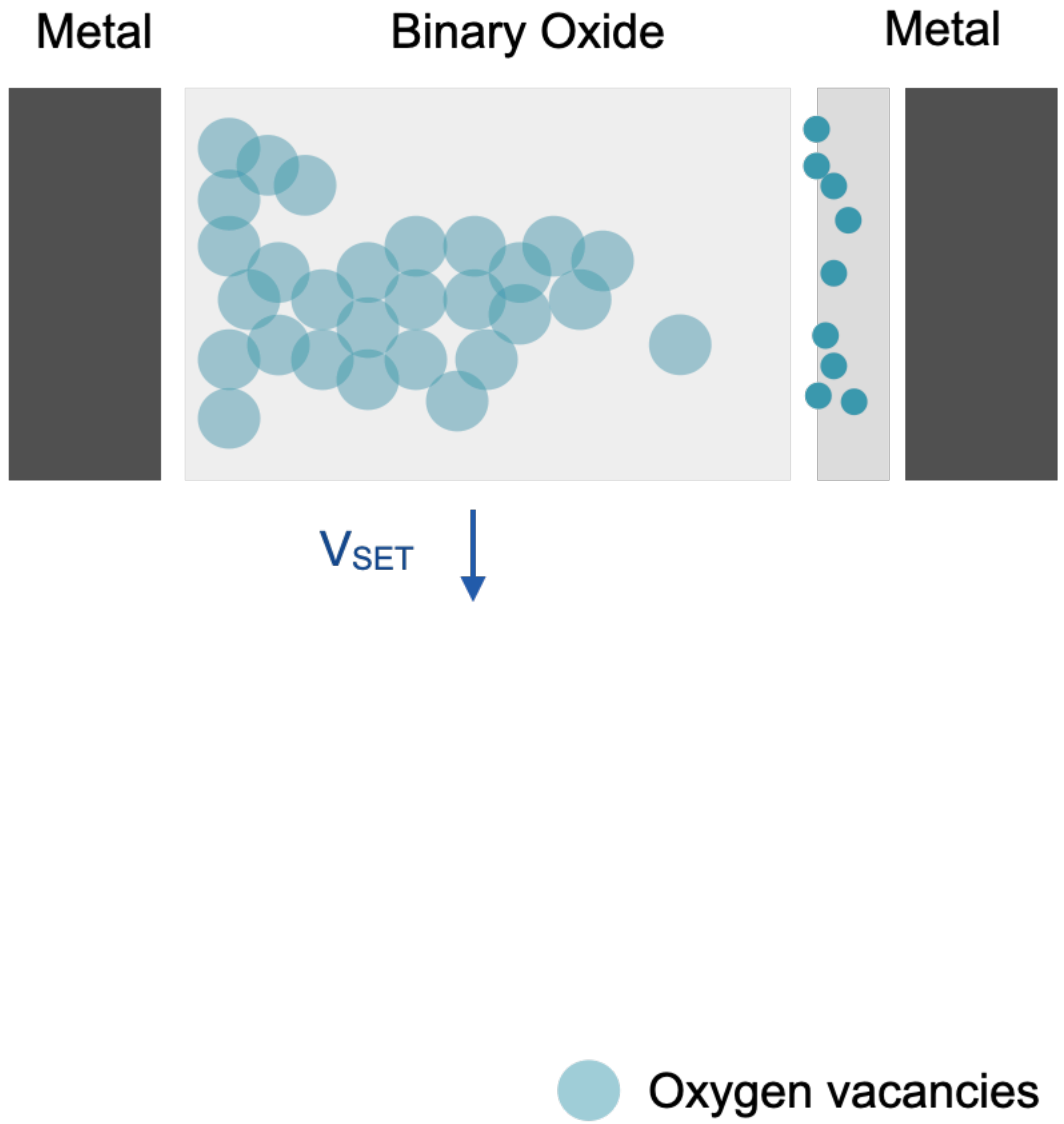
ETH zürich

Atomistic insights behind multi-level conductance transitions in HfOx memristors

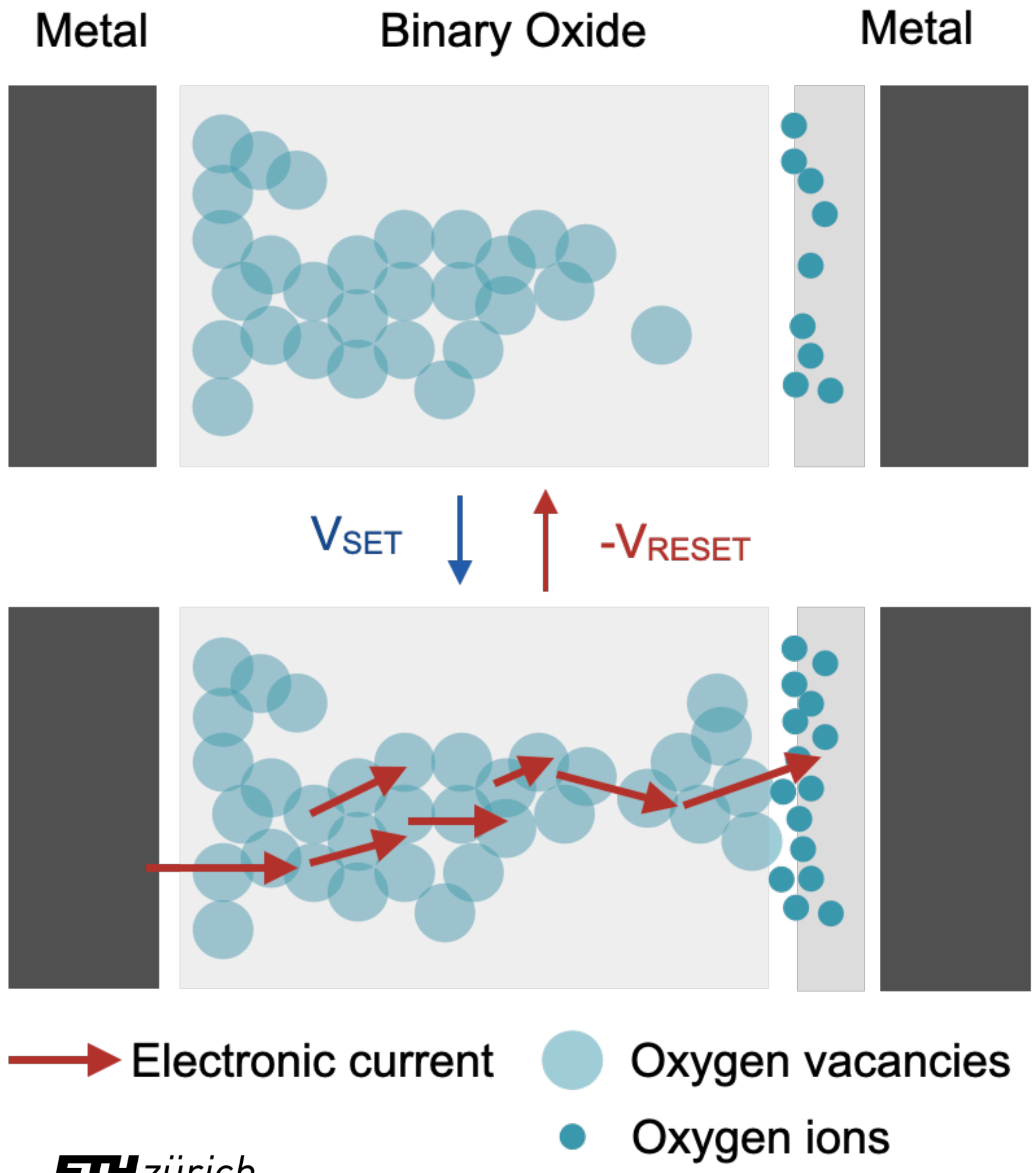
Manasa Kaniselvan
PhD Candidate, Institute for Integrated Systems
Computational Nanoelectronics Group

Coauthors: Marko Mladenovic, Jente Clarysse, Kevin Portner, Mathieu Luisier

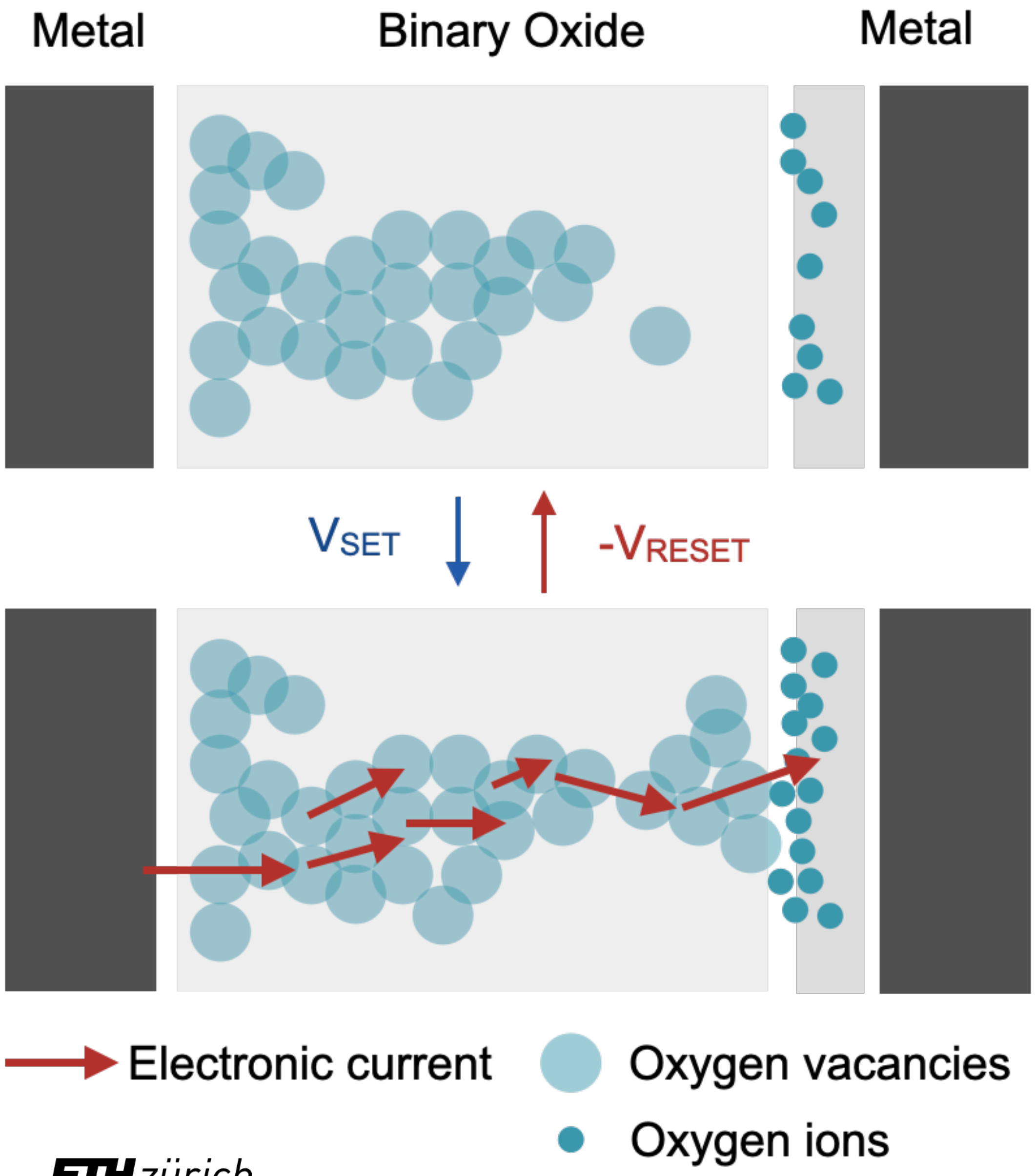
Oxide-based RRAM



Oxide-based RRAM



Oxide-based RRAM

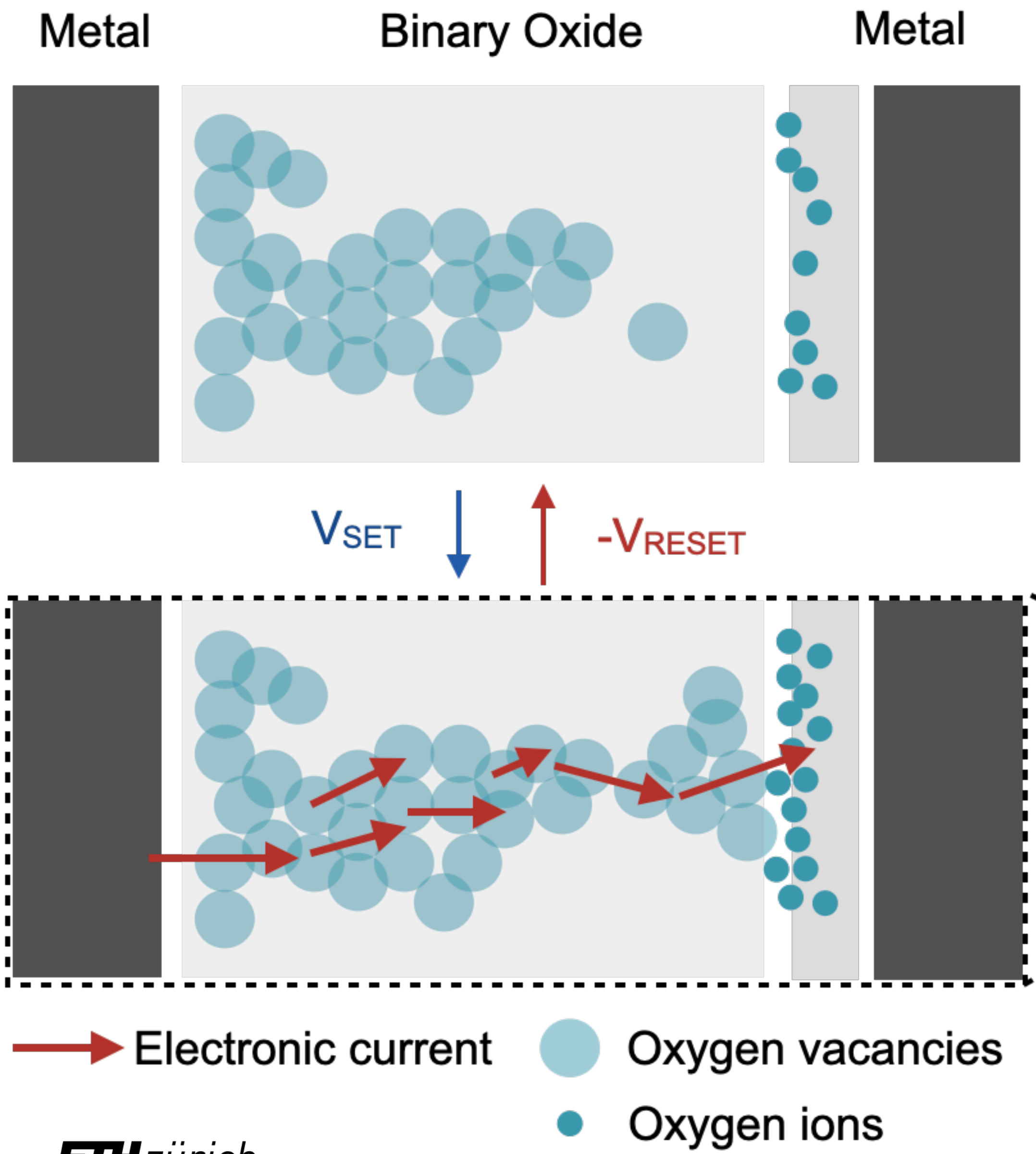


Emerging applications of these devices

- **Storage, on-chip memory (digital)**
- Synaptic weights (analog)

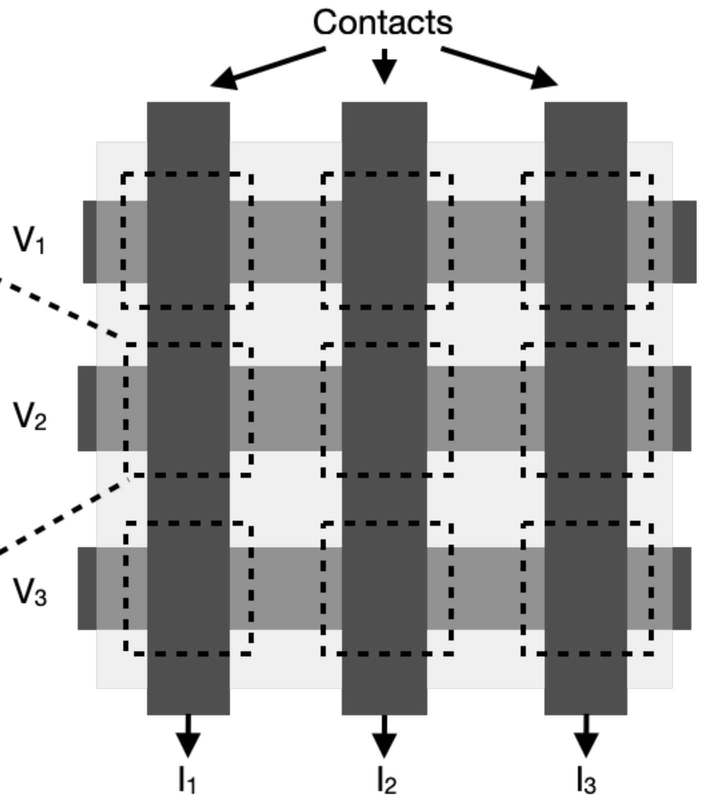
ETH zürich

Oxide-based RRAM



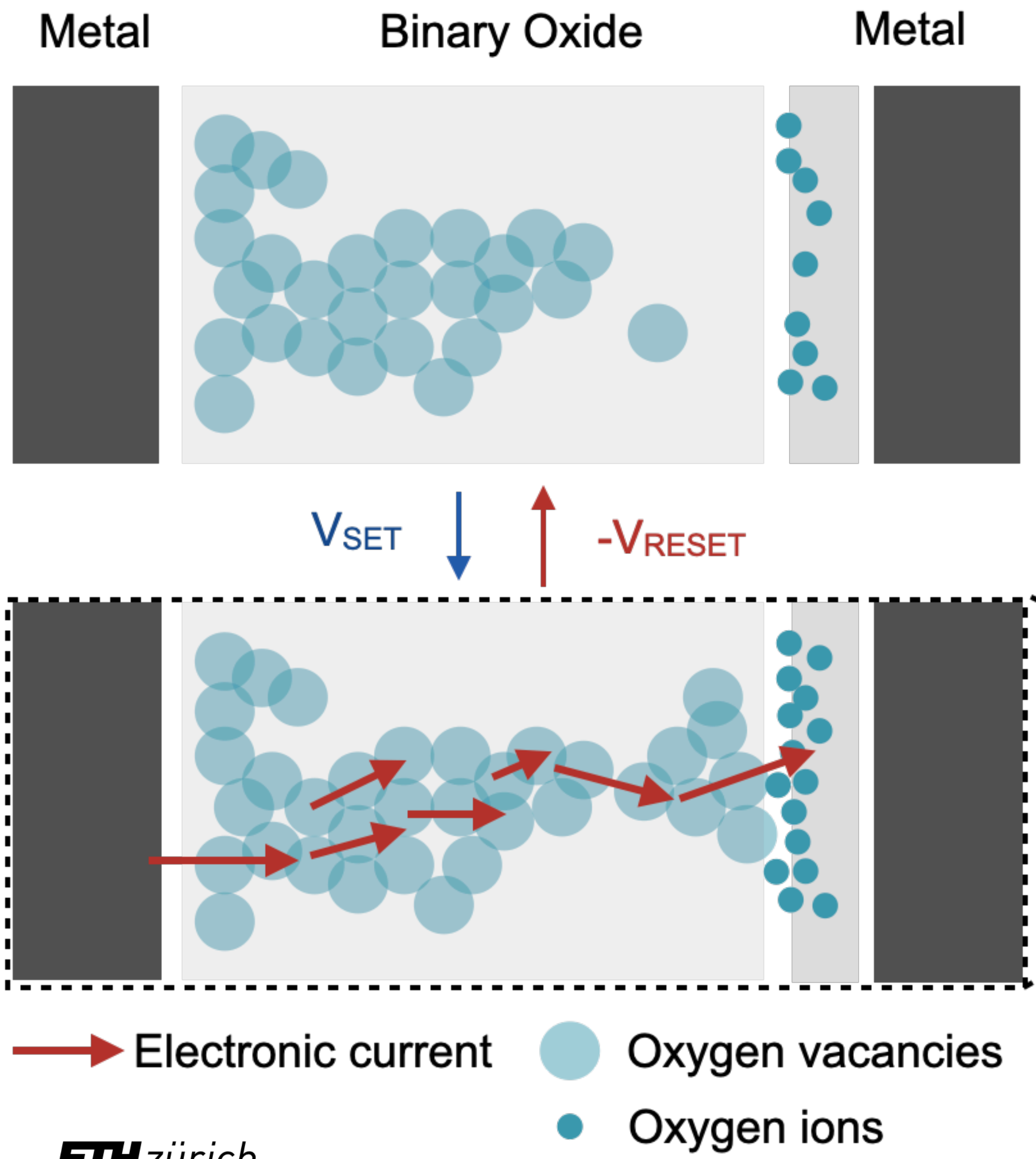
Emerging applications of these devices

- **Storage, on-chip memory (digital)**
- Synaptic weights (analog)



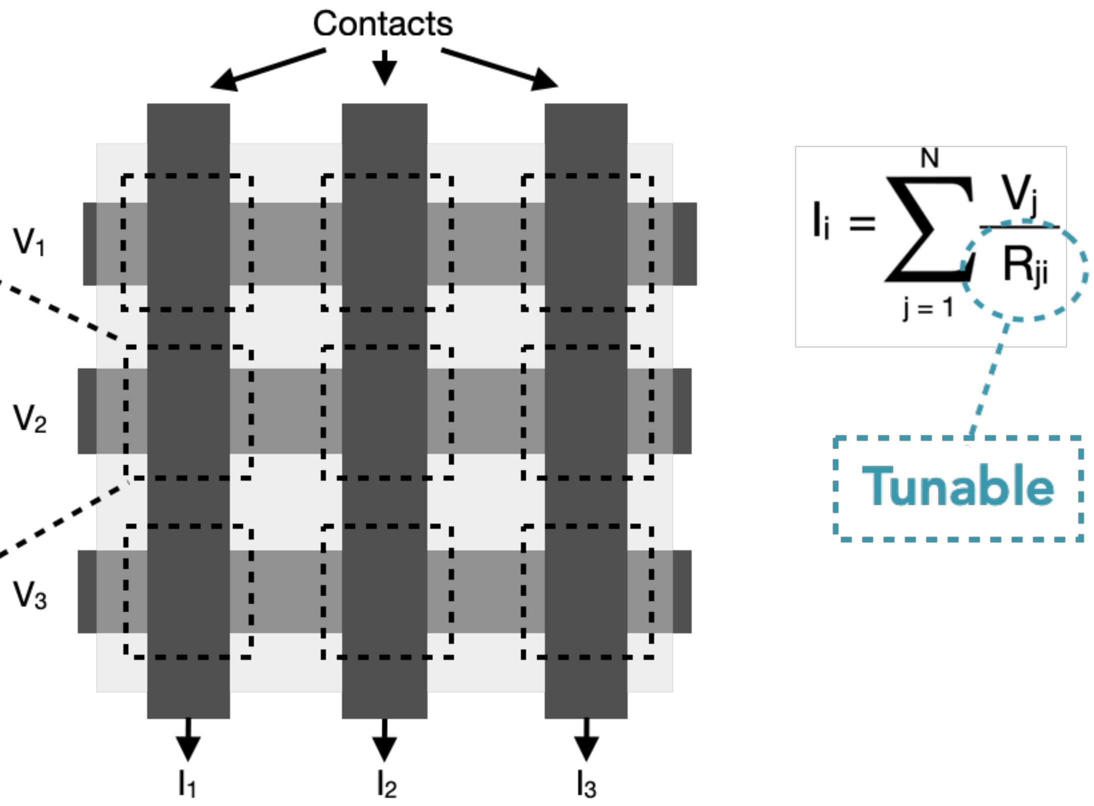
$$I_i = \sum_{j=1}^{N} \frac{V_j}{R_{ji}}$$

Oxide-based RRAM



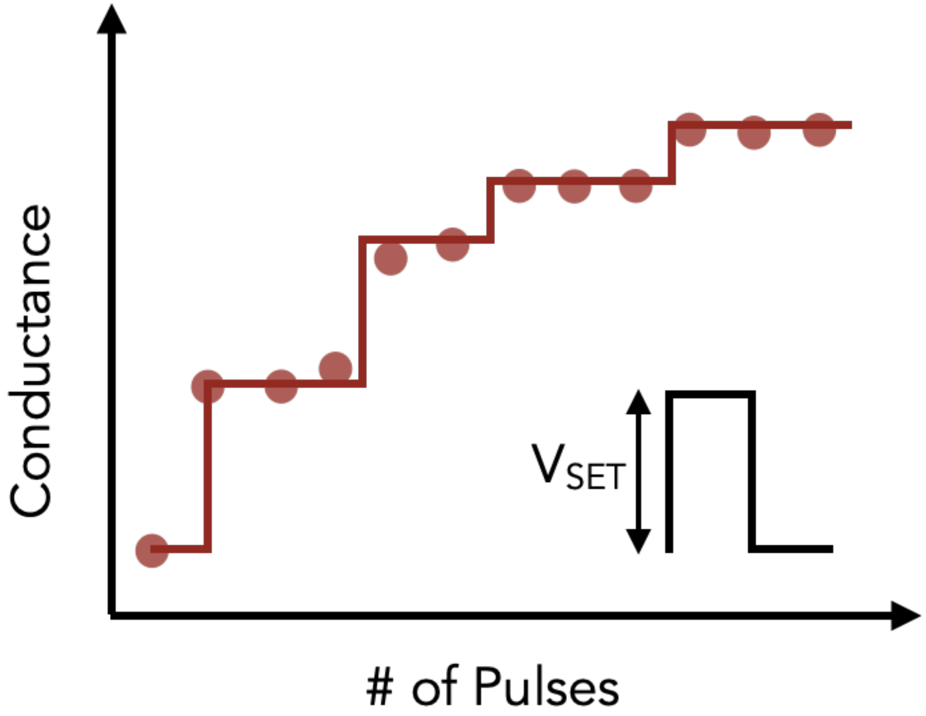
Emerging applications of these devices

- **Storage, on-chip memory (digital)**
- Synaptic weights (analog)



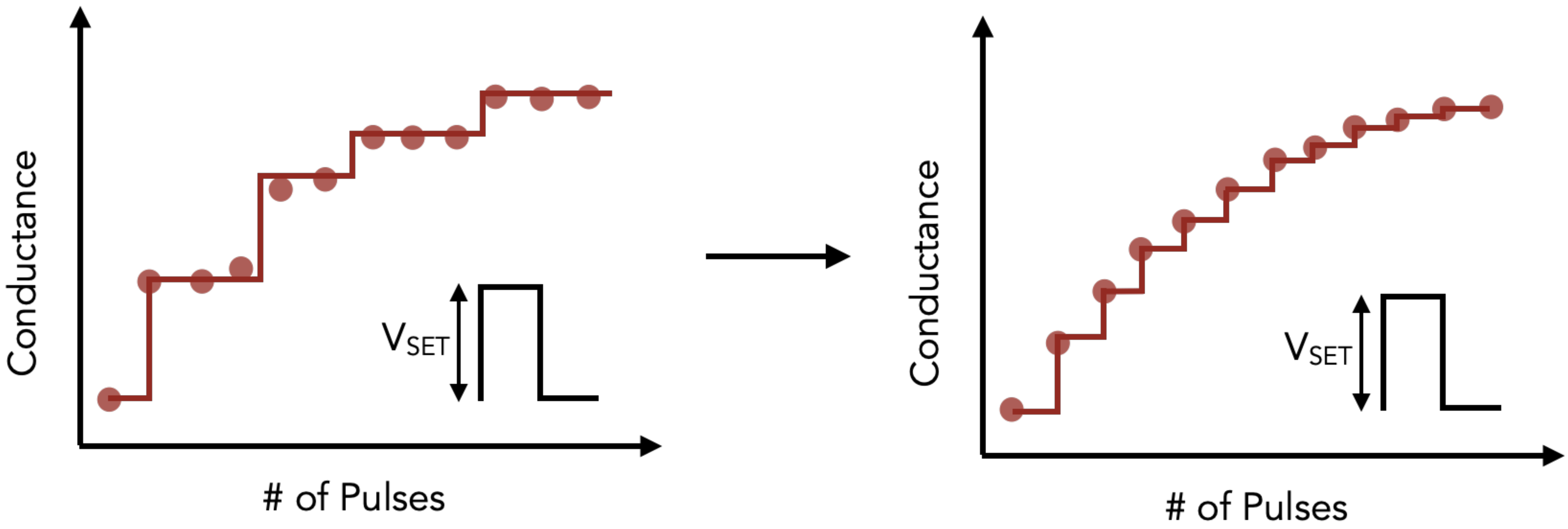
Challenges behind Designing Analog RRAM

- Increase the number of achievable conductances/synaptic weights



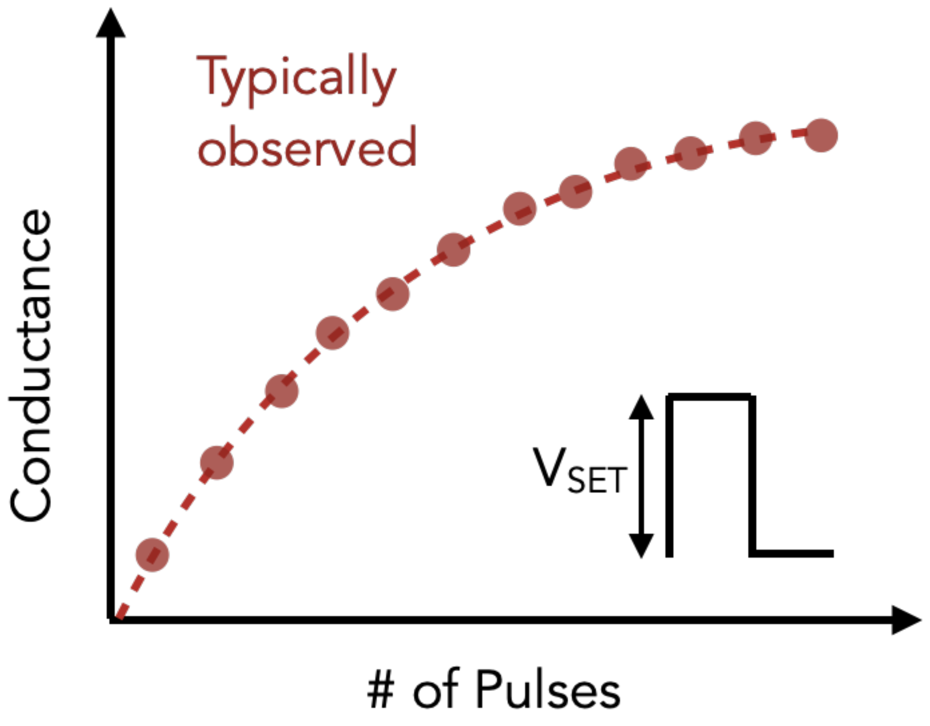
Challenges behind Designing Analog RRAM

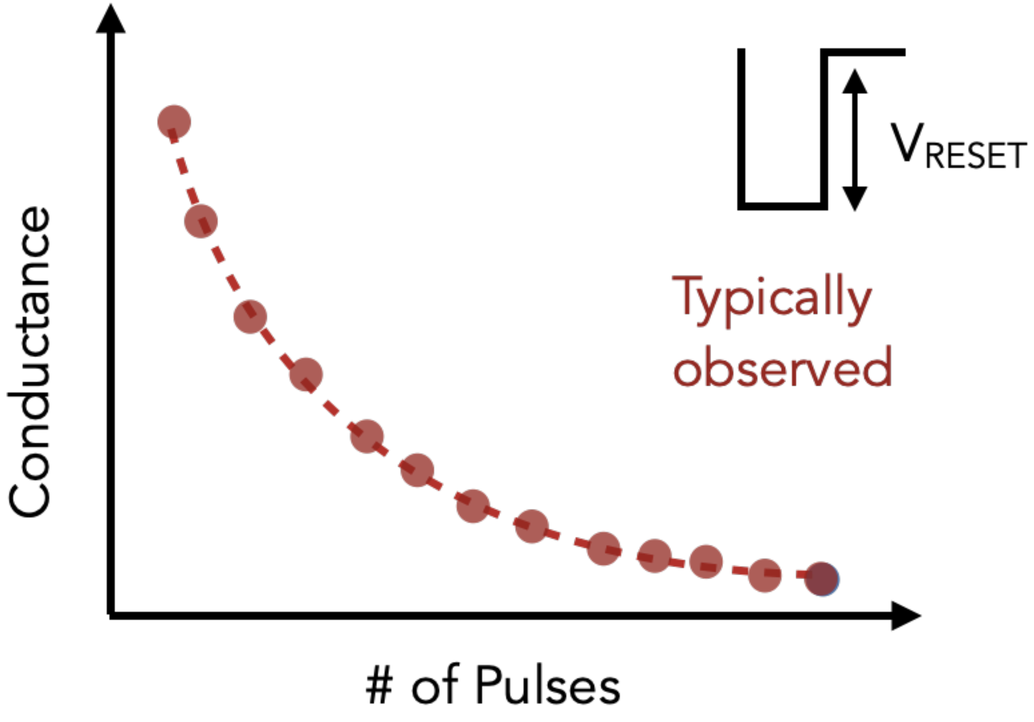
- Increase the number of achievable conductances/synaptic weights



Challenges behind Designing Analog RRAM

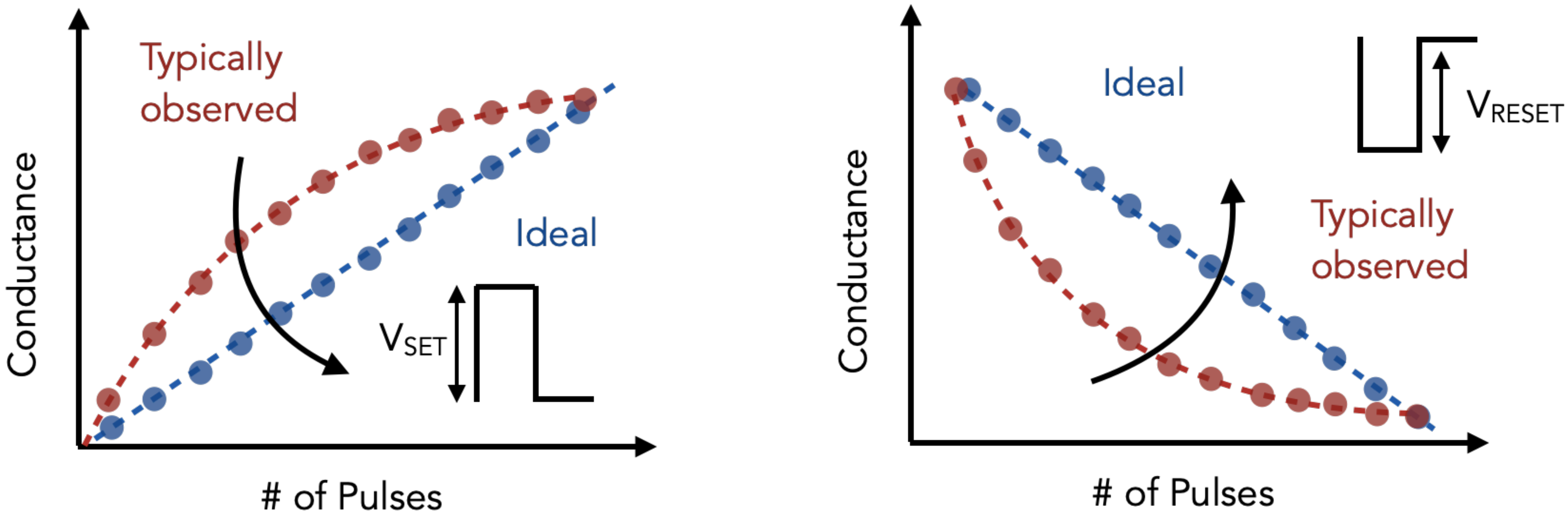
- Increase the number of achievable conductances/synaptic weights
- Linearize the transitions between these conductances/weights



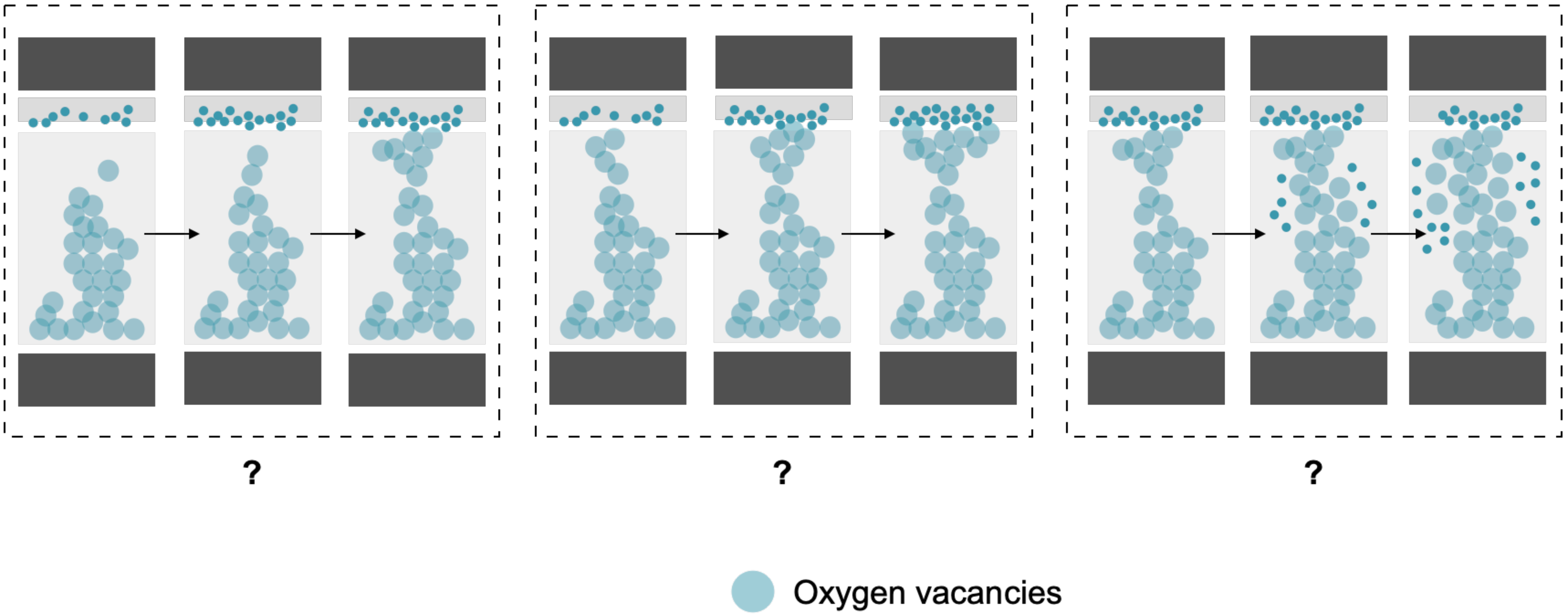


Challenges behind Designing Analog RRAM

- Increase the number of achievable conductances/synaptic weights
- Linearize the transitions between these conductances/weights



Switching Mechanisms for Intermediate States



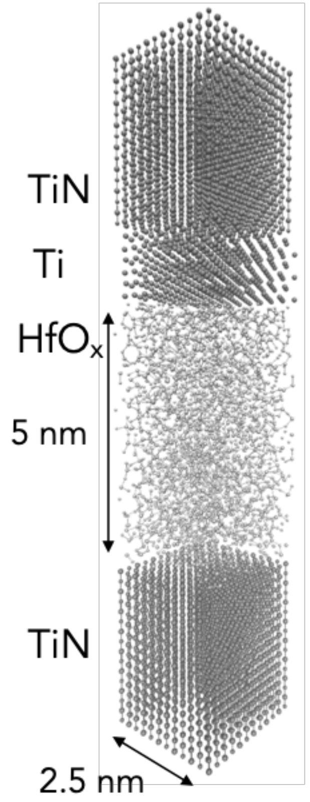
→ Investigate the **ionic kinetics** and **electronic current flow** behind analog device behaviour with **ab-initio** and **atomistic simulations**

→ Investigate the **ionic kinetics** and **electronic current flow** behind analog device behaviour with **ab-initio** and **atomistic simulations**

→ Provide **insight** towards device design

Simulation approach

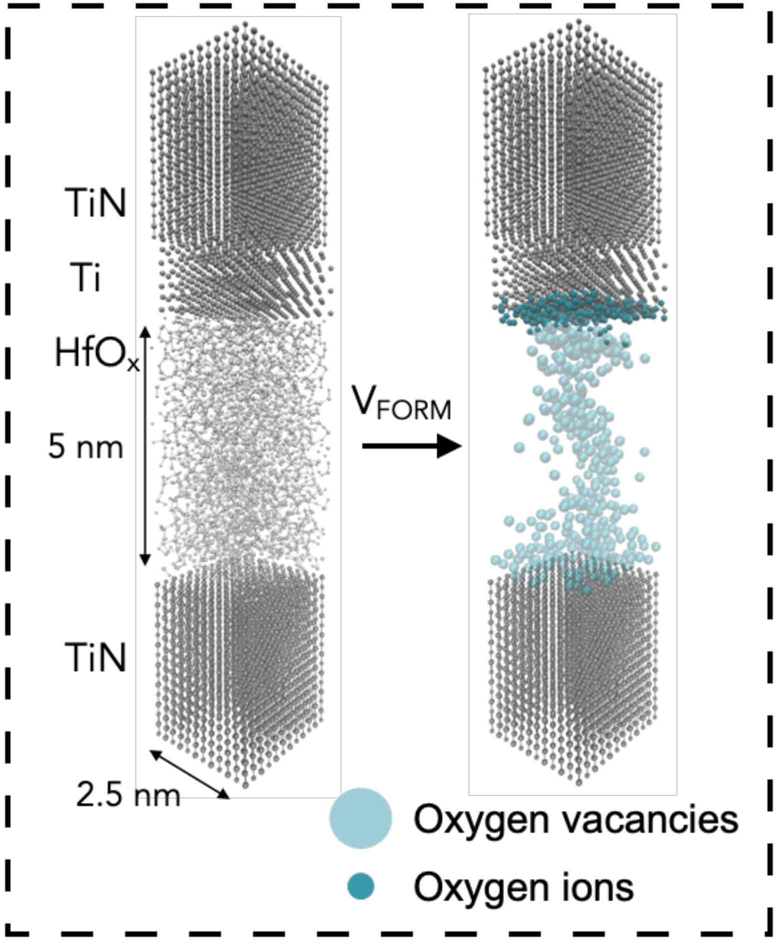
Kinetic Monte Carlo



Atomic Structure

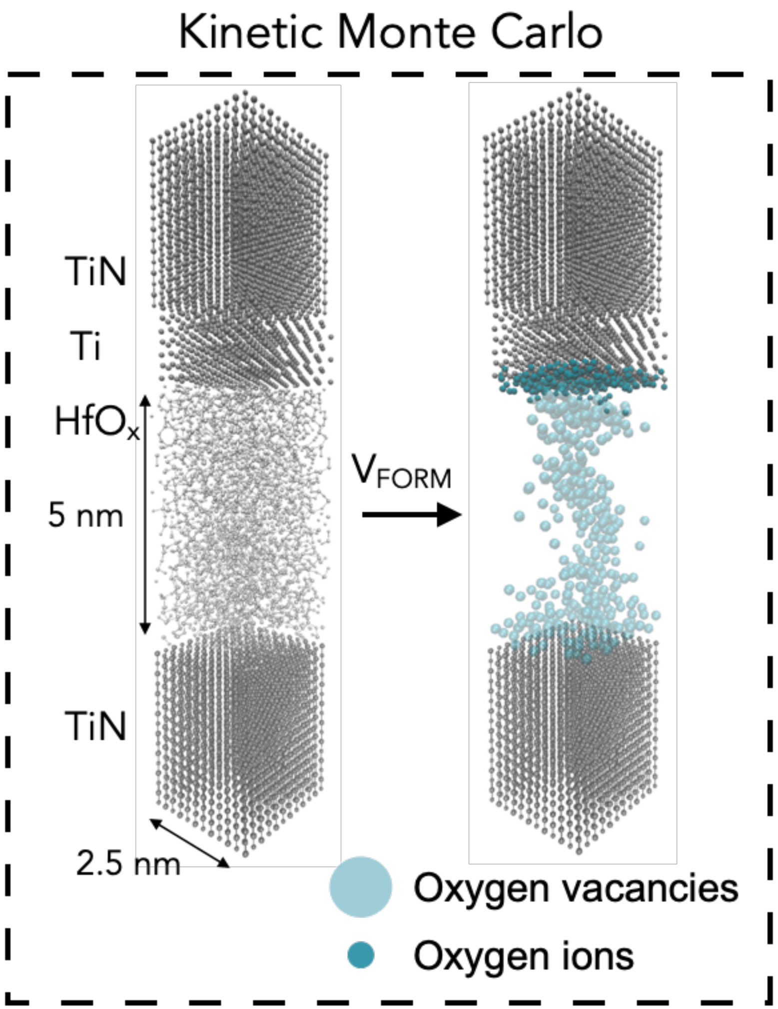
Simulation approach

Kinetic Monte Carlo

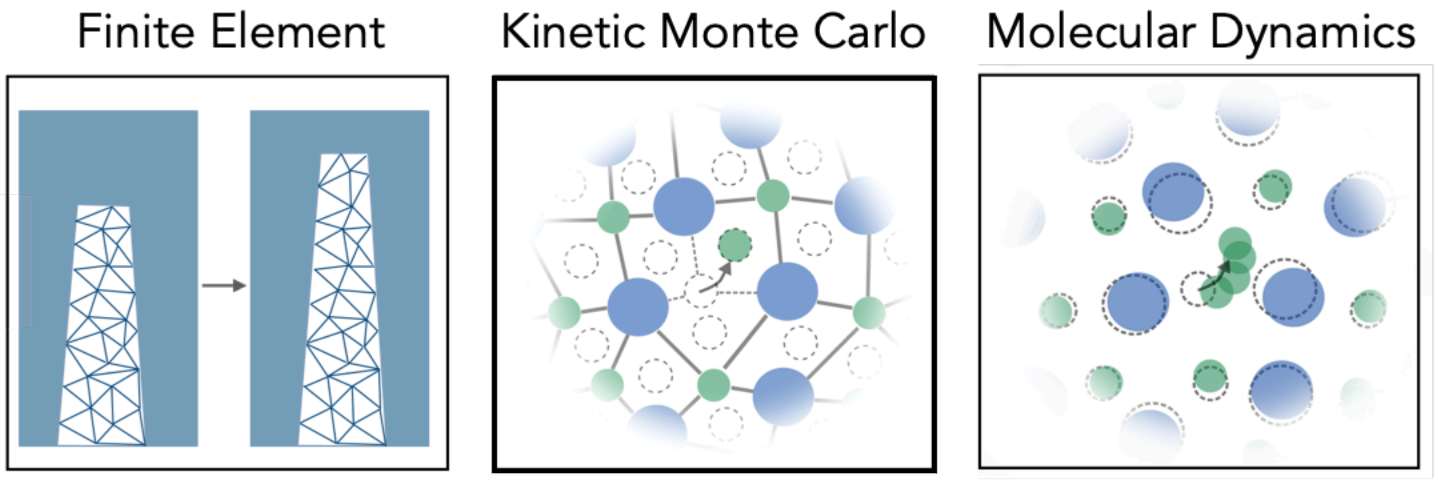


Atomic Structure

Simulation approach

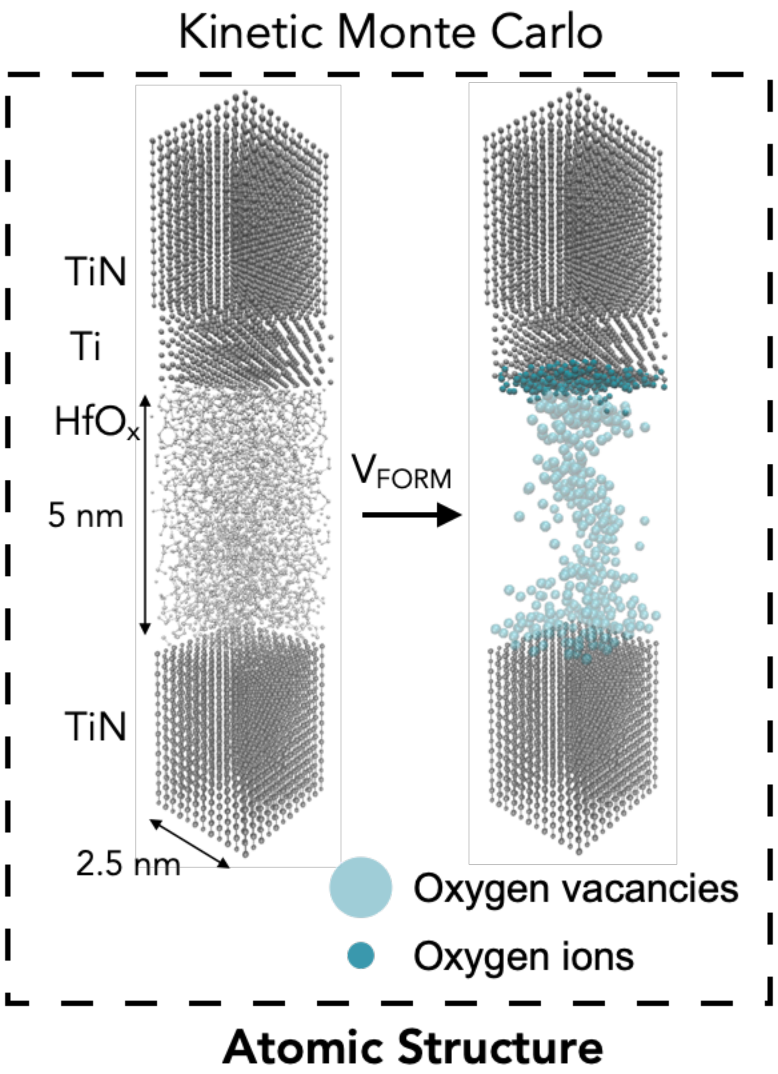


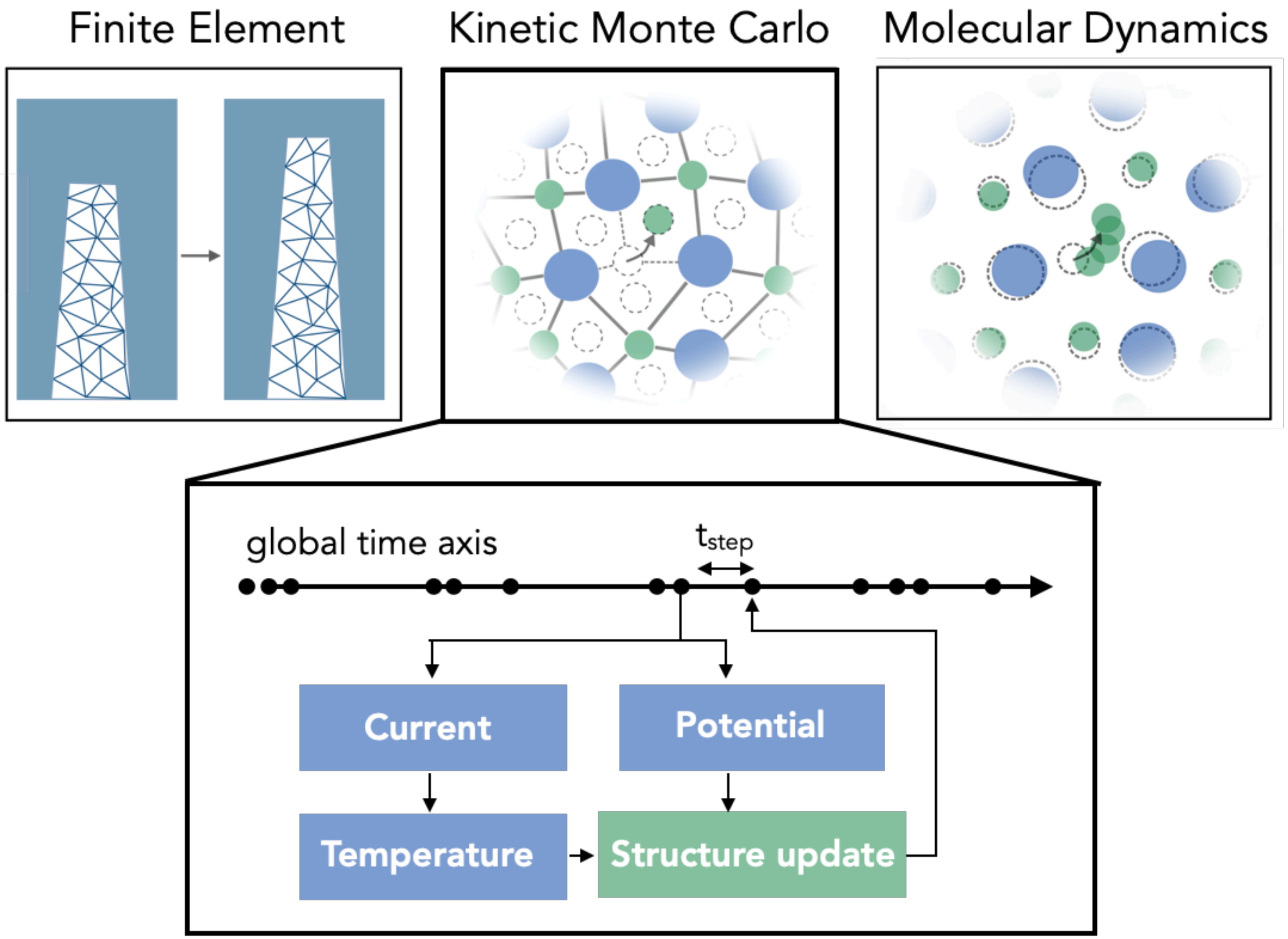
Atomic Structure



Kaniselvan, M*; Maeder, A*; Mladenović, M; Luisier, M; Ziogas, A.N; "Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays". (Accepted paper) *International Conference on High Performance Computing, Networking, Storage and Analysis (SC24)* 2024
Kaniselvan, M.; Luisier, M.; Mladenović, M; "An Atomistic Model of Field-Induced Resistive Switching in Valence Change Memory" *ACS Nano* 2023

Simulation approach

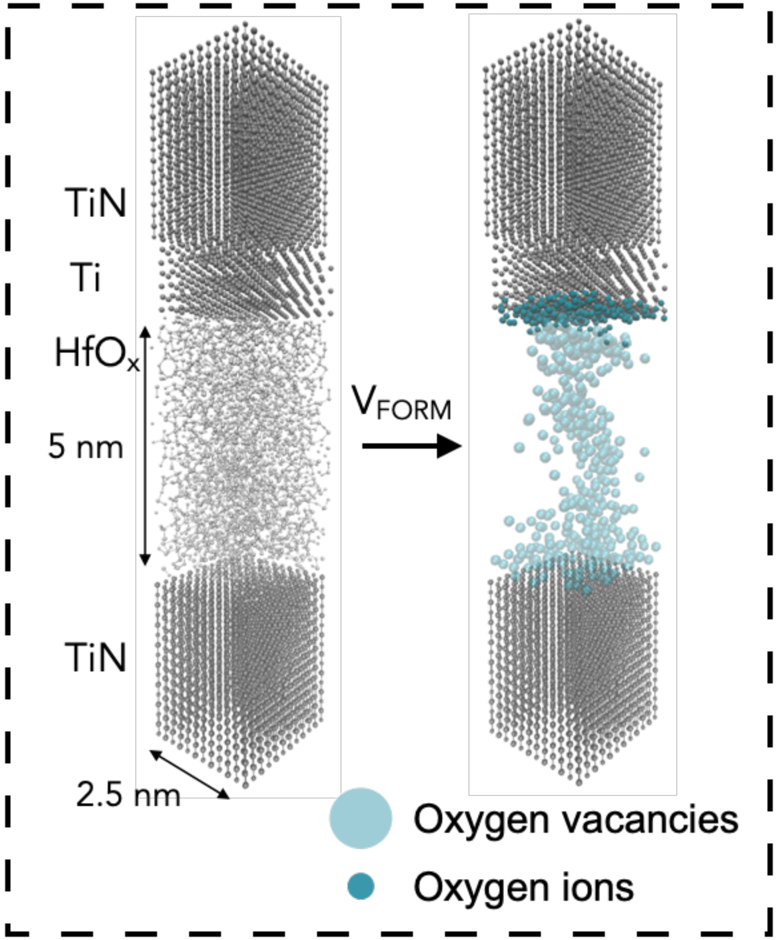




Kaniselvan, M*; Maeder, A*; Mladenović, M; Luisier, M; Ziogas, A.N; "Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays". (Accepted paper) *International Conference on High Performance Computing, Networking, Storage and Analysis (SC24)* 2024
Kaniselvan, M.; Luisier, M.; Mladenović, M; "An Atomistic Model of Field-Induced Resistive Switching in Valence Change Memory" *ACS Nano* 2023

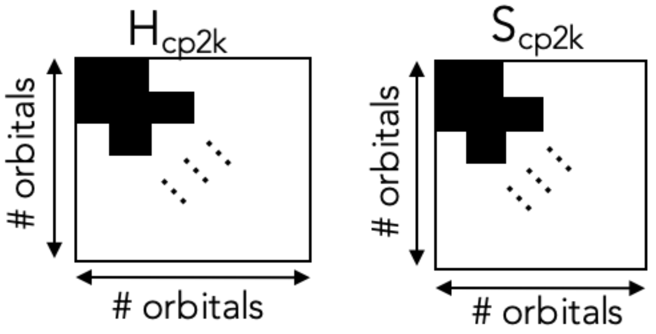
Simulation approach

Kinetic Monte Carlo



Atomic Structure

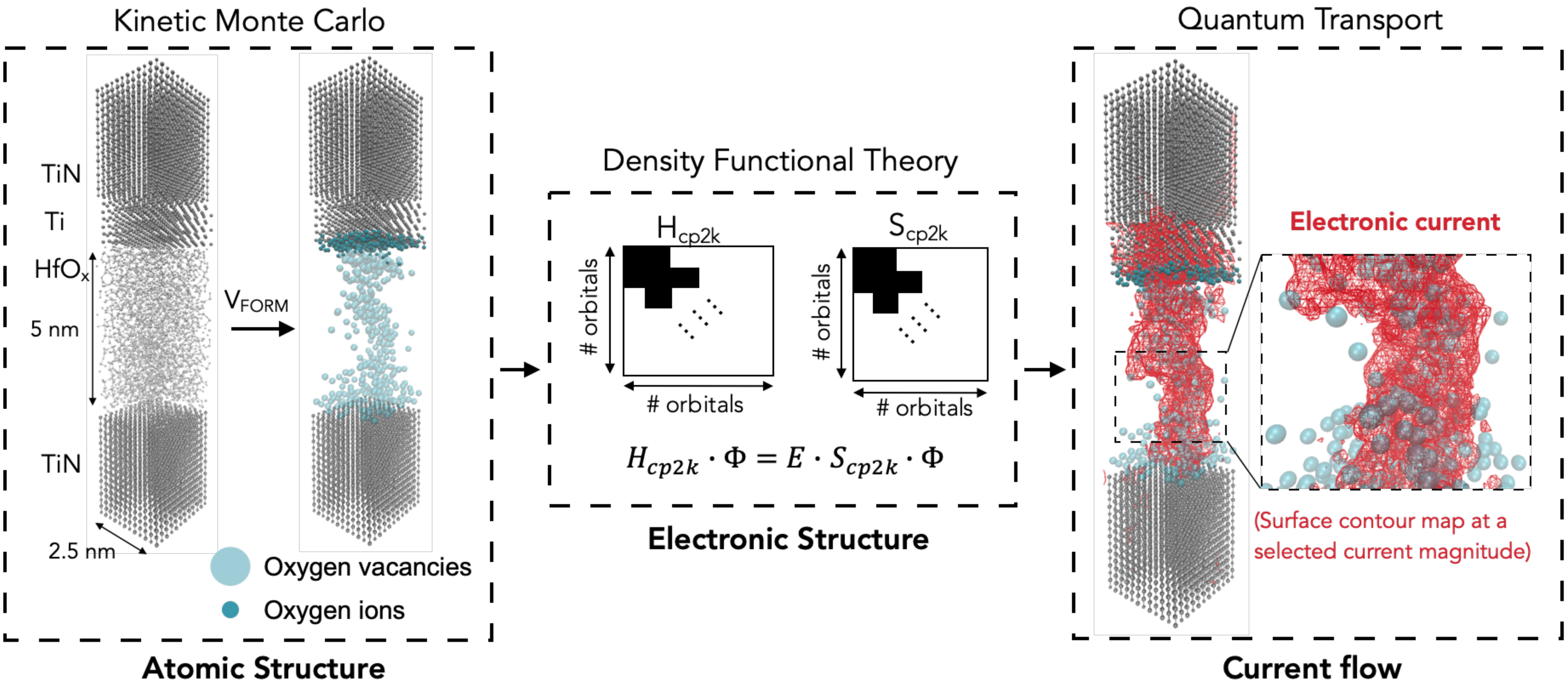
Density Functional Theory



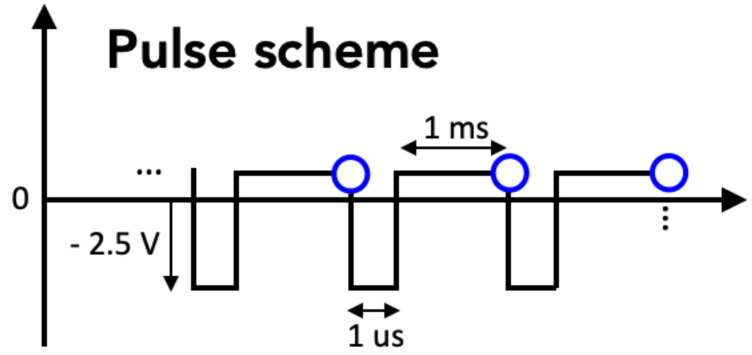
$$H_{cp2k} \cdot \Phi = E \cdot S_{cp2k} \cdot \Phi$$

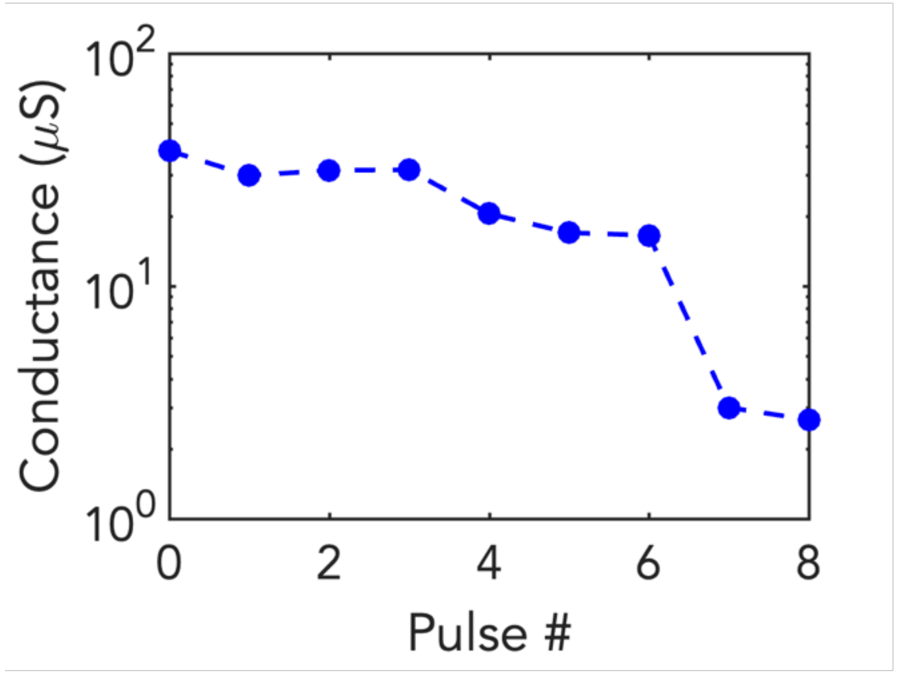
Electronic Structure

Simulation approach

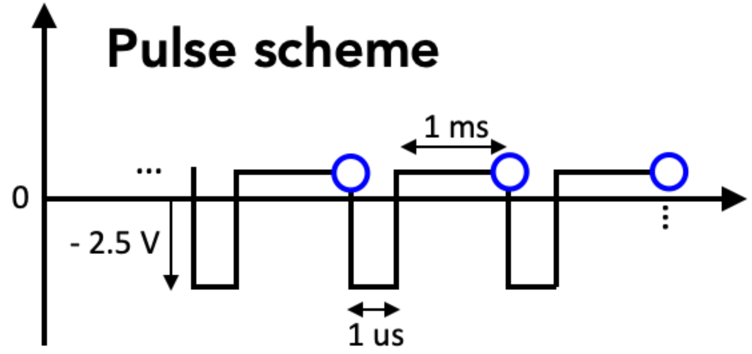


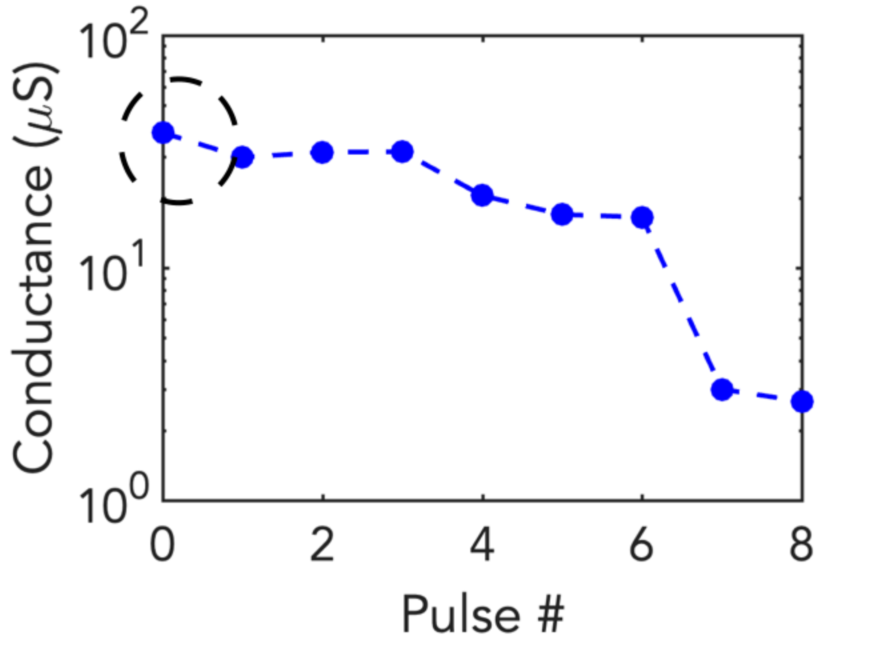
Gradual Conductance Decreases

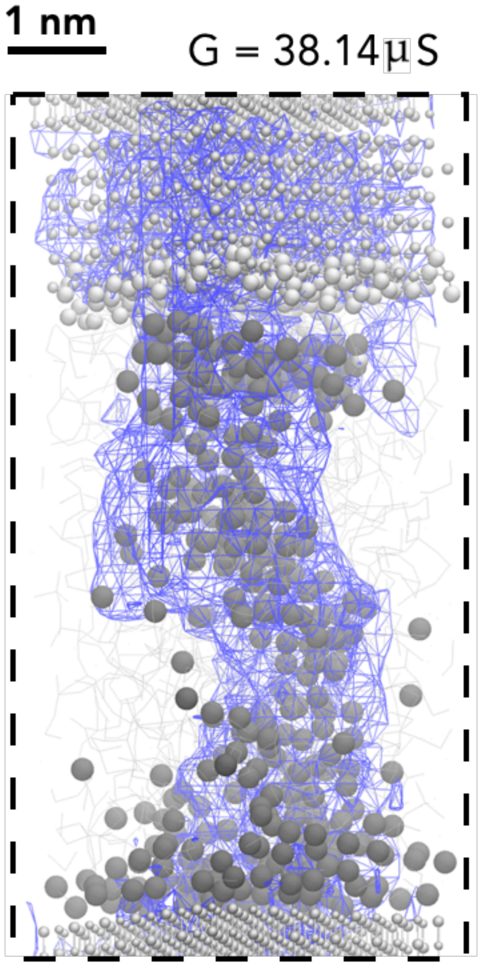




Gradual Conductance Decreases

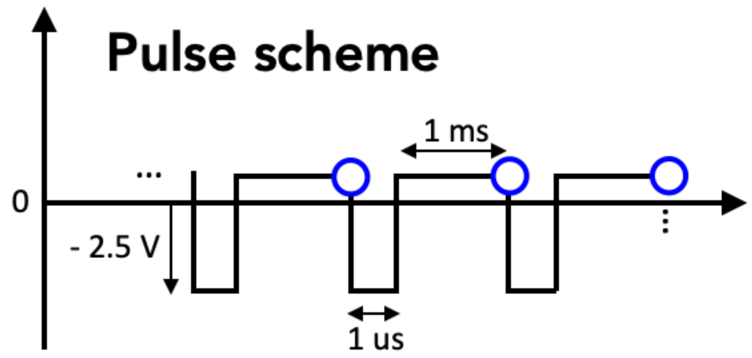


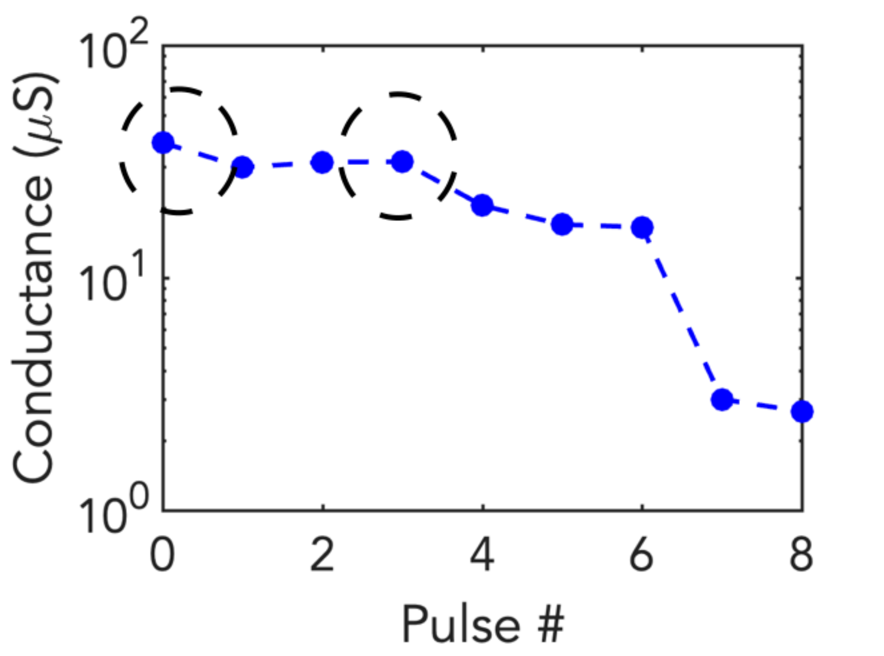


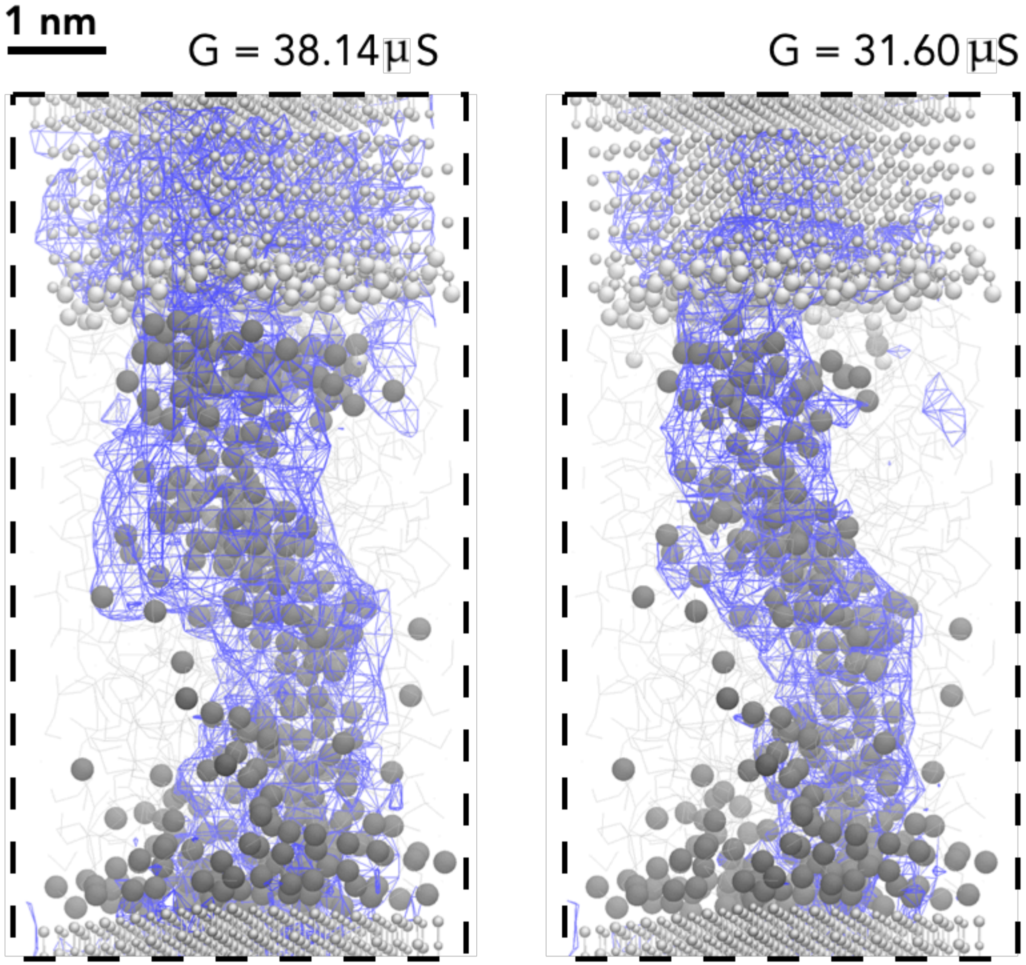


ETH zürich

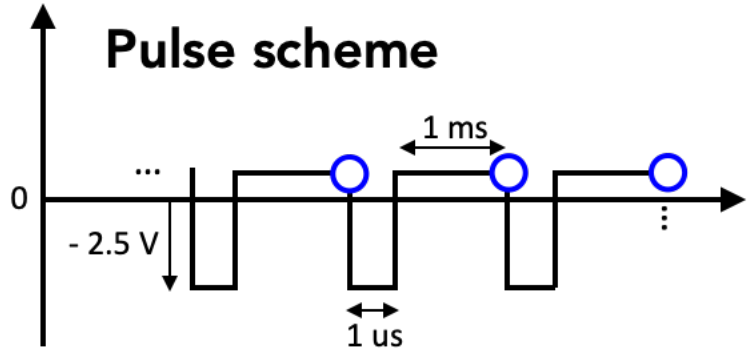
Gradual Conductance Decreases

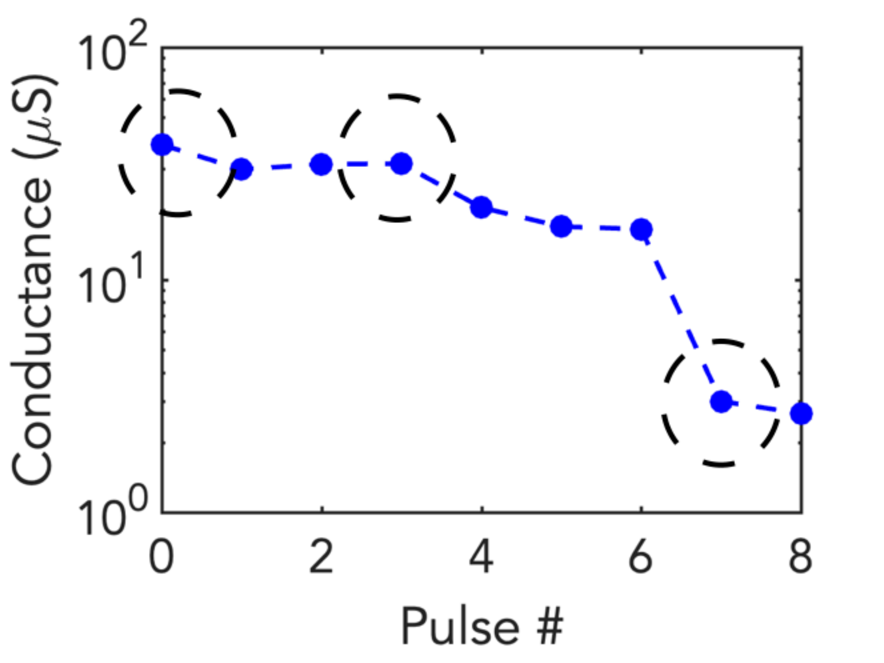


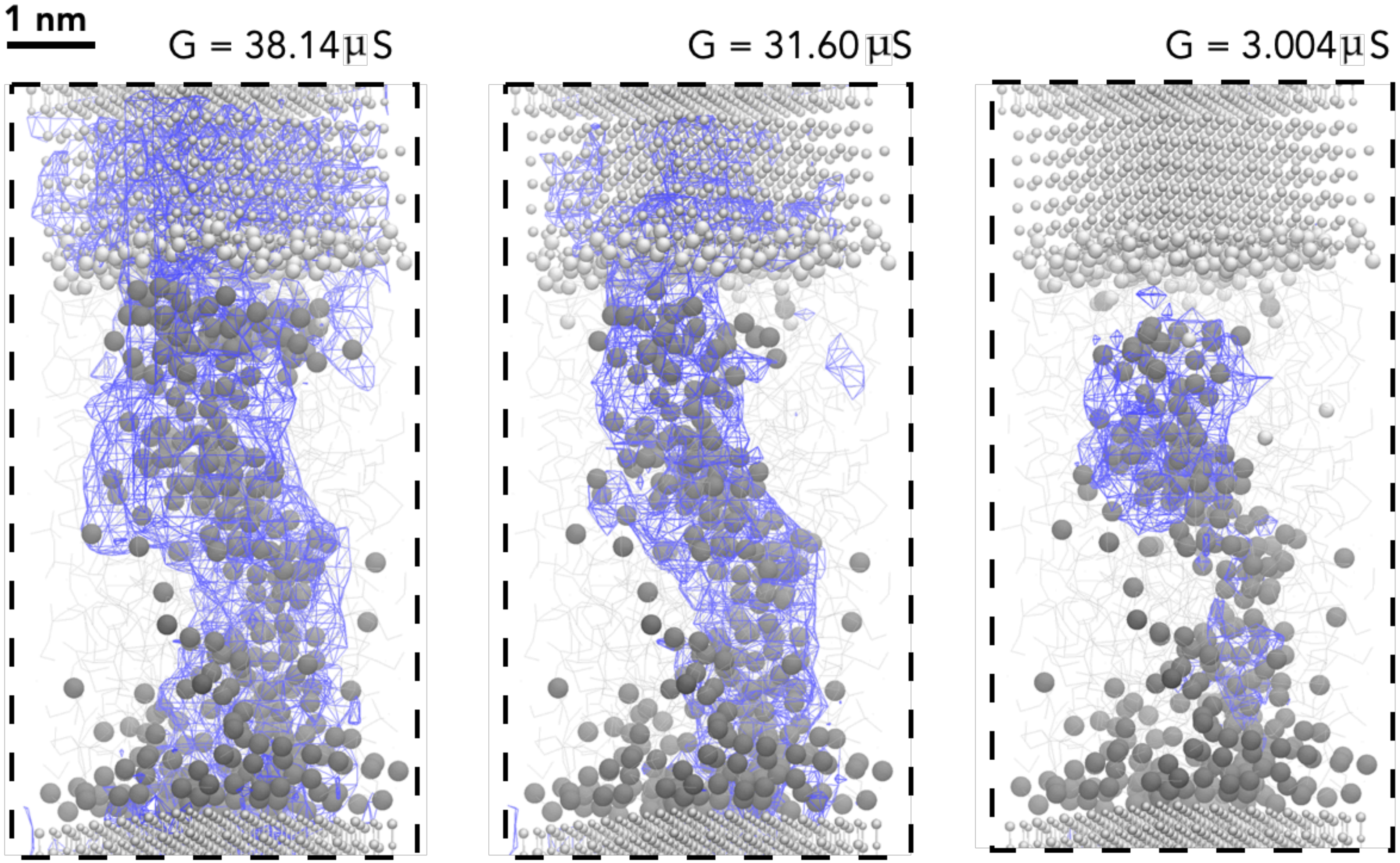




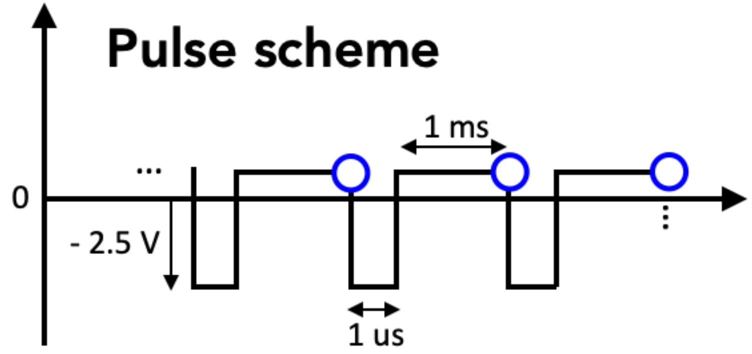
Gradual Conductance Decreases

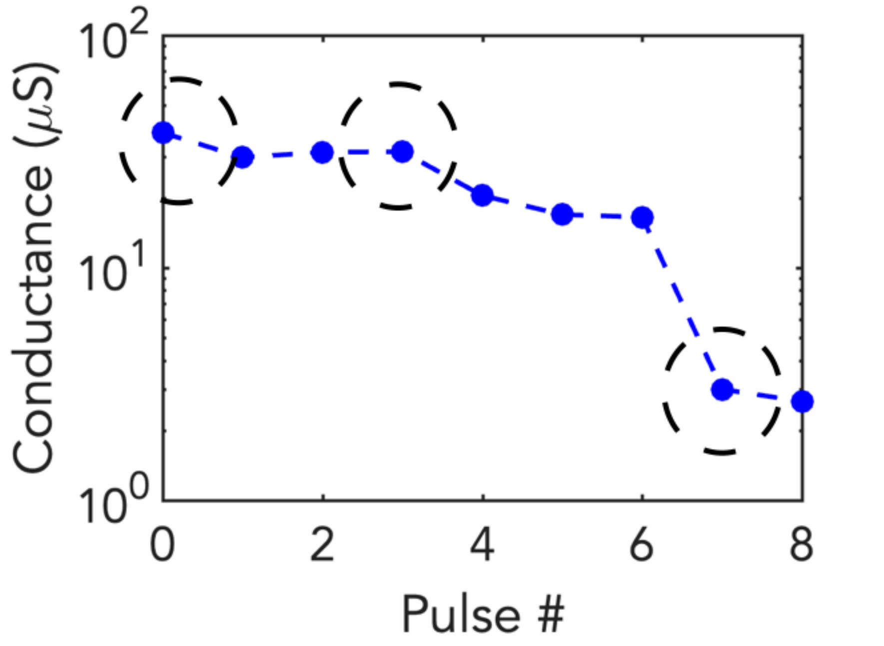


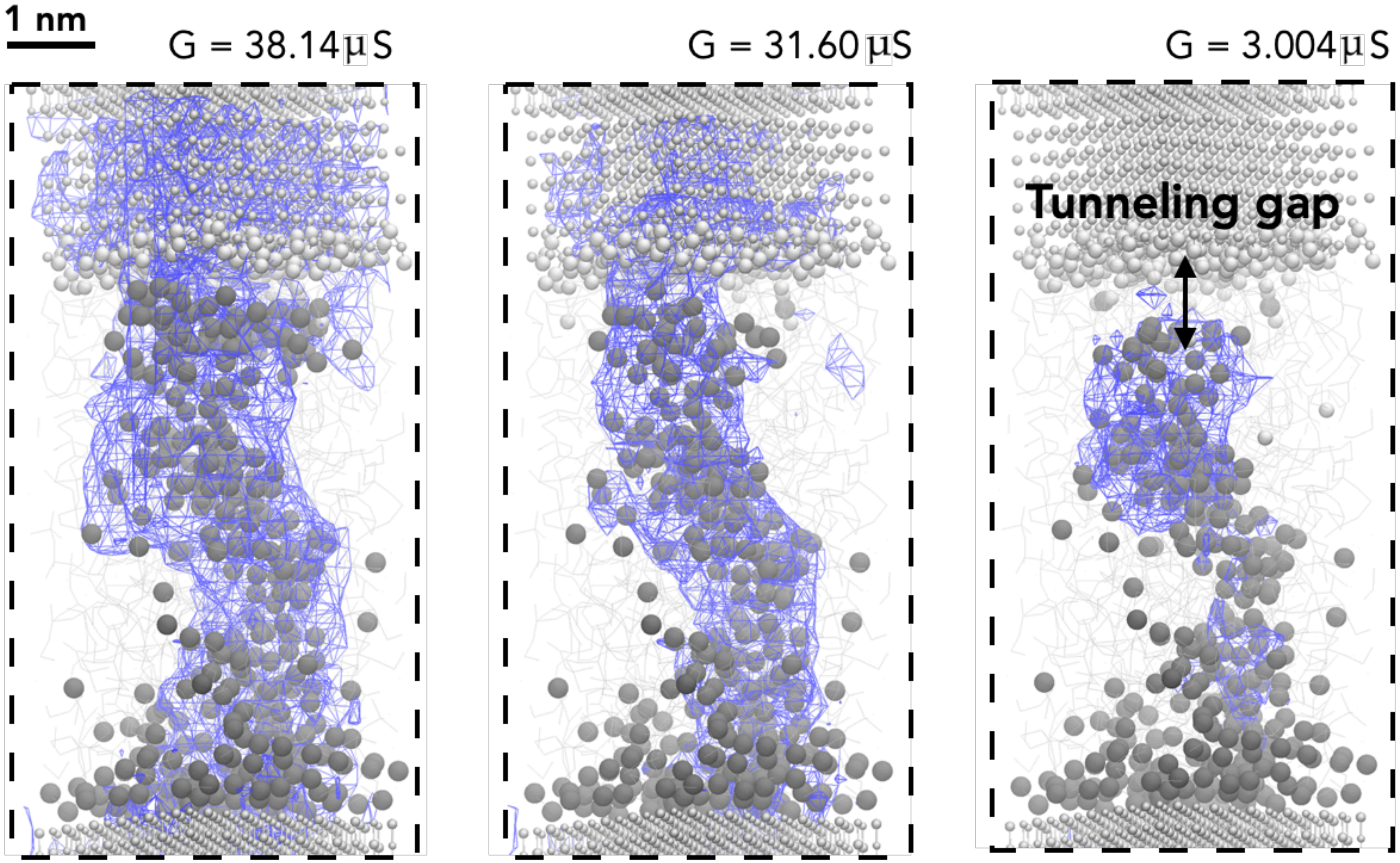




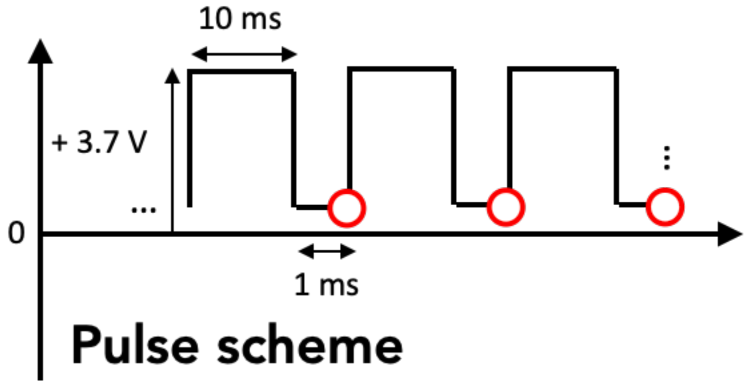
Gradual Conductance Decreases

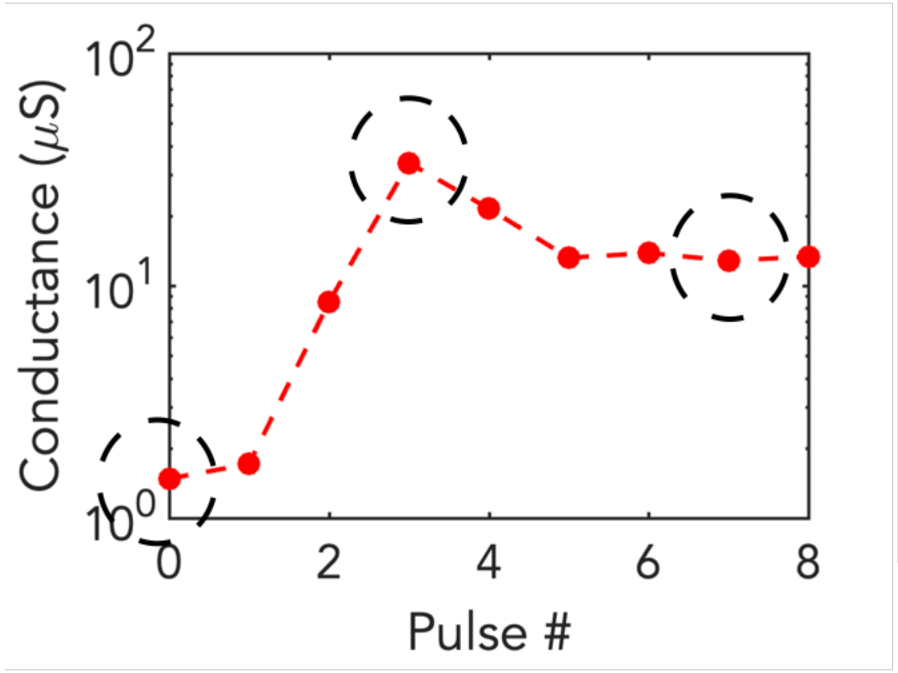


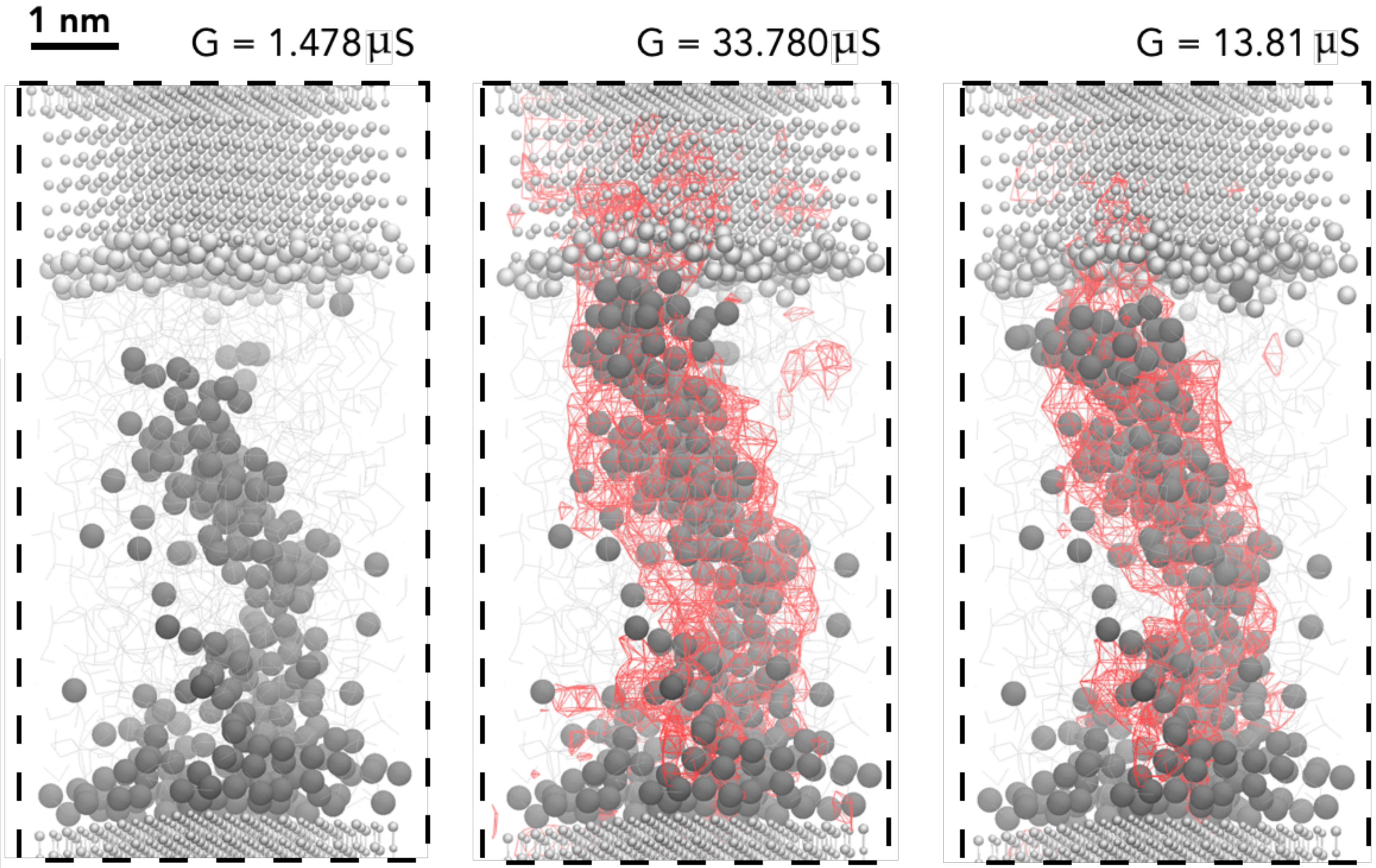




Gradual Conductance Increases



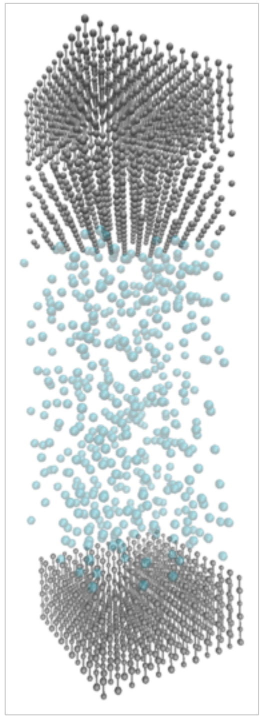




ETH zürich

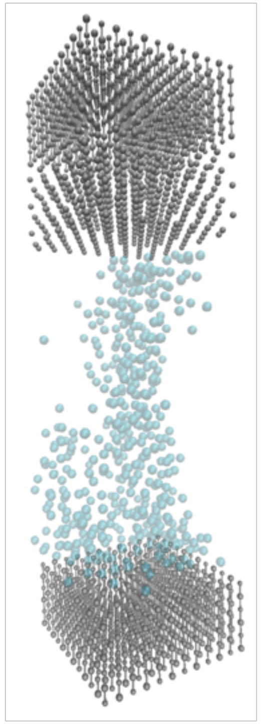
Current flow through HfOx

Non-Filamentary



HfO_x : x = 1.512

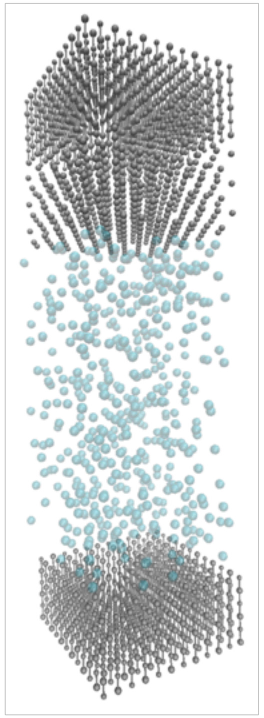
Filamentary

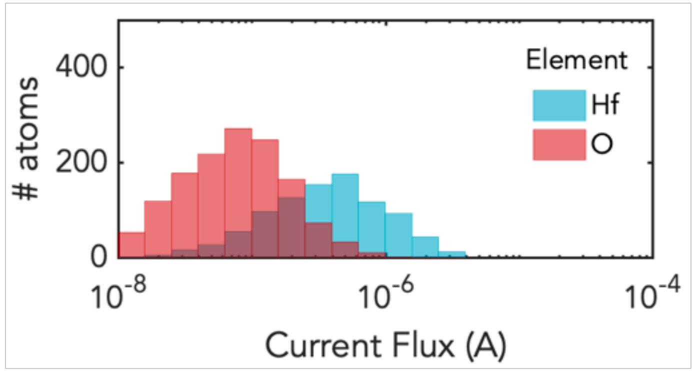


HfO_x : x = 1.512

Current flow through HfOx

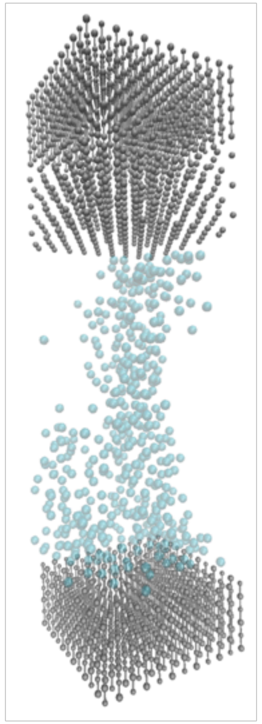
Non-Filamentary

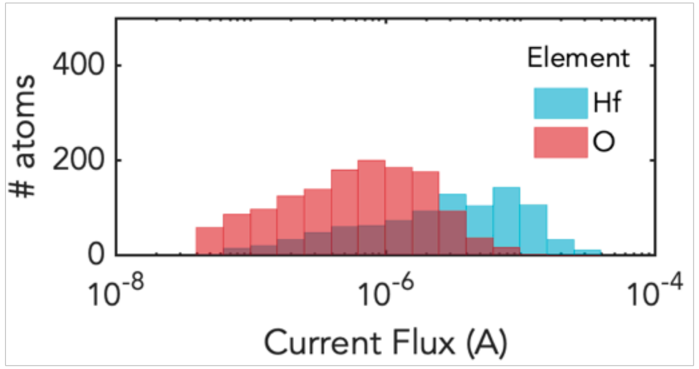




HfO_x : x = 1.512

Filamentary

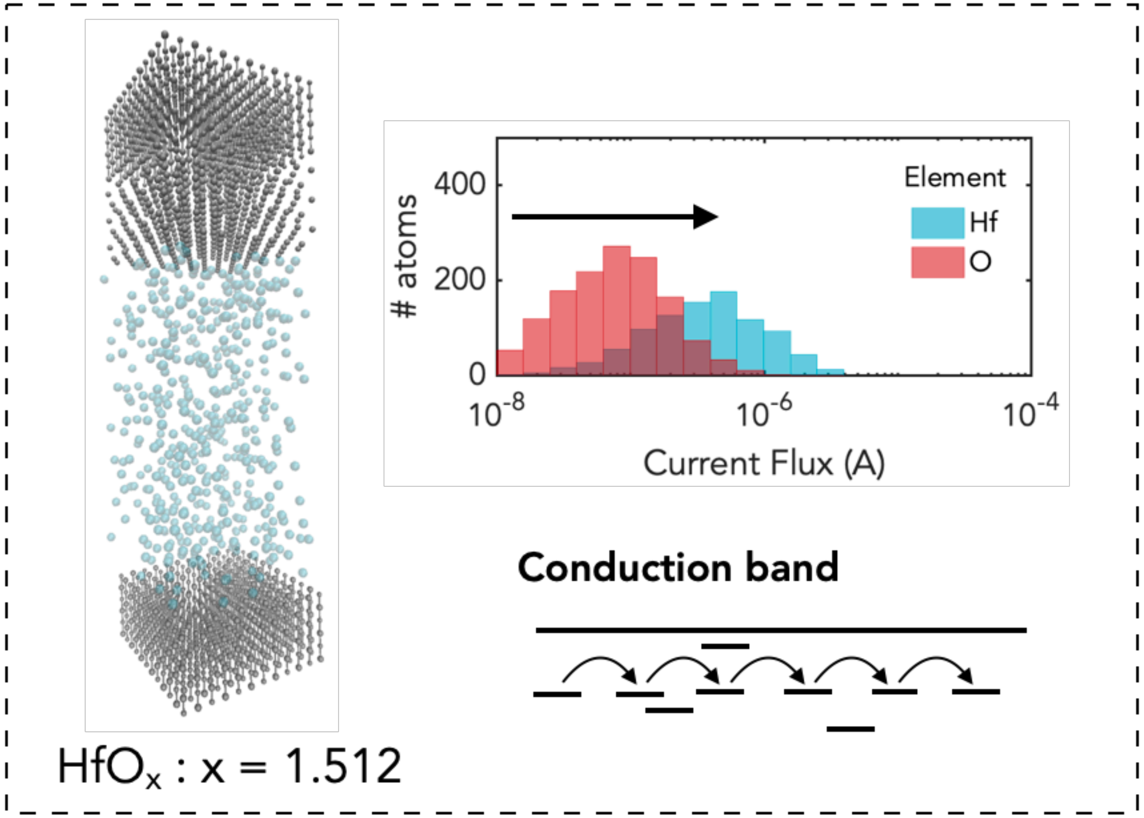




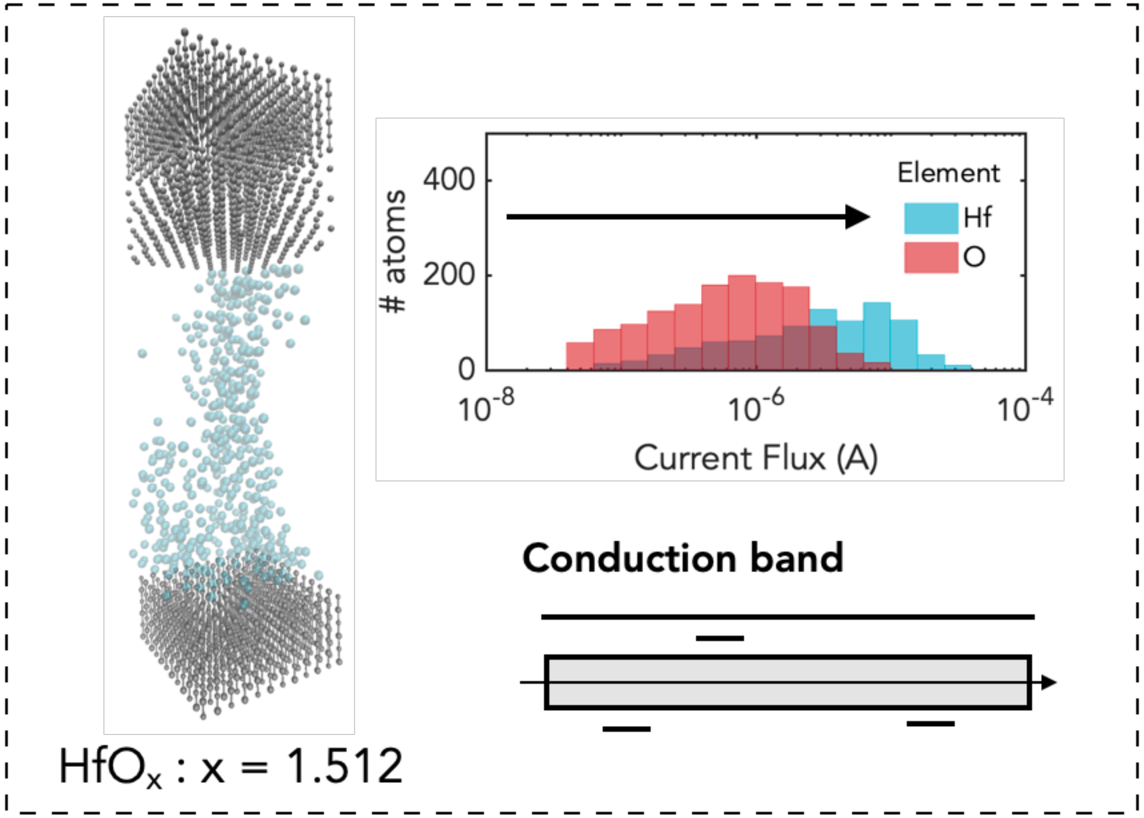
HfO_x : x = 1.512

Current flow through HfOx

Non-Filamentary



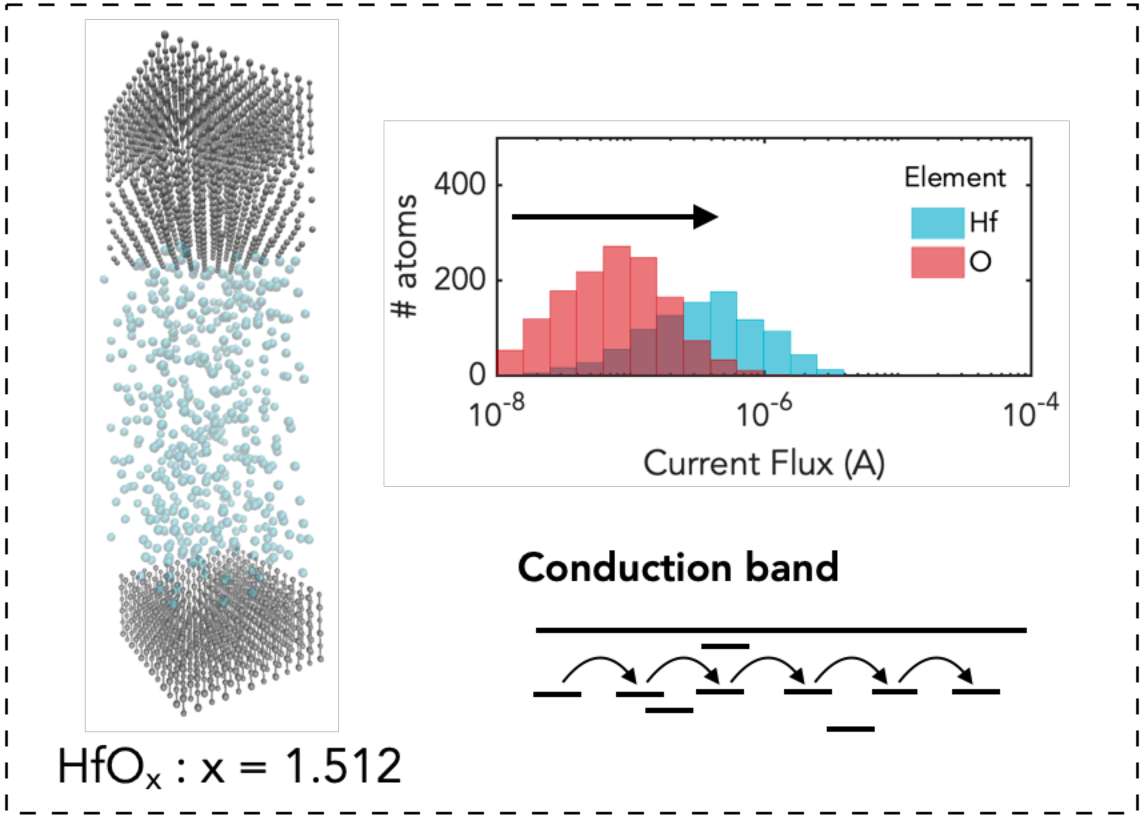
Filamentary



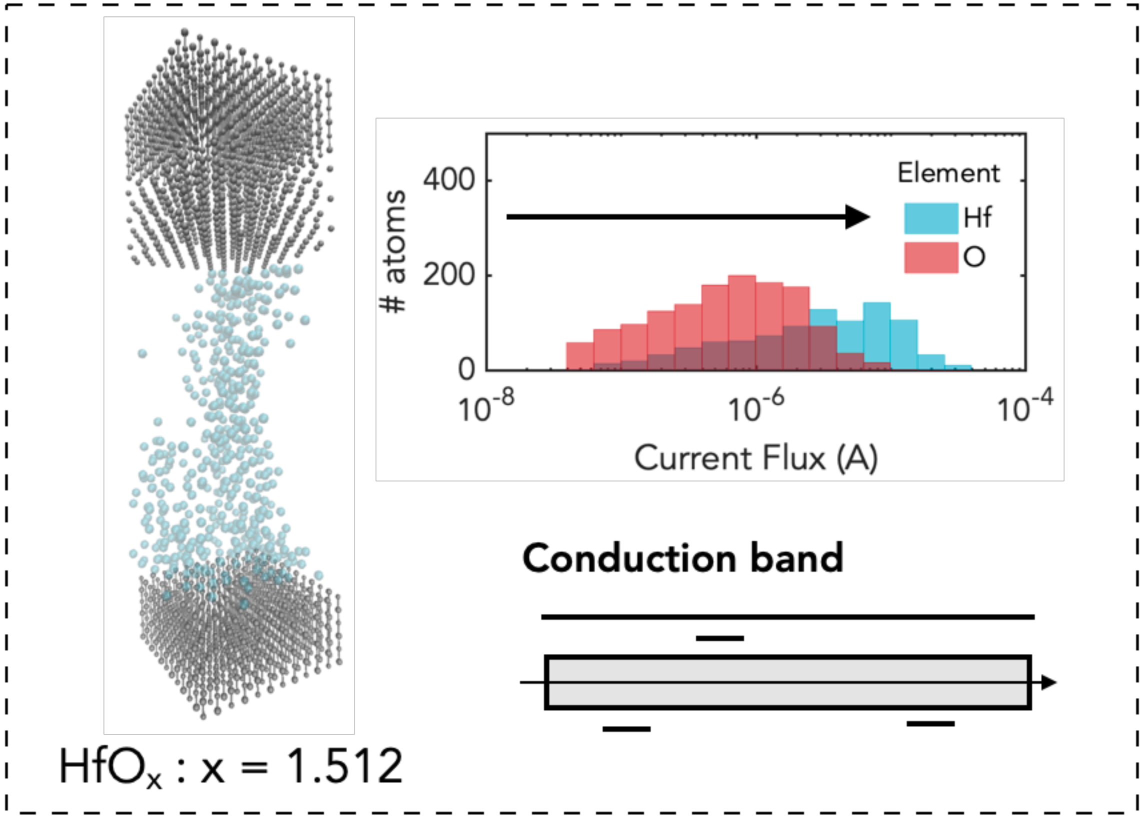
- The magnitude of current is increased in the presence of filamentary vacancy clusters

Current flow through HfOx

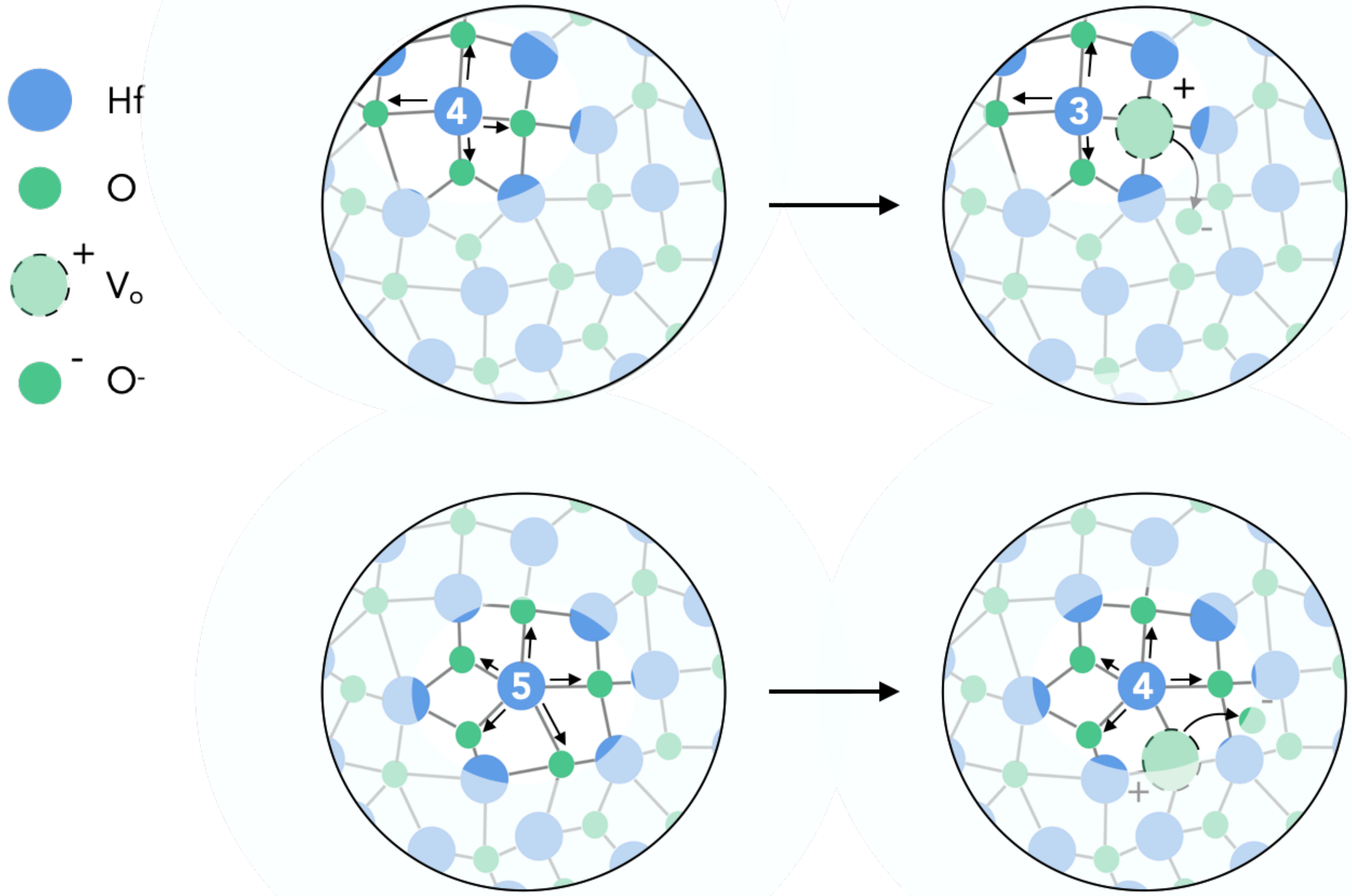
Non-Filamentary



Filamentary



- The magnitude of current is increased in the presence of filamentary vacancy clusters
- Current flows through Hf atoms

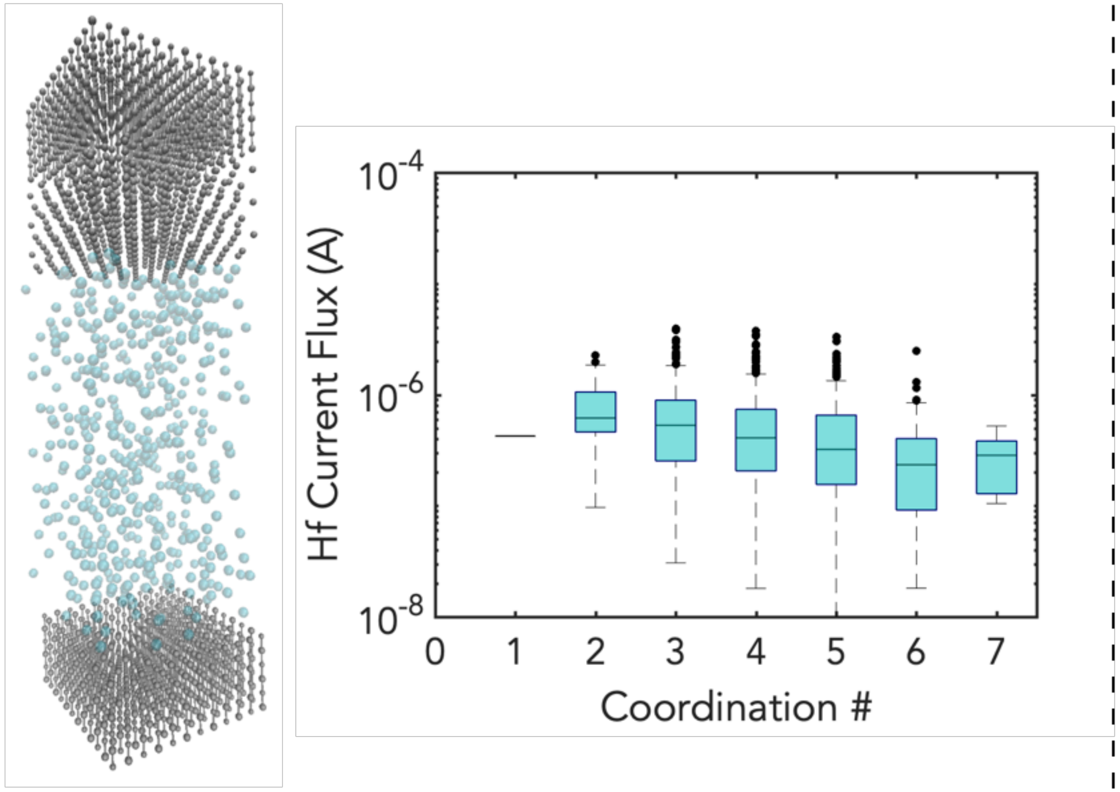


Oxygen coordination is affected by…

- Underlying atomic connectivity
- Presence of Oxygen vacancy defects

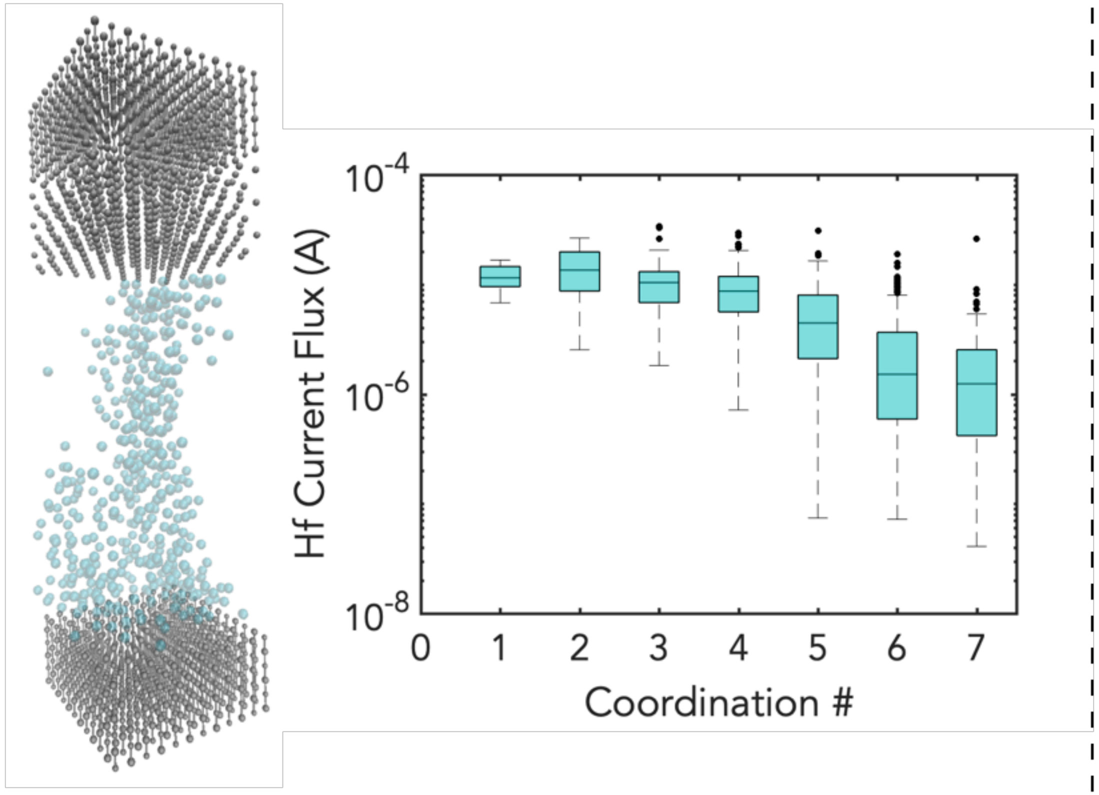
Current flow through the defective oxide

Non-Filamentary



HfO_x : x = 1.512

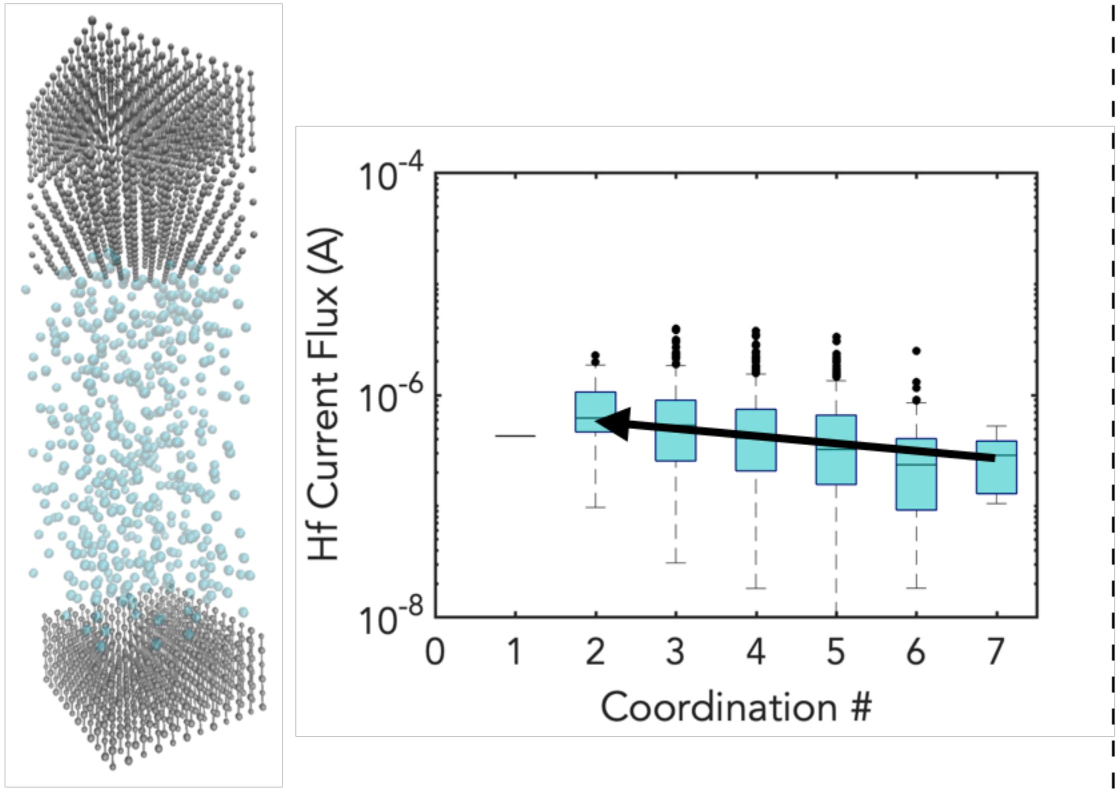
Filamentary



HfO_x : x = 1.512

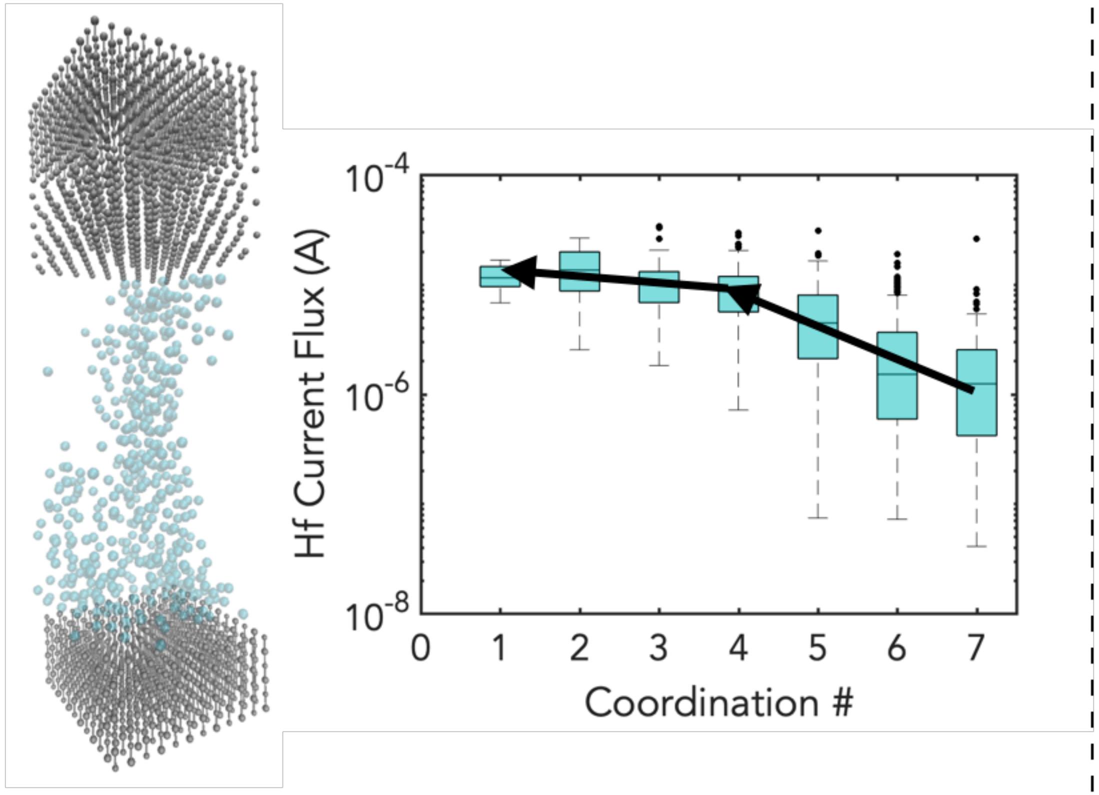
Current flow through the defective oxide

Non-Filamentary



HfO_x : x = 1.512

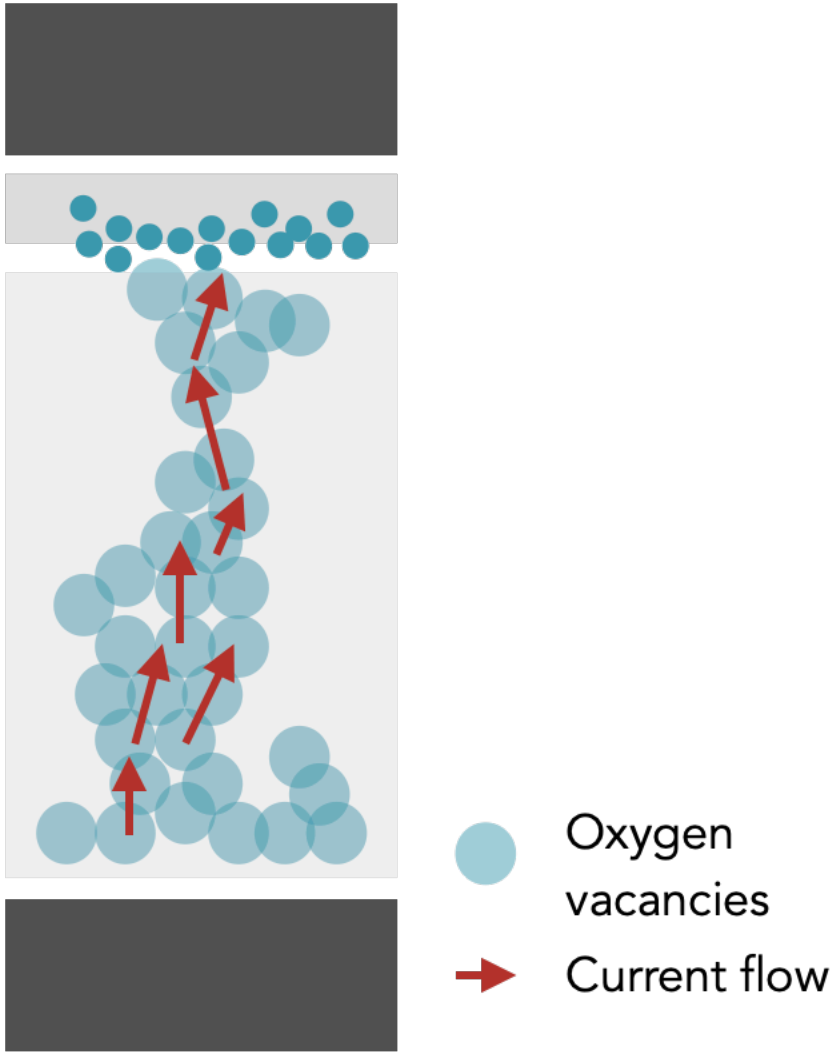
Filamentary



HfO_x : x = 1.512

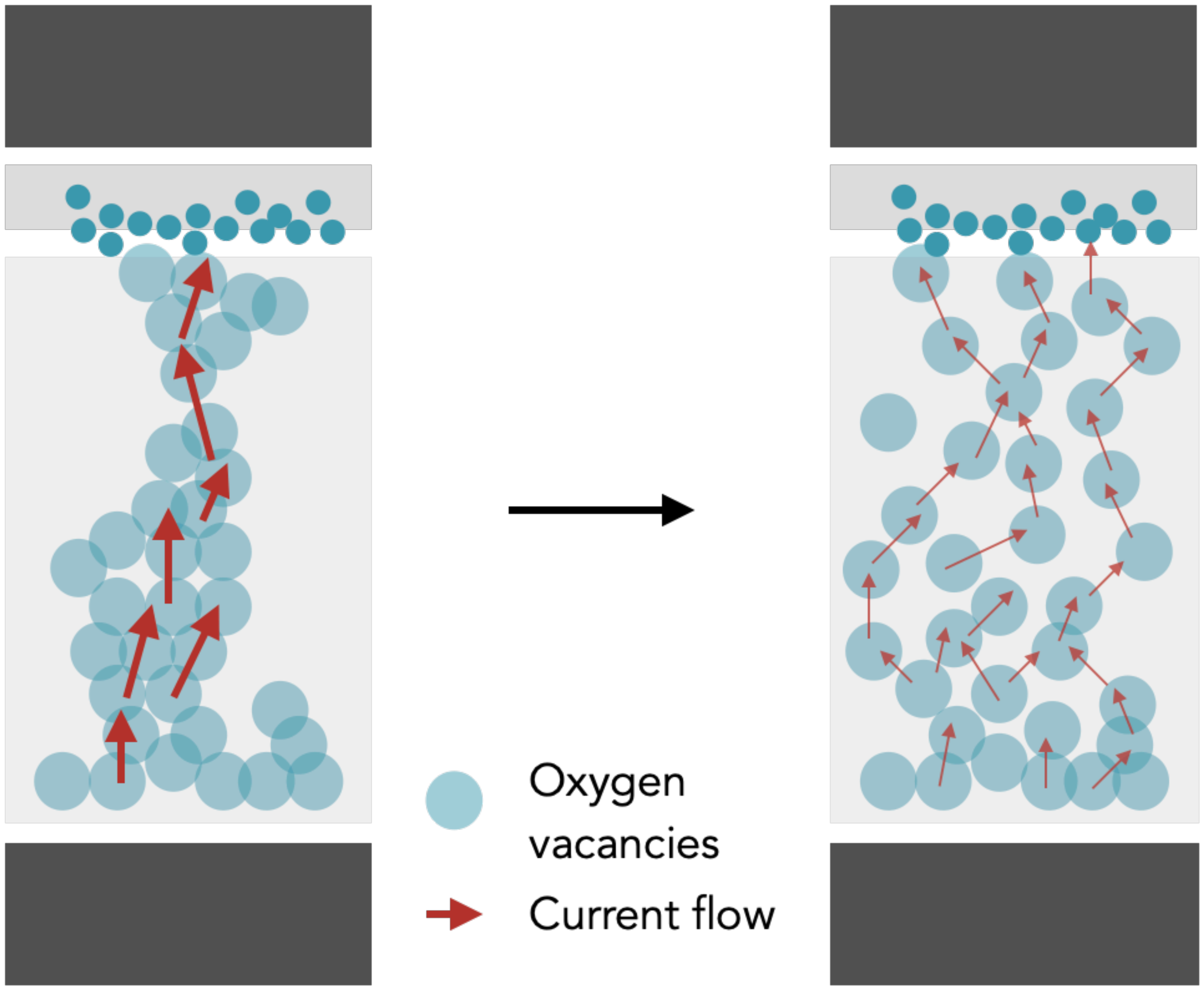
Summary

Some atoms direct **more** of the electronic current



Summary

Some atoms direct **more** of the electronic current



Individual atoms direct **less** of the electronic current

Outlook: Methods to improve analog operation

Chemical/compositional

- Adding dopants/nucleation sites
- Engineered bilayers with interface-type switching

Thermal

- Thermal Enhancement Layers
- Optical pulses
- Operating at higher temperatures

Outlook: Methods to improve analog operation

Chemical/compositional

- Adding dopants/nucleation sites
- Engineered bilayers with interface-type switching

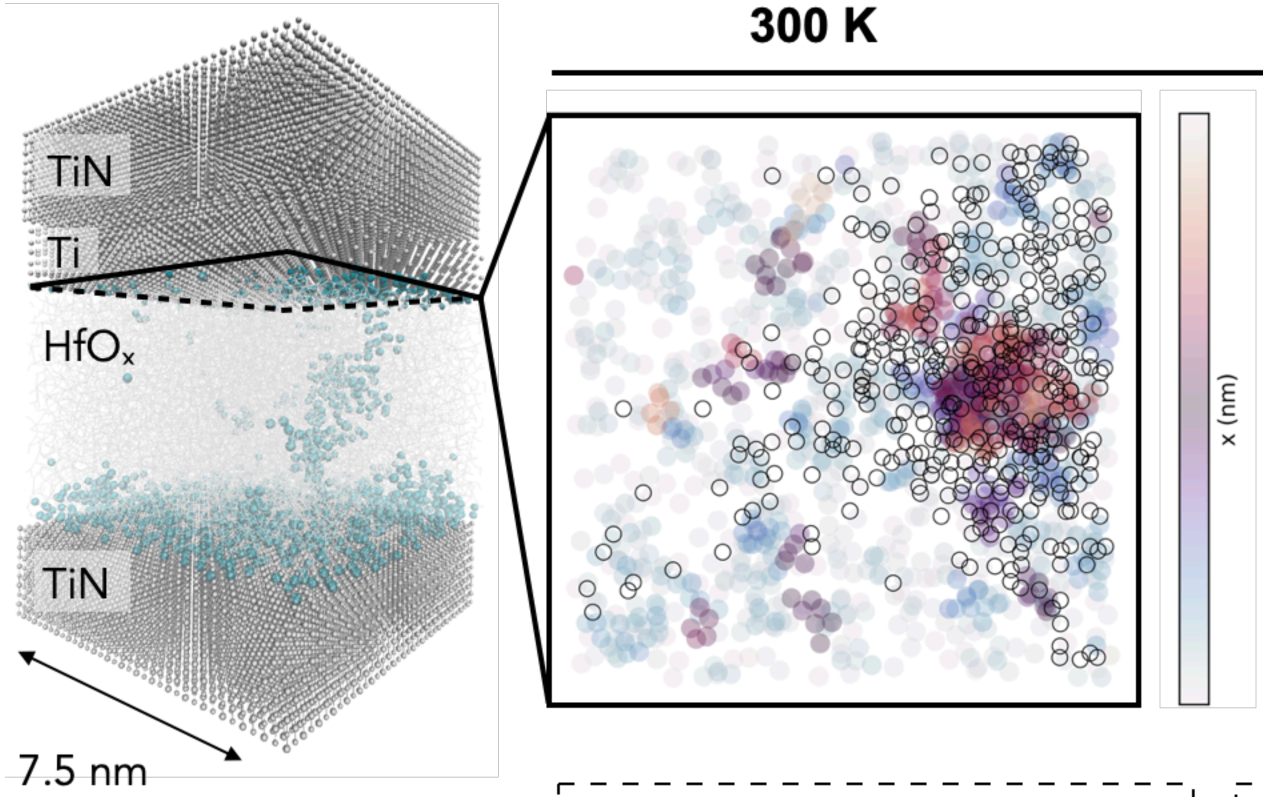
Thermal

- **Thermal Enhancement Layers**
- **Optical pulses**
- **Operating at higher temperatures**

Outlook: Thermal engineering

Increasing electroforming temperature at fixed V_{FORM} = 6.0 V

300 K **350 K** **400 K**

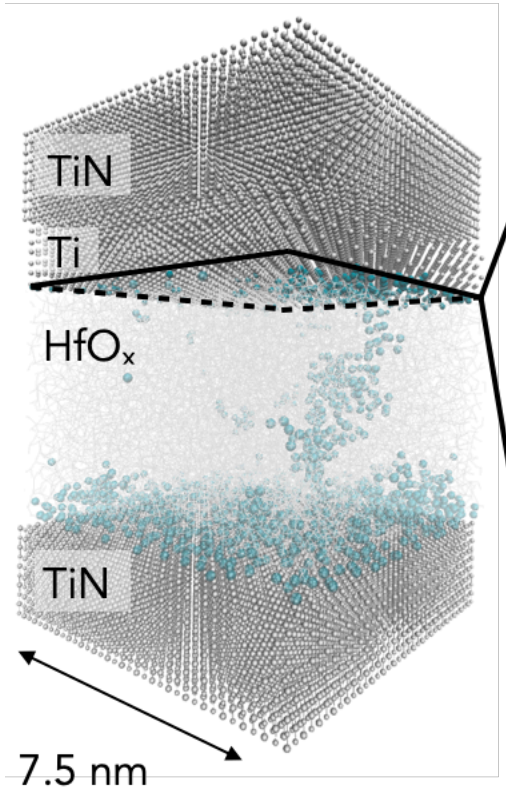


Oxygen ion in Ti reservoir

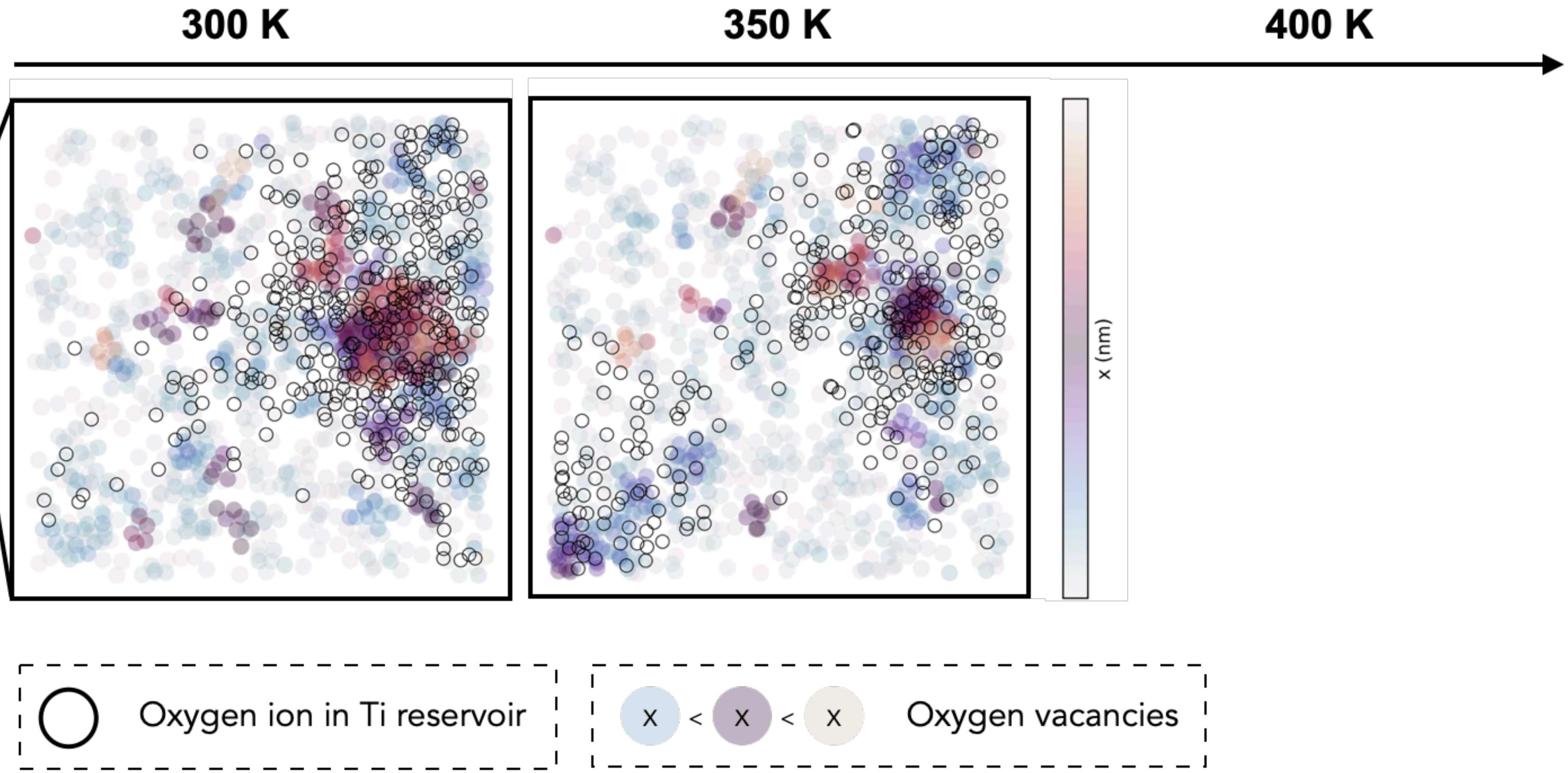
x < x < x Oxygen vacancies

ETH zürich

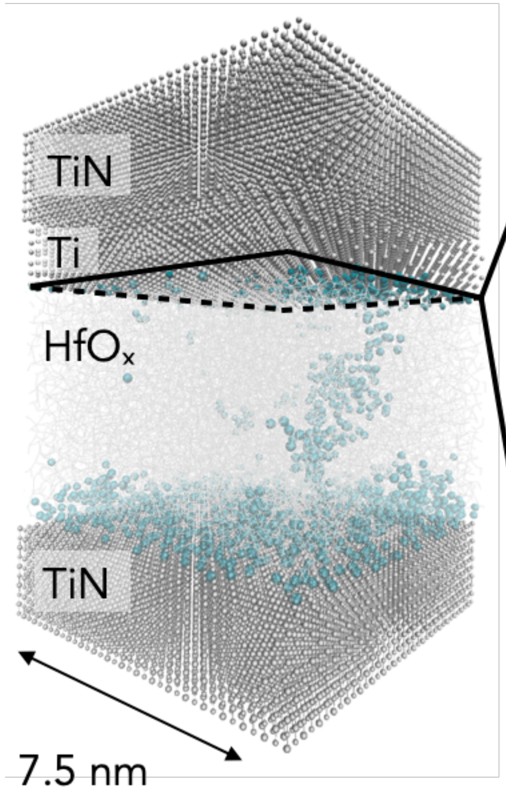
Outlook: Thermal engineering



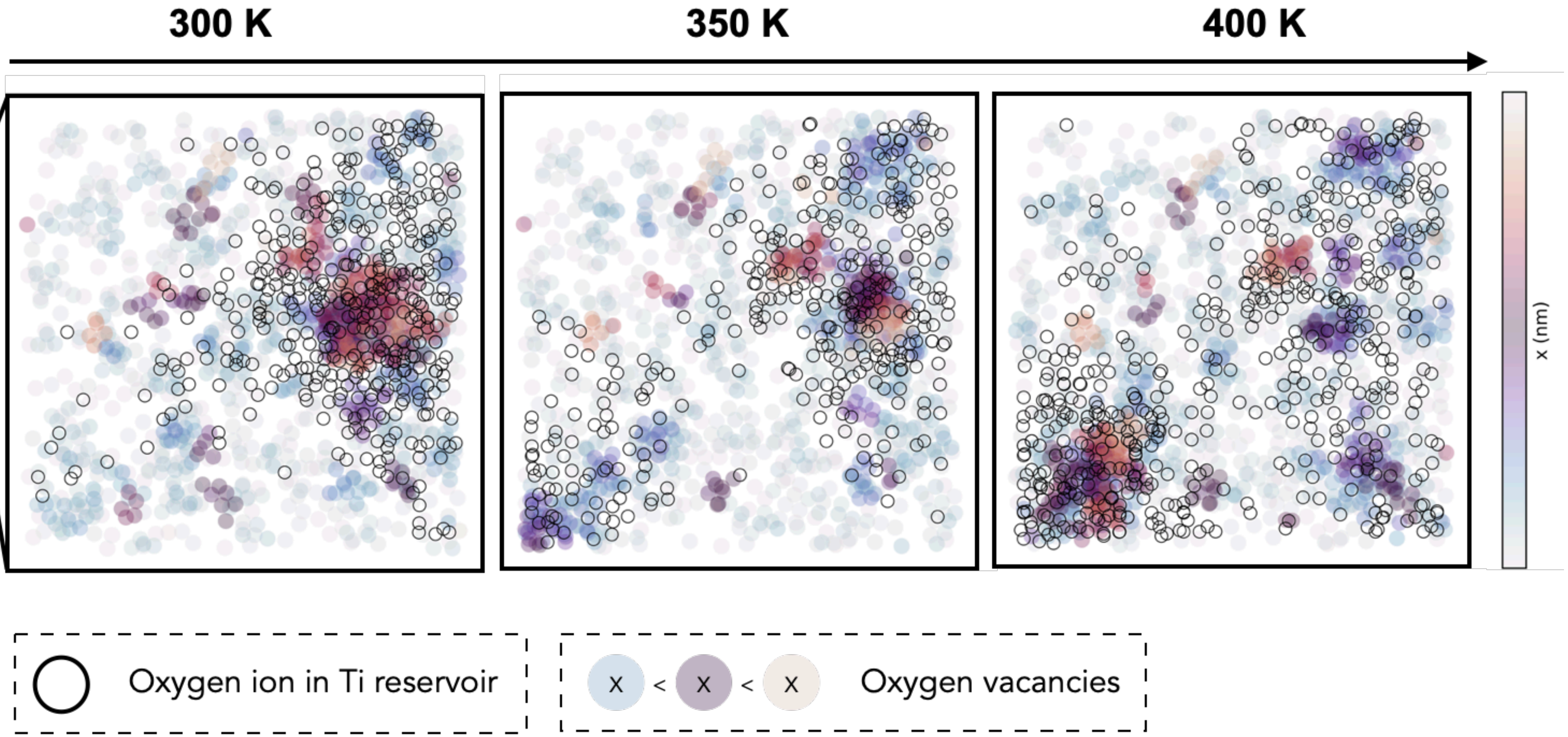
Increasing electroforming temperature at fixed V_{FORM} = 6.0 V



Outlook: Thermal engineering



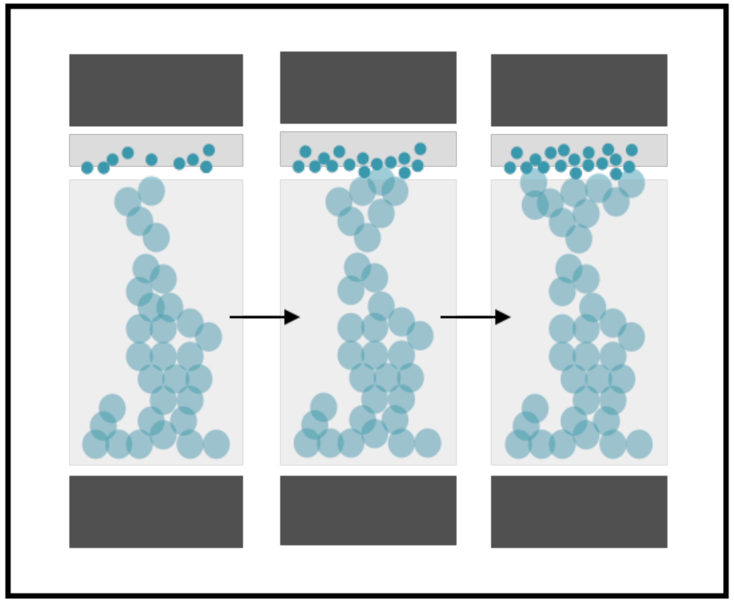
Increasing electroforming temperature at fixed V_{FORM} = 6.0 V



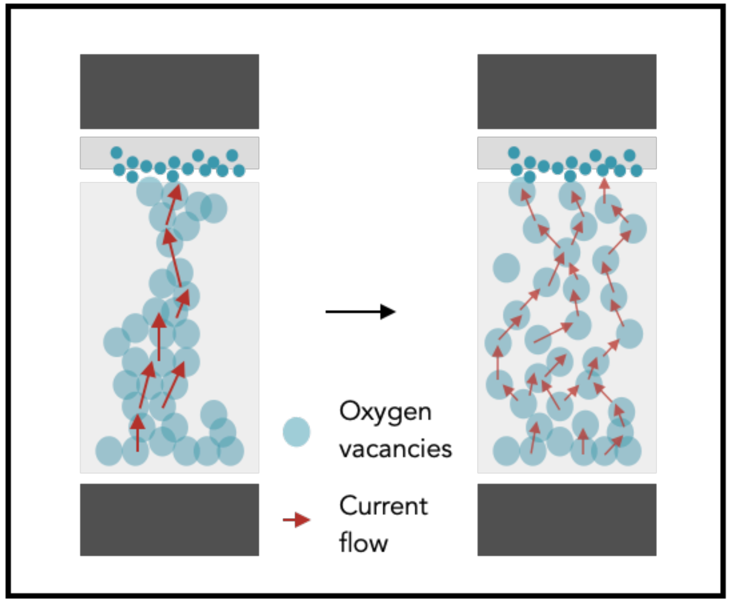
ETH zürich

Summary and Acknowledgements

Origin of non-linear conductance updates

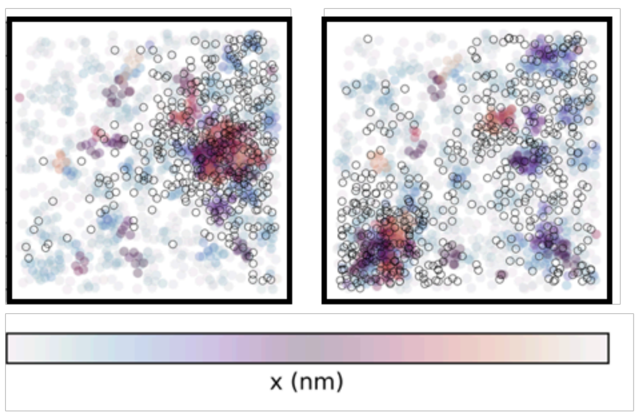


Coordination-dependance of current flow



Methods to achieve more uniformly defective oxides

Environment temperature during electroforming step



Discussions, moral support:

Marko Mladenović
Jente Clarysse
Kevin Portner
Mathieu Luisier

Computational Resources

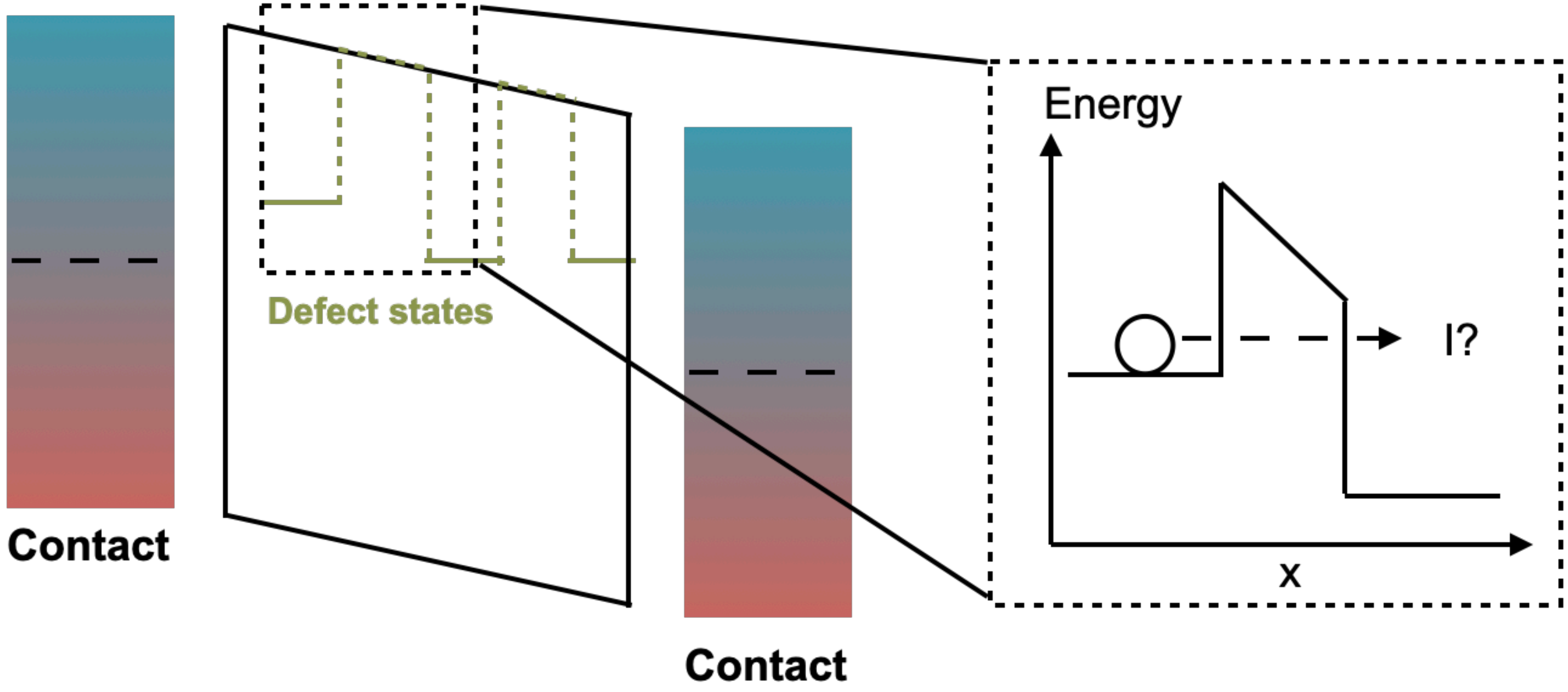
CSCS

Funding

Swiss National Science Foundation

NSERC CRSNG

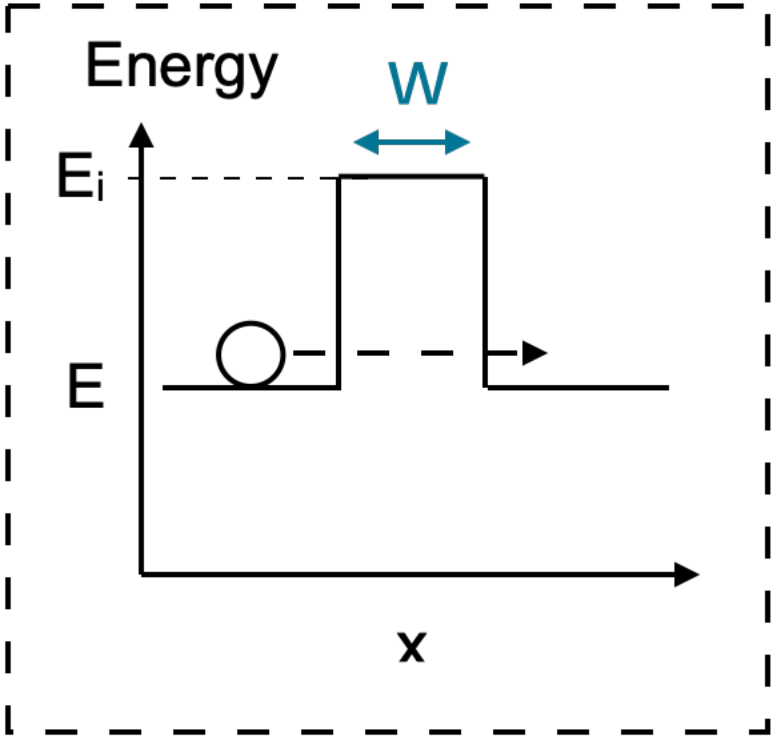
Mechanisms of Current Flow: Tunneling

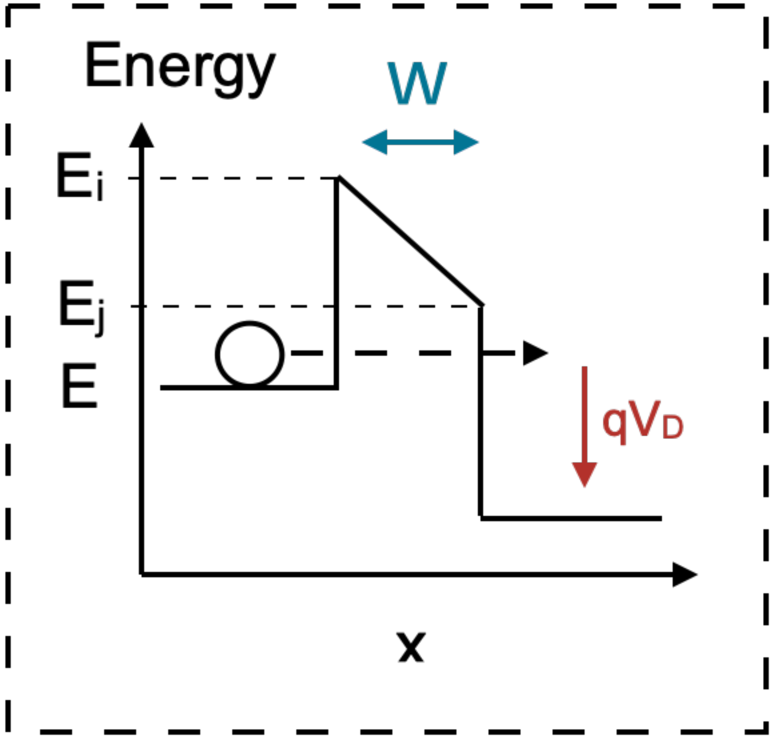


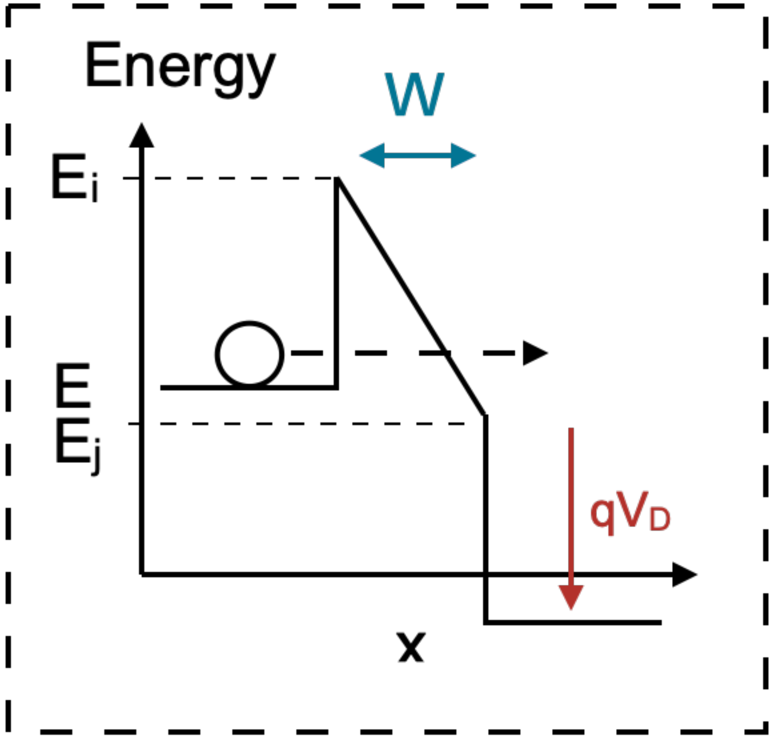
$$E = \frac{\hbar^2 k^2}{2m}$$

$$T(E) = exp(-\int Im(k(E)dx)) \longrightarrow T(E) = exp(-\frac{2m_e}{\hbar}\int \sqrt{E}dx)$$

Mechanisms of Current Flow: Tunneling







$$T(E) = exp(-\frac{\sqrt{2m_e}}{\hbar} \cdot \sqrt{E_i} \cdot W)$$

$$T(E) = exp(-\frac{\sqrt{2m_e}}{\hbar} \cdot \frac{2W}{3(E_i - E_j)} \cdot (E_i^{3/2} - E_j^{3/2}))$$

$$T(E) = exp(-\frac{\sqrt{2m_e}}{\hbar} \cdot \frac{2W}{3(E_i - E_j)} \cdot E_i^{3/2})$$