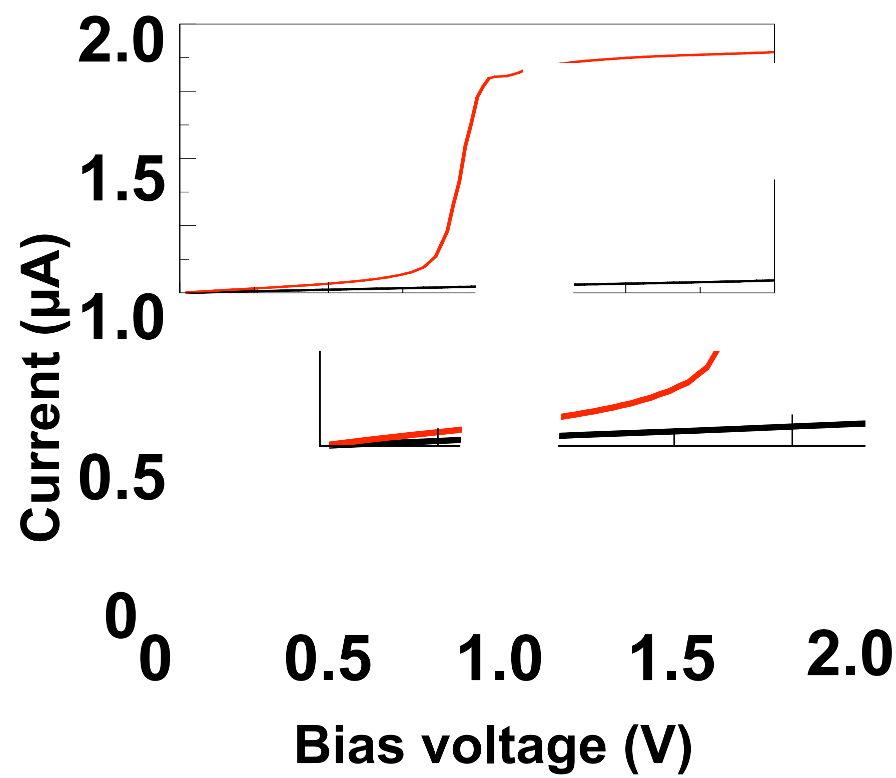
**Defect: single oxygen vacancy**



# How is the leakage current affected by the defects?

**Defect: single oxygen vacancy**



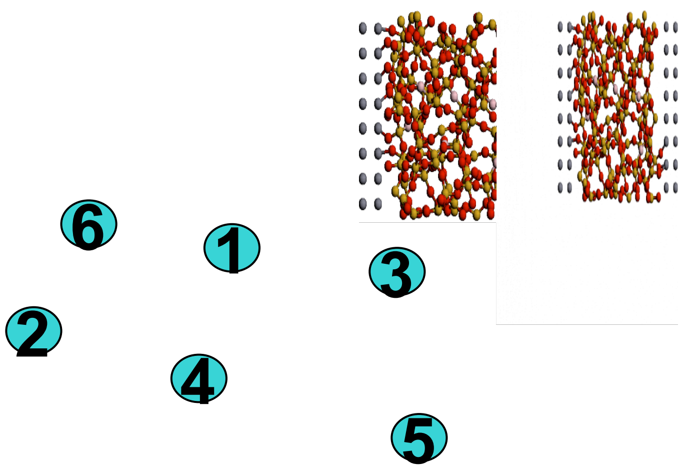

***Transport energy window***

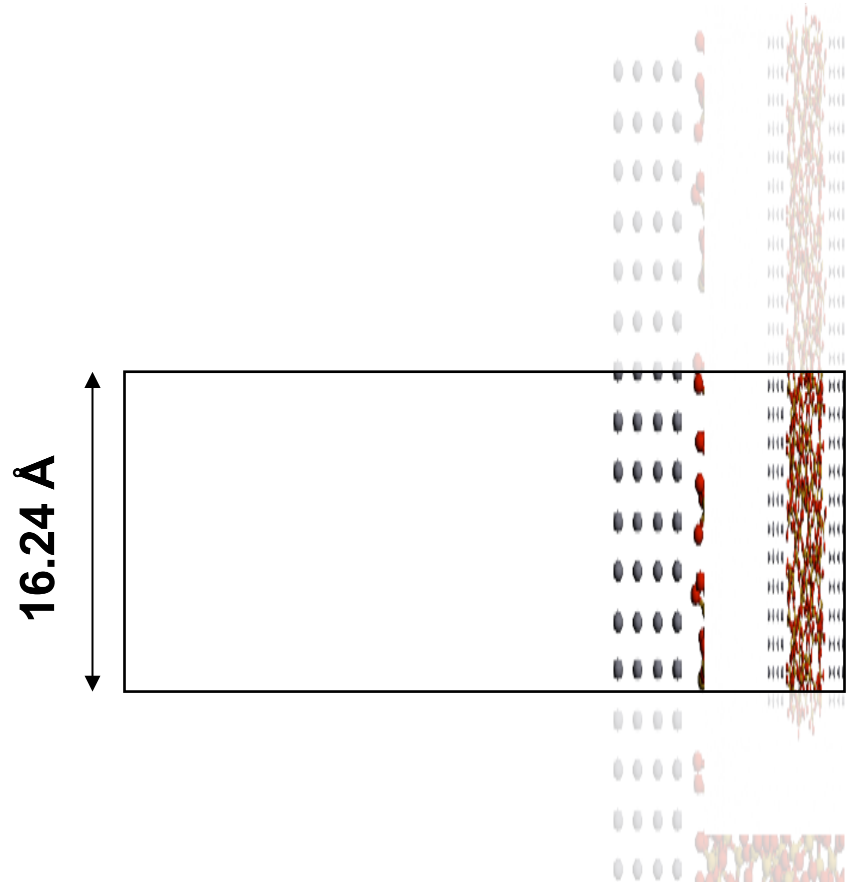
**from $-V_b/2$ to $+V_b/2$**

# Amorphous $SiO_2$ leakage currents

## Creating defects in a-$SiO_2$

Number of oxygen to be removed:
from 1 to 6




556 atoms in scattering region

16.24 Å

*Nikolai Sergueev*

# How is the leakage current affected by the defects?

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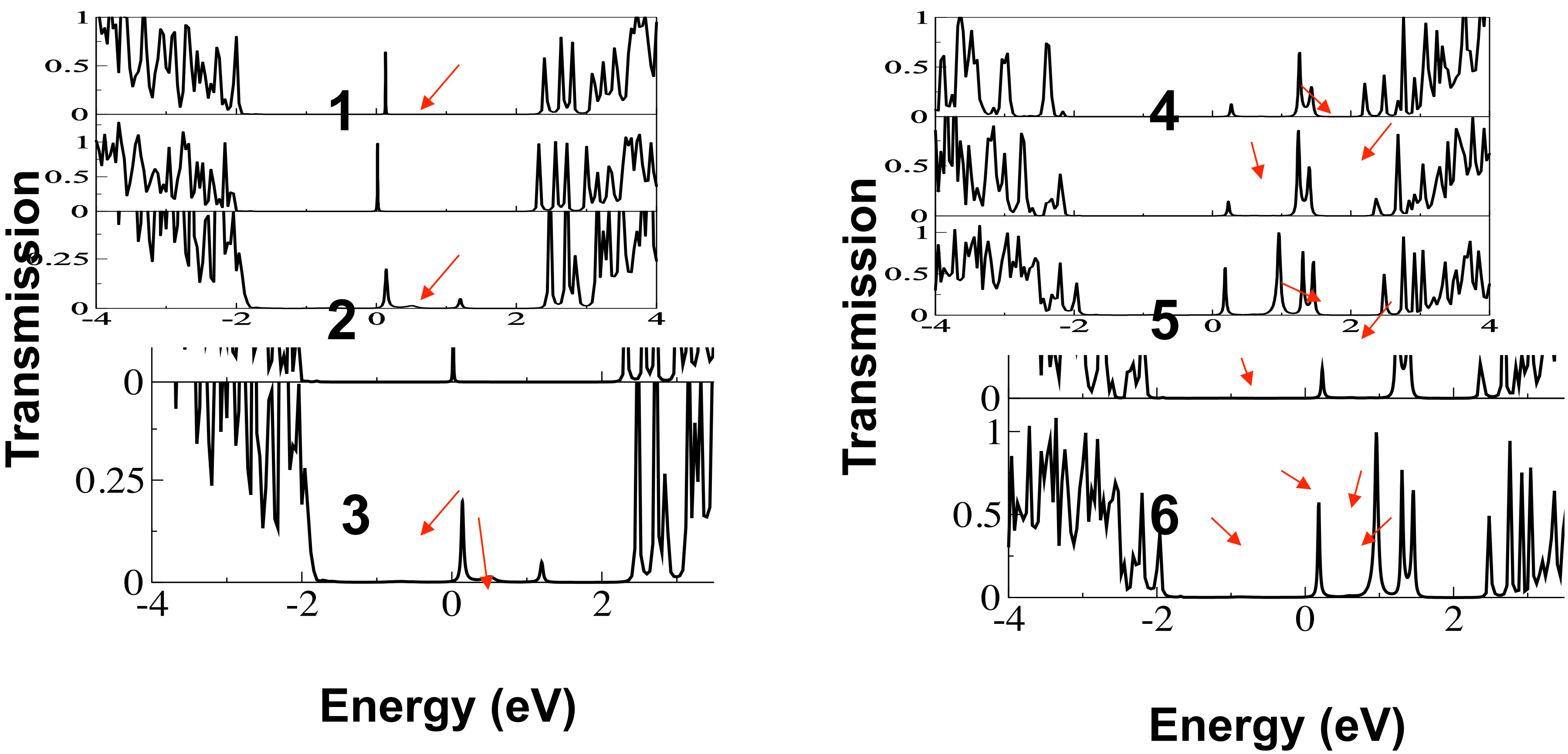
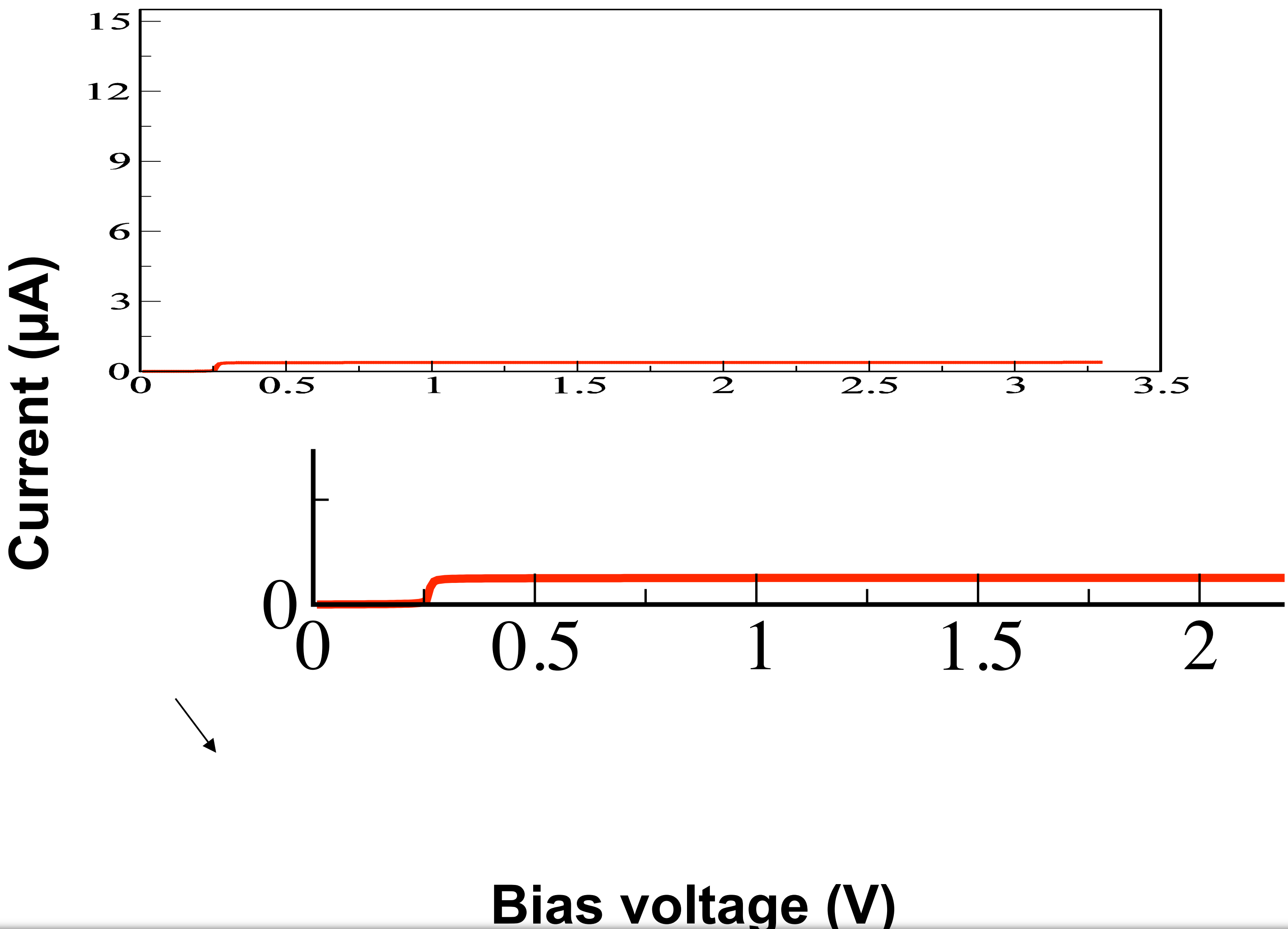
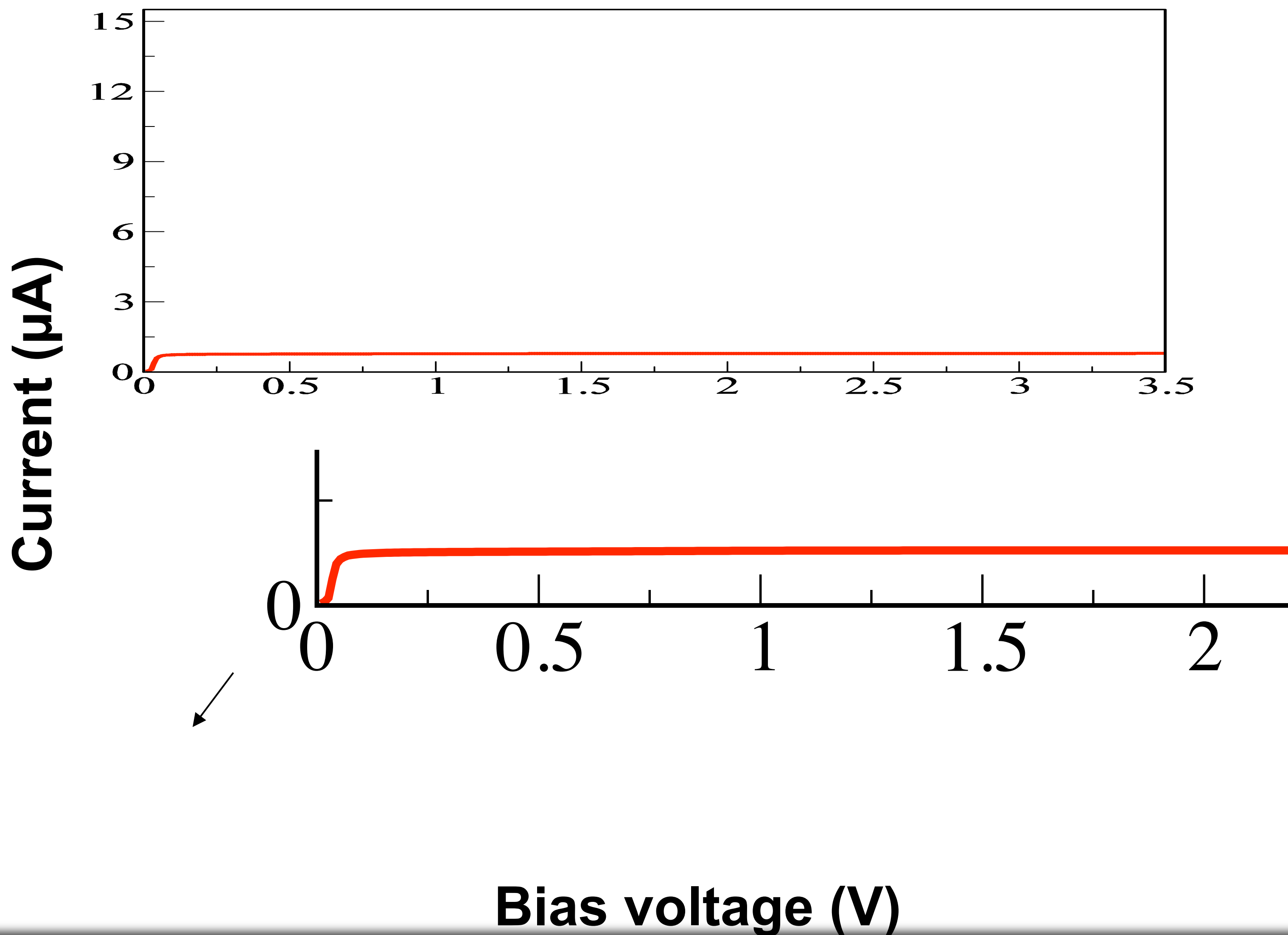
**Increasing number of defects …**



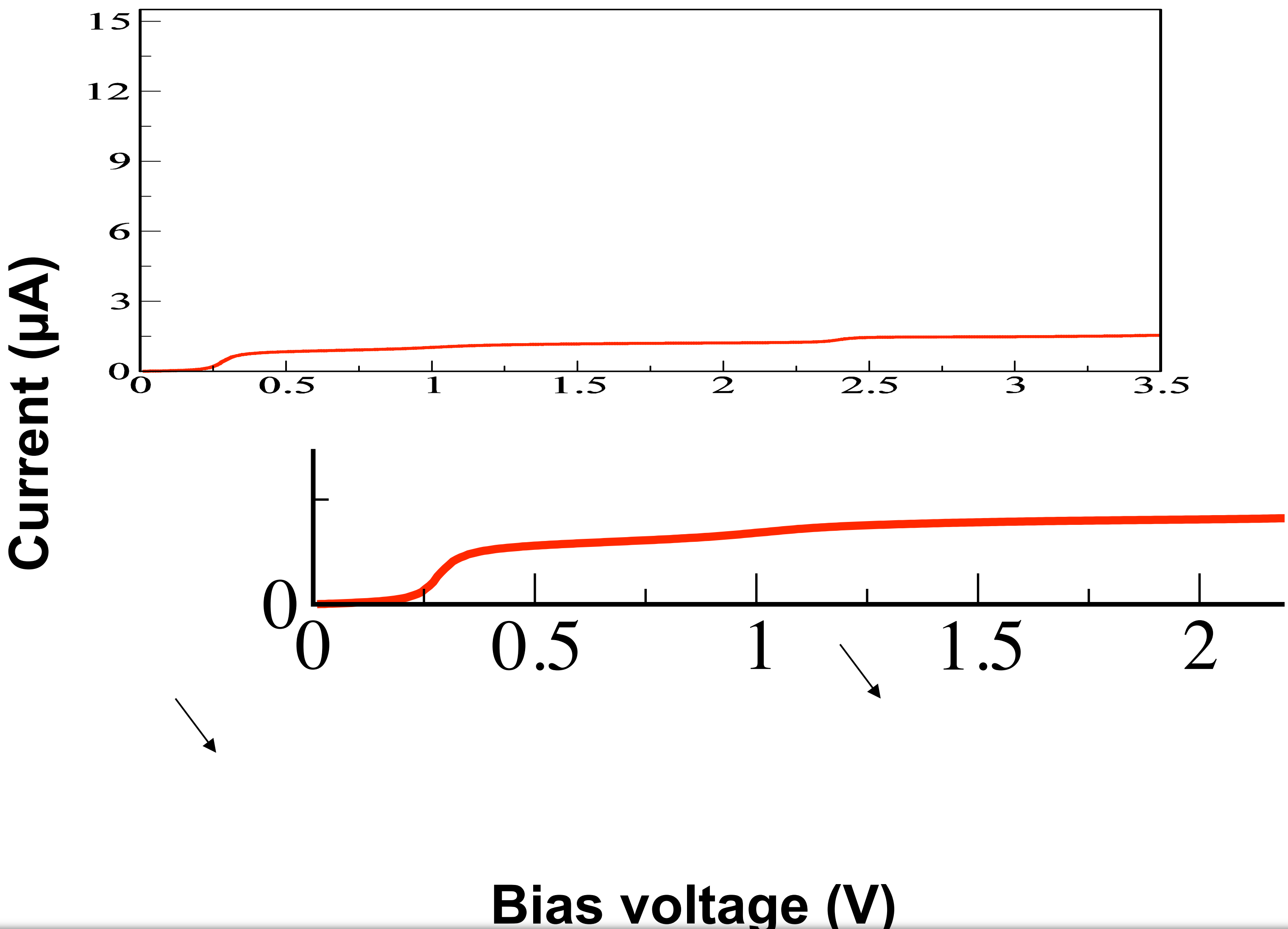
# 1 defect



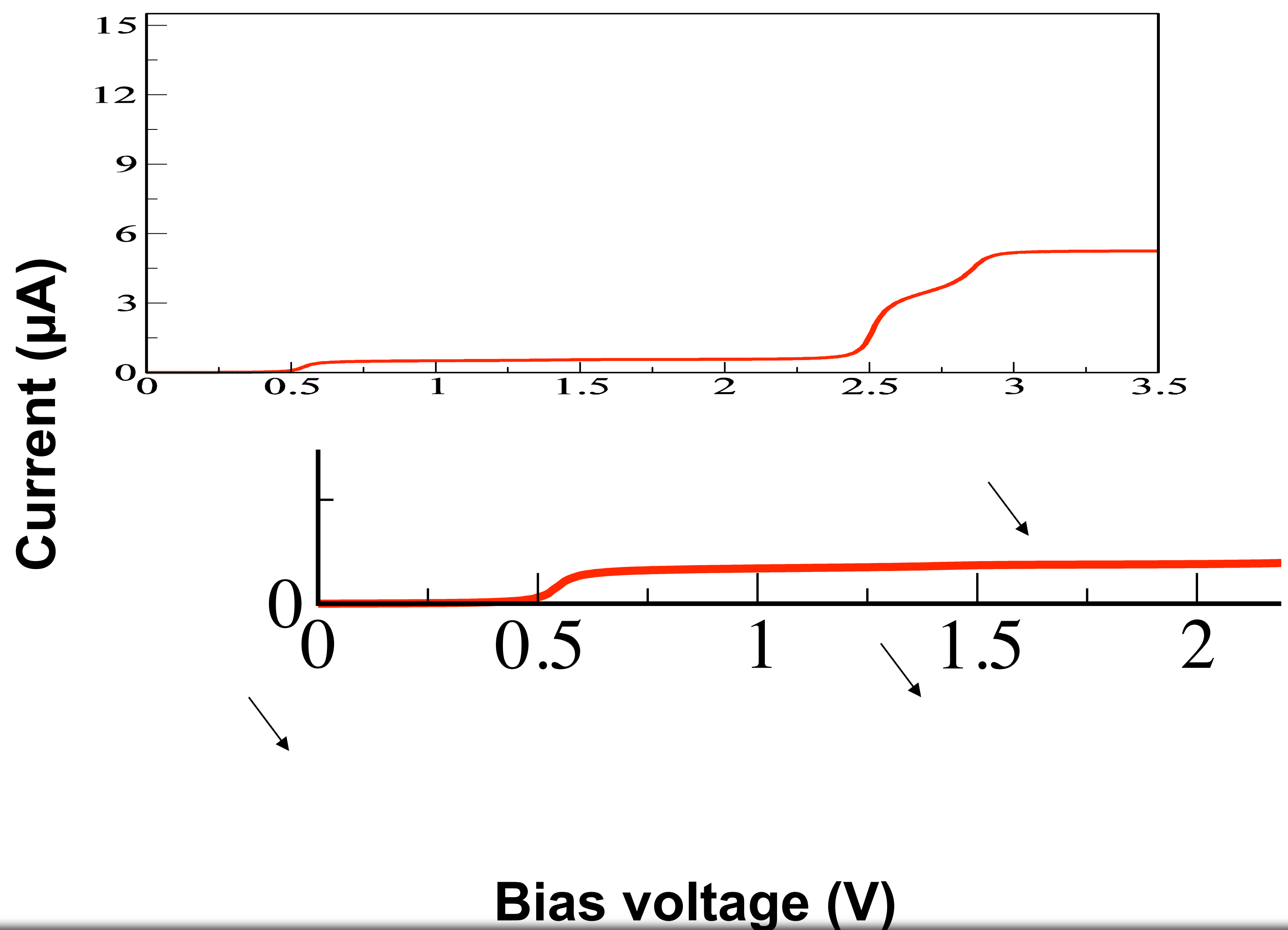
# 2 defects



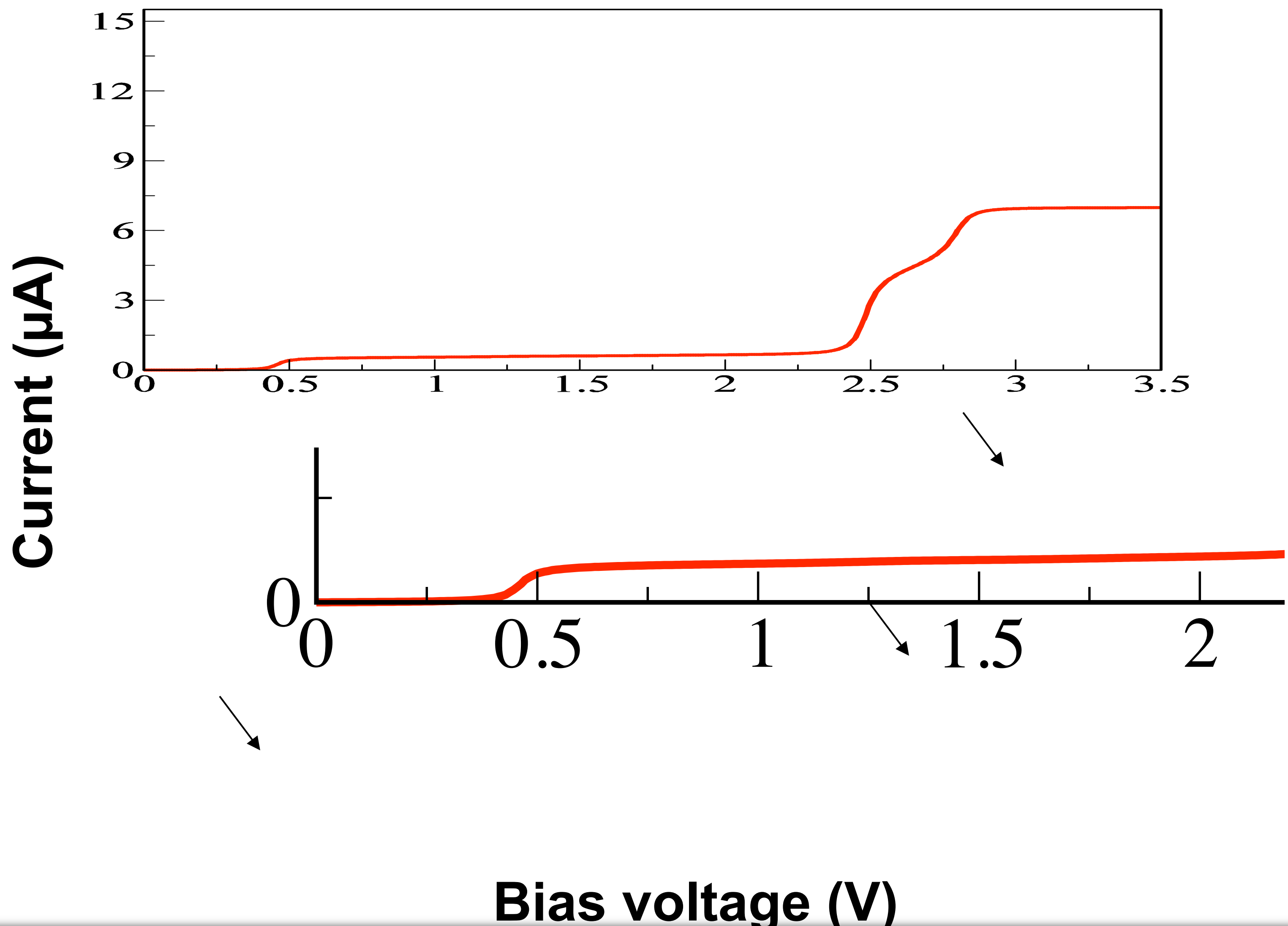
# 3 defects



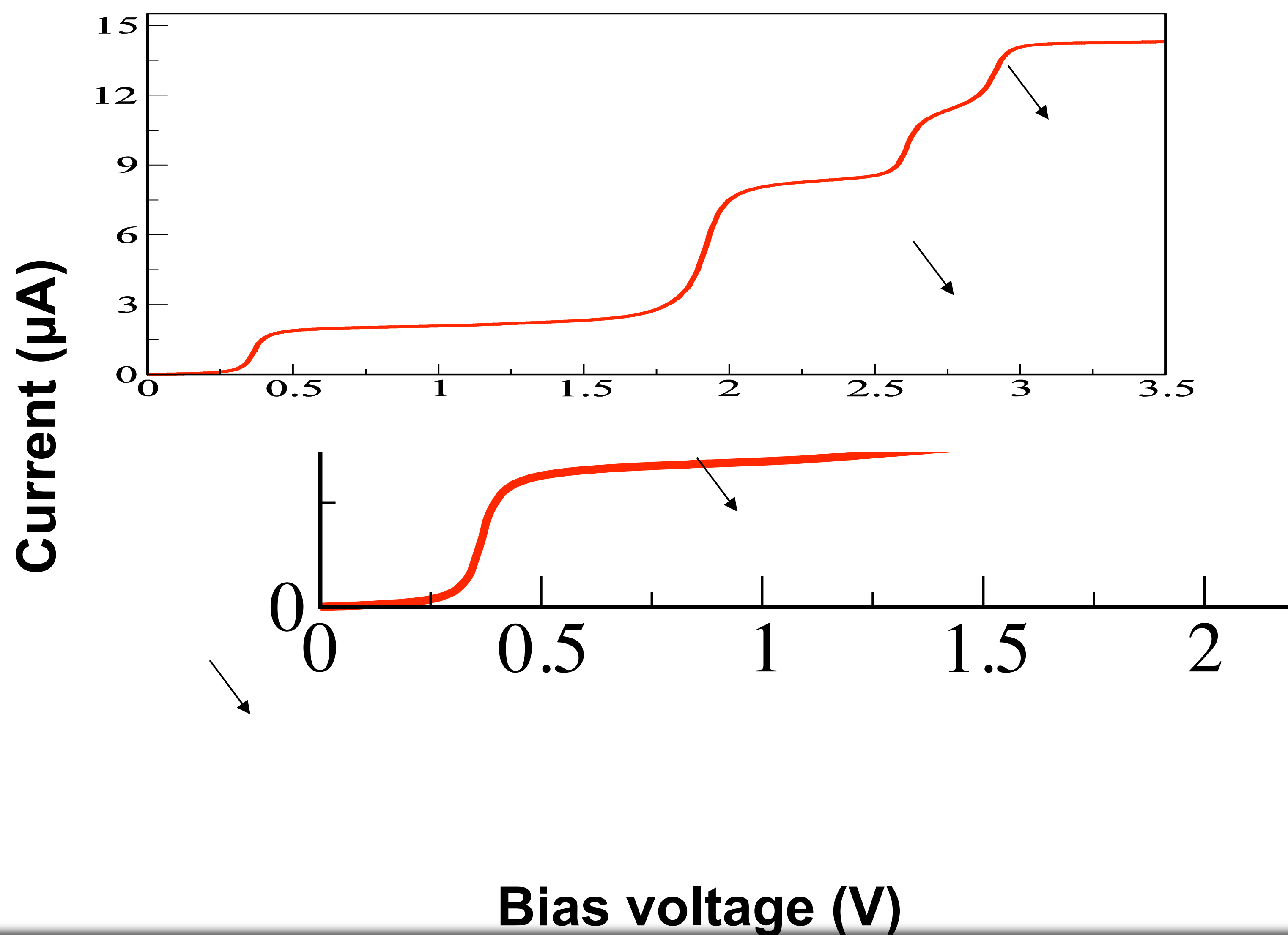
# 4 defects



# 5 defects



# 6 defects



# Conclusions

We performed first principles quantum mechanical transport calculations and we obtained the following:

- conductance vs. oxide thickness dependence is correct
- current-voltage dependence qualitatively agrees with experiment
- the defects result in the step-like functions of the IV
- current increases with number of defects

Going from atomic-scale to mesoscale description …

***First Principles Transport QM Model*** → ***parameters*** → ***Percolation Model***

# Ion-Induced Leakage Currents
## III. Percolation Model

M. J. Beck[1], N. Sergueev[1], Y. S. Puzyrev[1],
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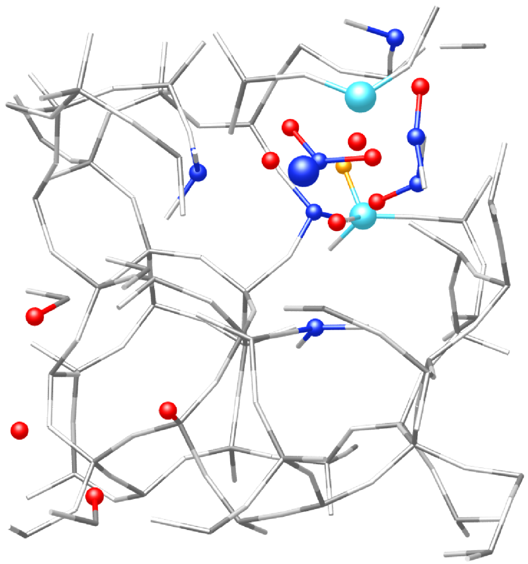
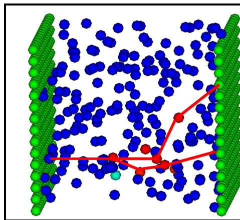
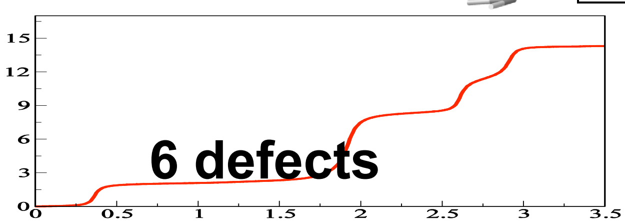
# Multi-scale calculation

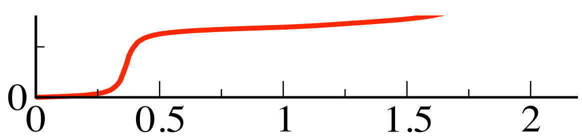
## *From QM transport to I-V device characteristics*

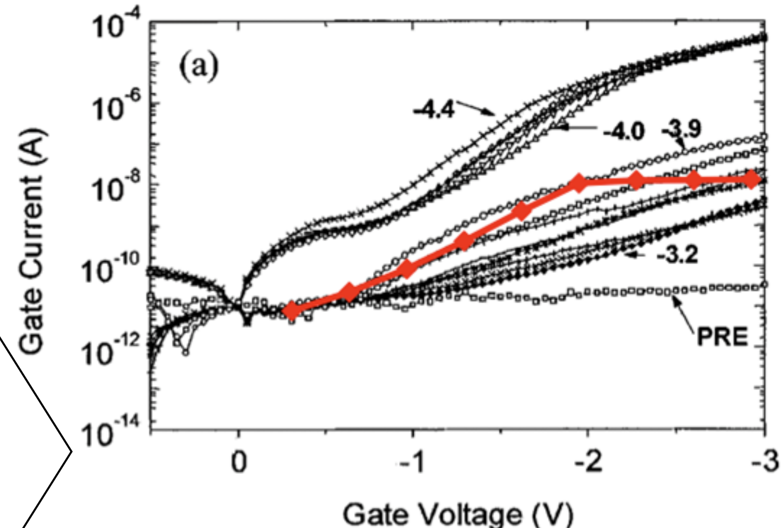


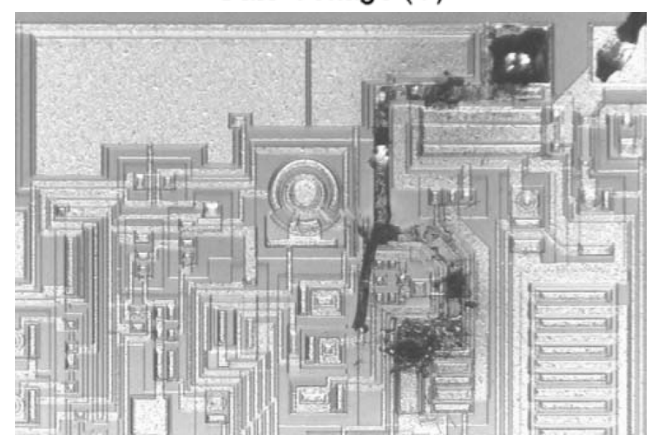
Mott's defect-defect tunneling





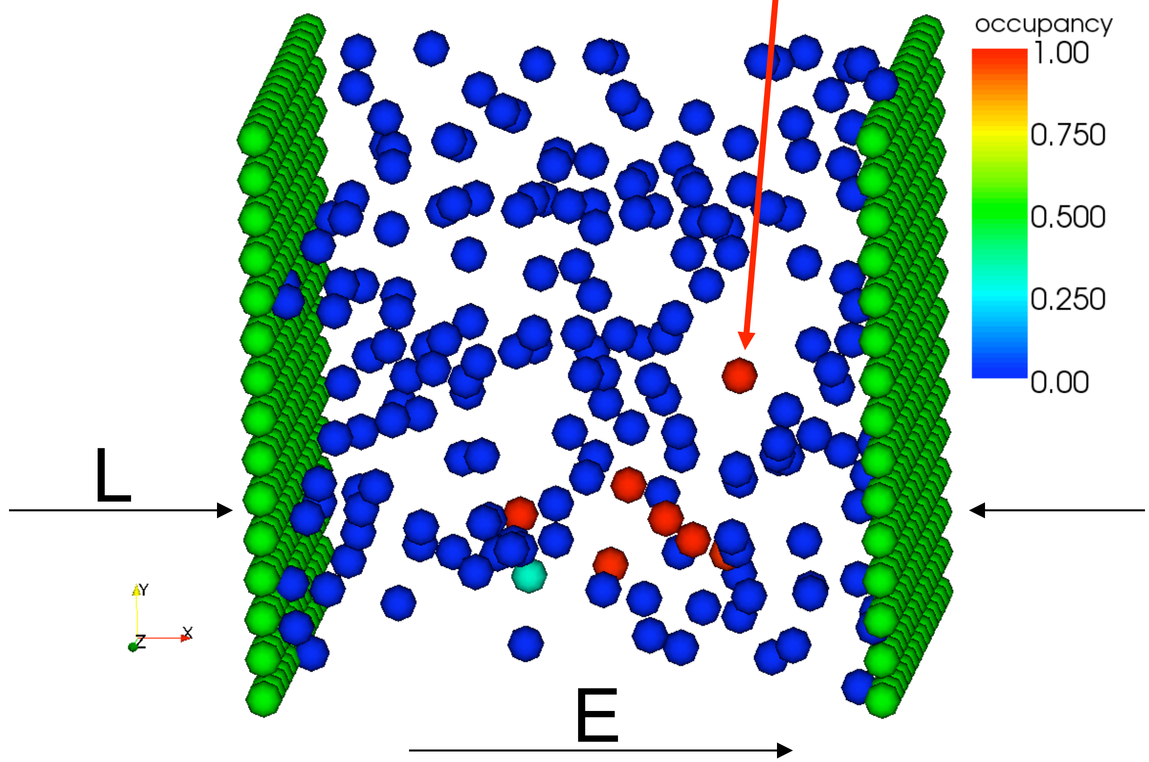
# Defect-to-defect tunneling

- L =1.4 nm
- Defect energy levels
- Defect atomistic map

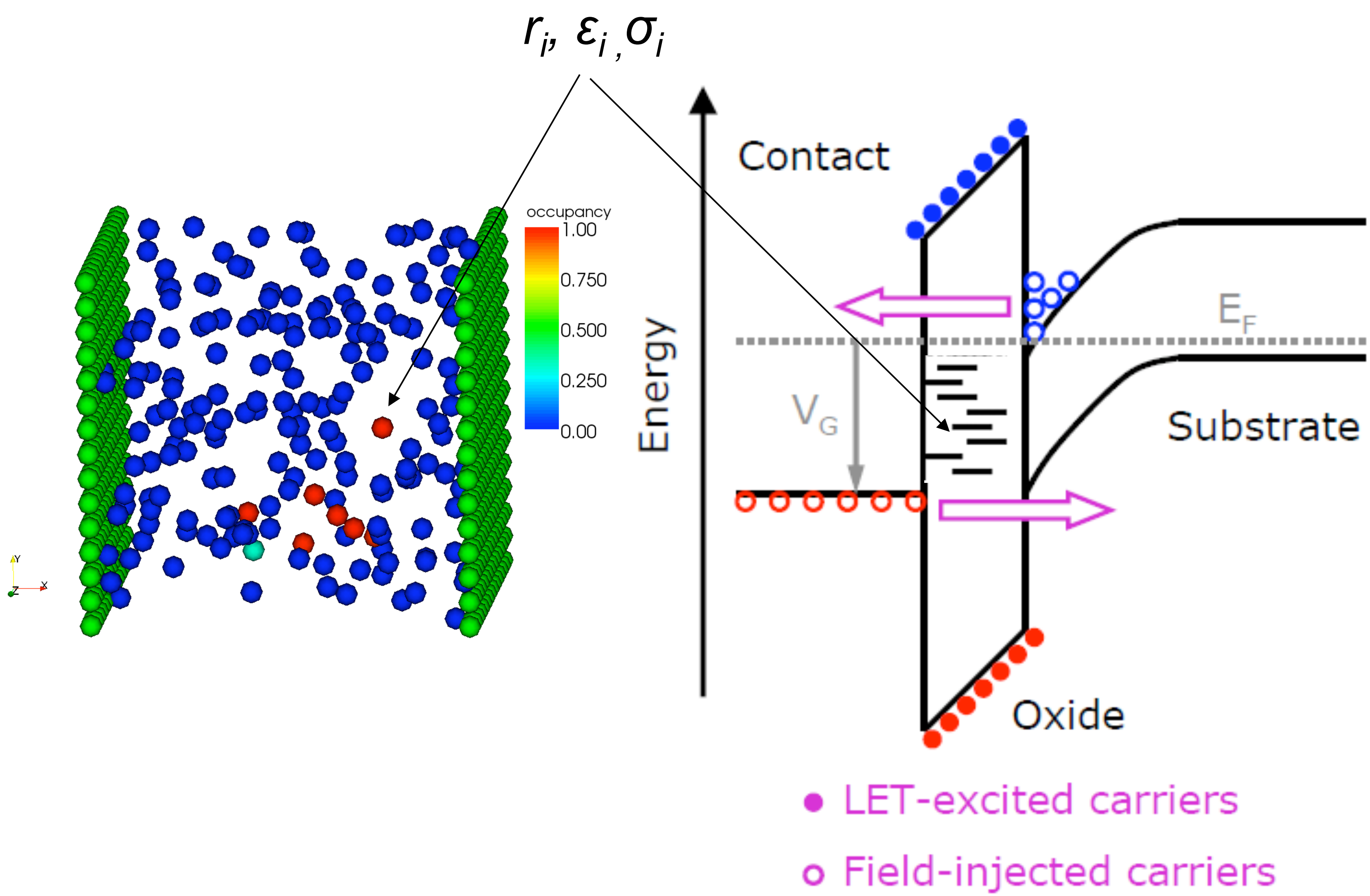
time = 78fs
22 defects

**Defects DOS**

$r_i, \varepsilon_i, \sigma_i$



# Defect-to-defect tunneling



# Defect-to-defect tunneling

Low-resistivity paths through oxide

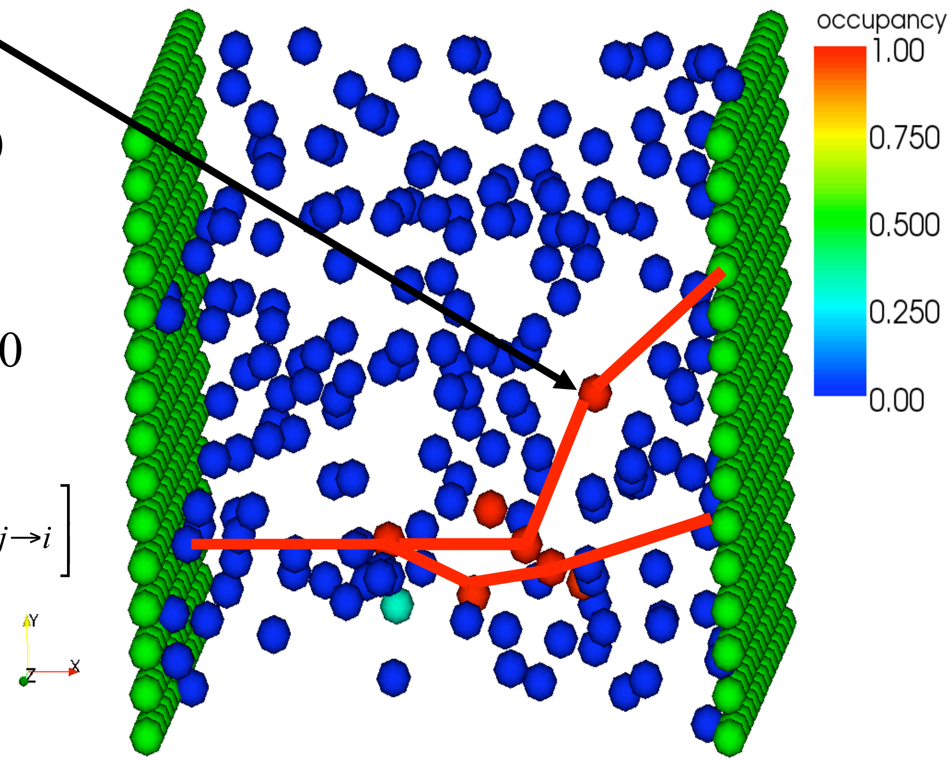
$$J = v_0 \Sigma_{ij} (\sigma_i^{boundary} - \sigma_j)$$

$$v_0 = 1.15 \times 10^{13}\ s^{-1}$$

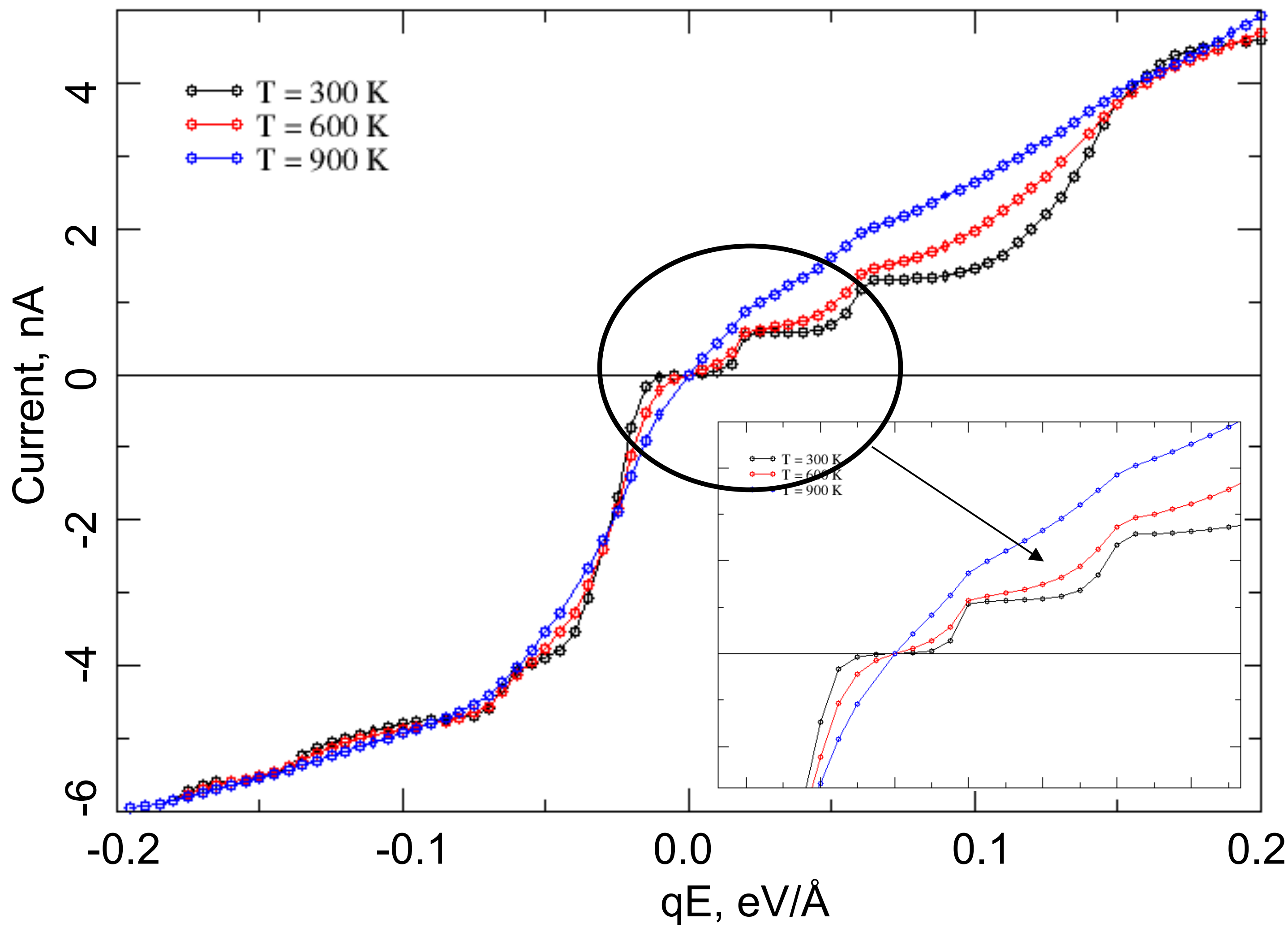
$$\Delta\varepsilon_{i\to j} = \left(\varepsilon_j - \varepsilon_i\right) + qE\left[\hat{e}_x \cdot \left(\vec{r_j} - \vec{r_i}\right)\right]$$

$$P_{i\to j} = \begin{cases} \exp\left(\dfrac{-\left|\vec{r_j} - \vec{r_i}\right|}{r_0}\right), & \Delta\varepsilon_{i\to j} \le 0 \\ \exp\left(\dfrac{-\left|\vec{r_j} - \vec{r_i}\right|}{r_0} + \dfrac{-\Delta\varepsilon_{i\to j}}{kT}\right), & \Delta\varepsilon_{i\to j} > 0 \end{cases}$$

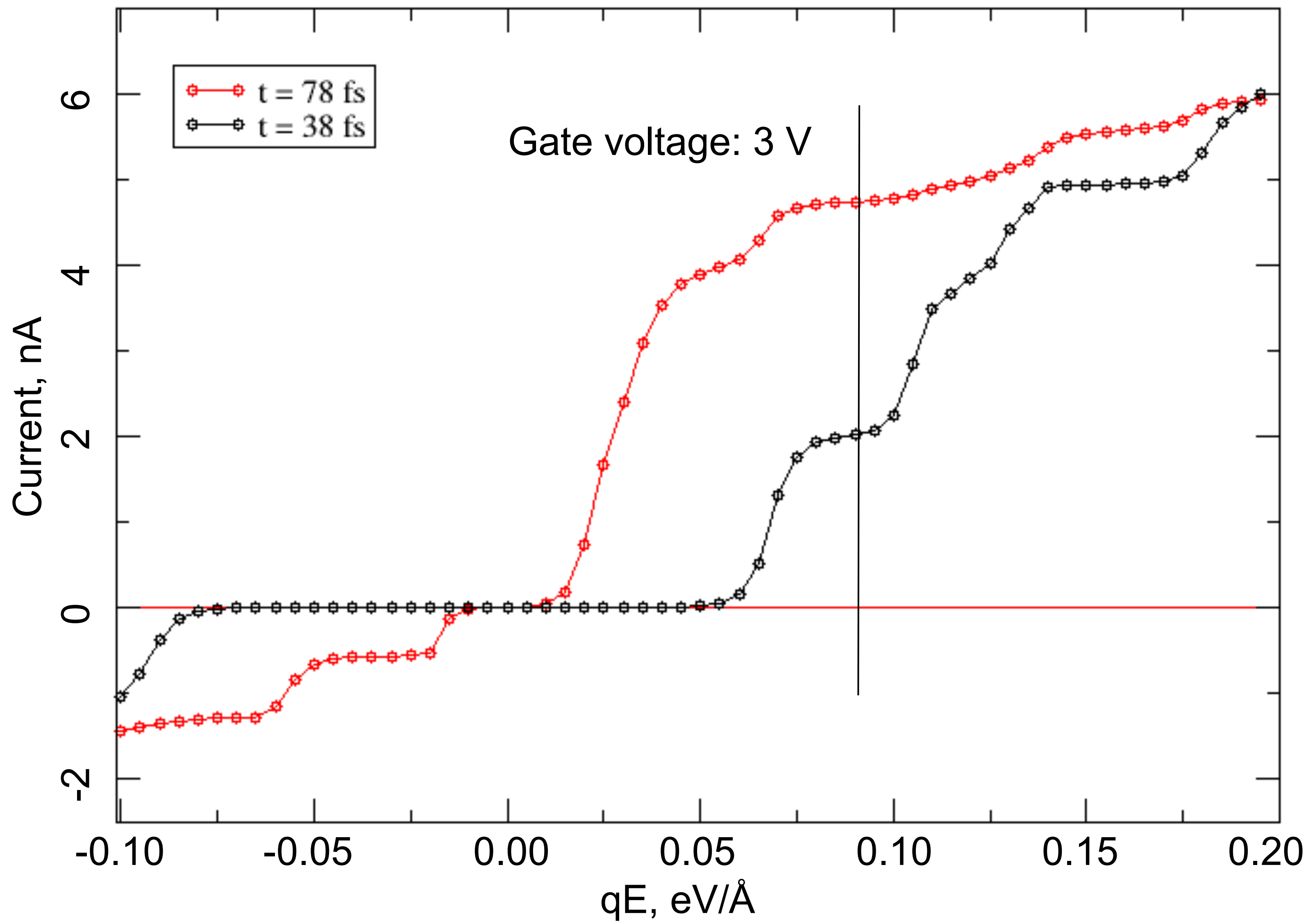
$$\sigma_j^{s+1} = \sigma_j^s + \sum_i \left[\sigma_i^s\left(1 - \sigma_j^s\right)P_{i\to j} - \sigma_j^s\left(1 - \sigma_i^s\right)P_{j\to i}\right]$$



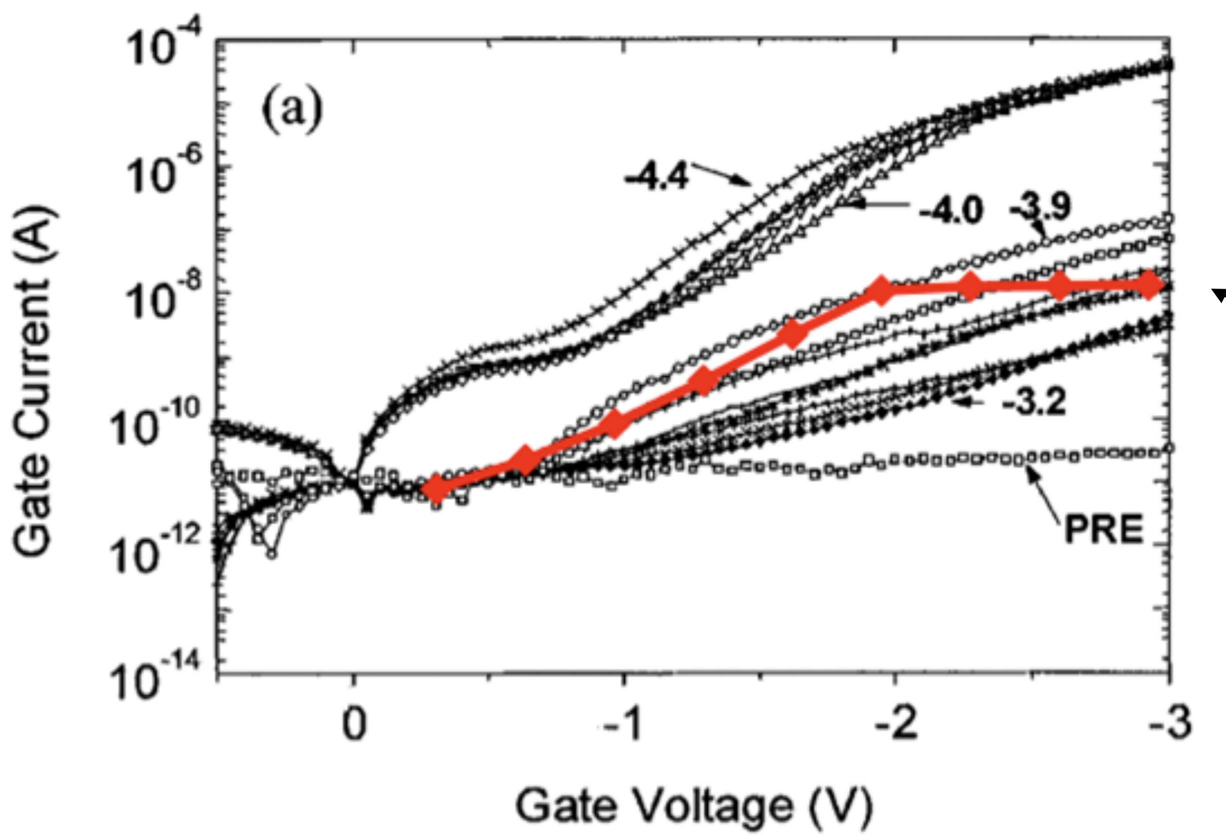
# Leakage Current Temperature Dependence



# Leakage Current Time Dependence



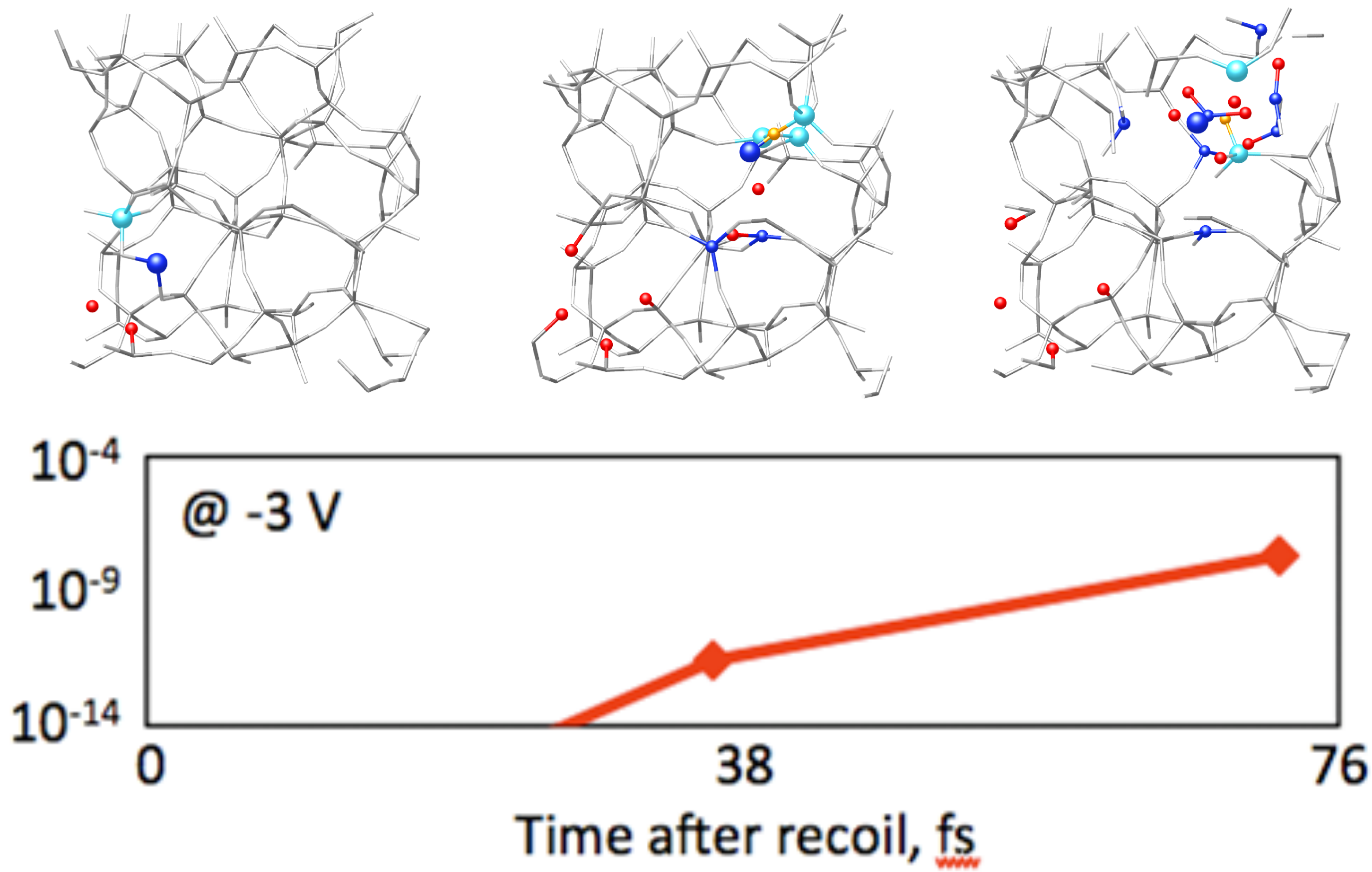
# Direct comparison with experiment

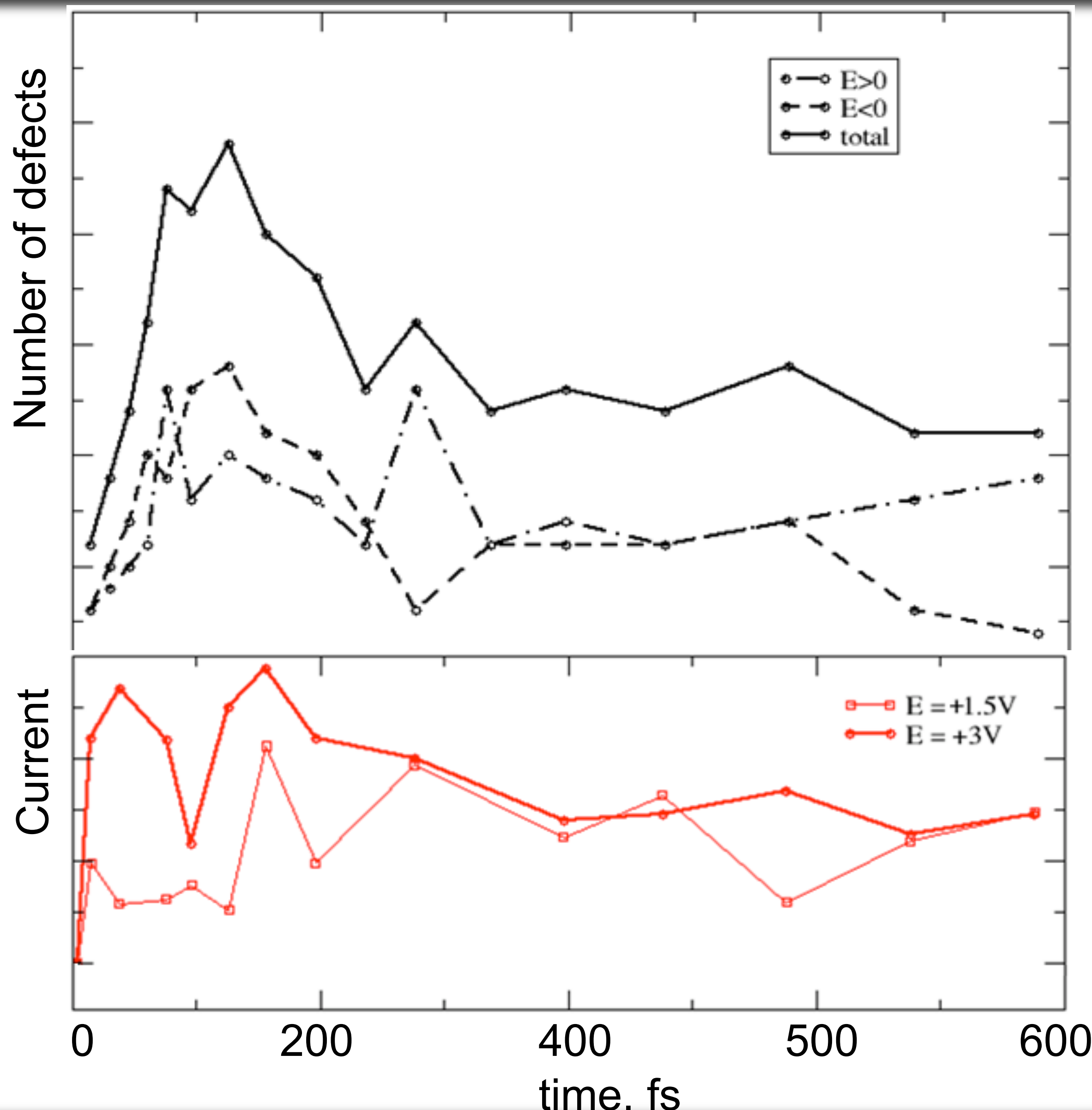



Quantitative agreement!

Massengill, et al., IEEE TNS 48 1904 (2001)

# Model results in real-time defect evolution and transient currents






Defect time evolution

*Energy*

*Space*

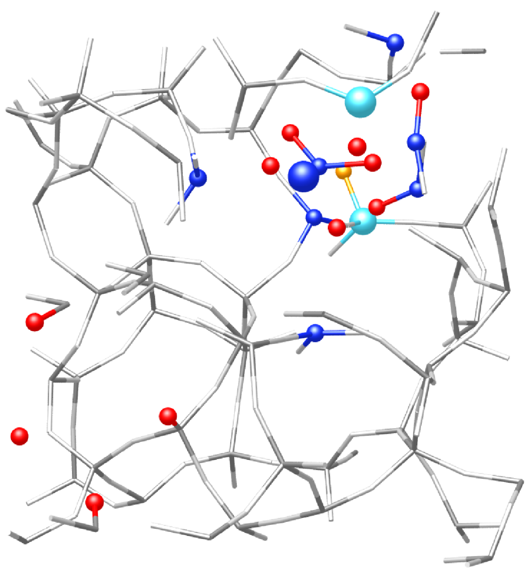
Transient current
Keeps going

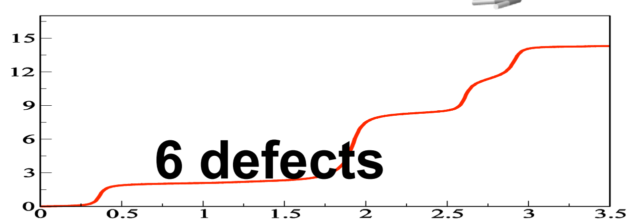
# Conclusion

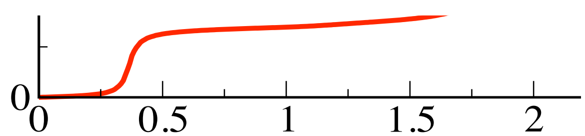
- Displacement damage lead to appreciable current
- Low-resistivity paths through oxide layers
- 3D Mott defect-to-defect calculation of leakage currents

# Conclusion

## ***From QM transport to I-V device characteristics***






Quantitative agreement!