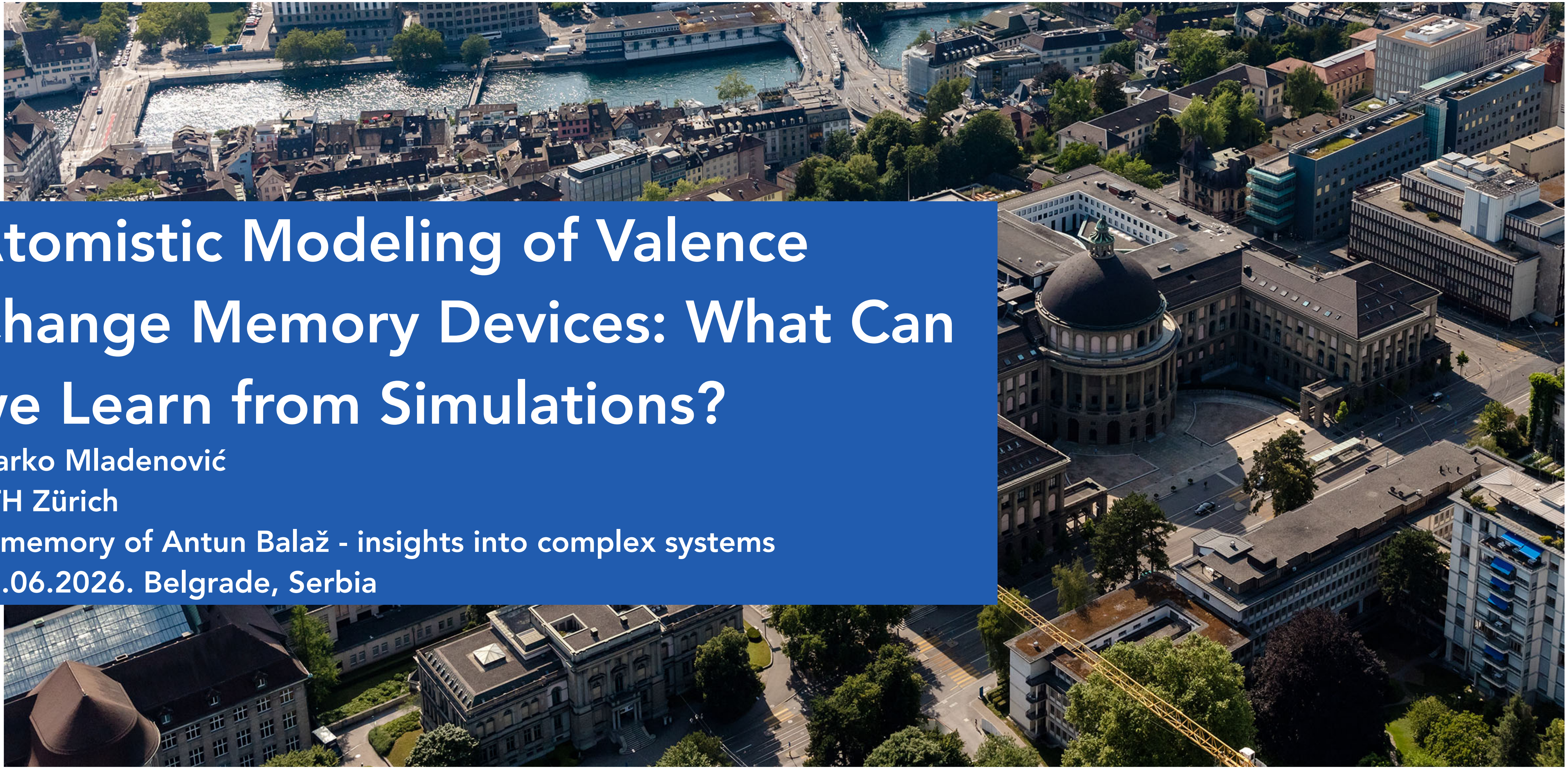

Atomistic Modeling of Valence Change Memory Devices: What Can we Learn from Simulations?

Marko Mladenović
ETH Zürich

In memory of Antun Balaž - insights into complex systems
12.06.2026. Belgrade, Serbia

Outline

Valence Change Memory Cells: General

Atomistic Simulations: Overview of Different Methods

Example 1: Modeling of Resistive Switching in VCM

Example 2: Termination-Dependent Resistive Switching in $SrTiO_3$

Valence Change Memory Cells: General

Valence change memory (VCM) cells: memristors whose resistance (conductance) is altered by changing the coordination of metal ions through oxygen vacancies

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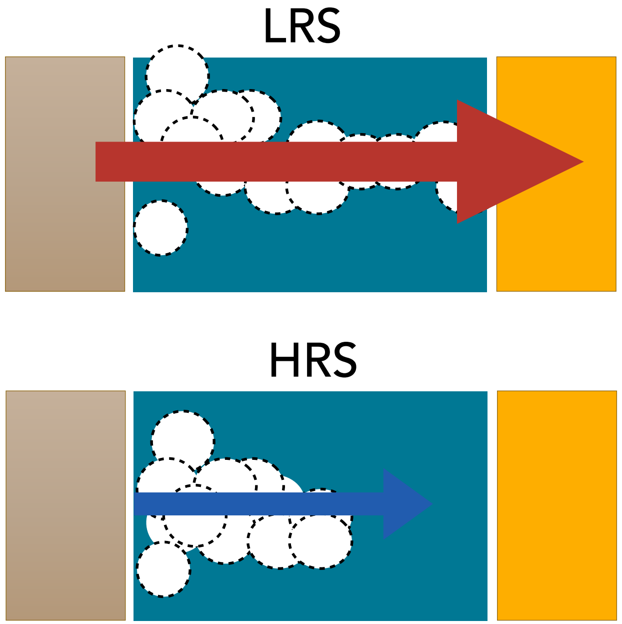

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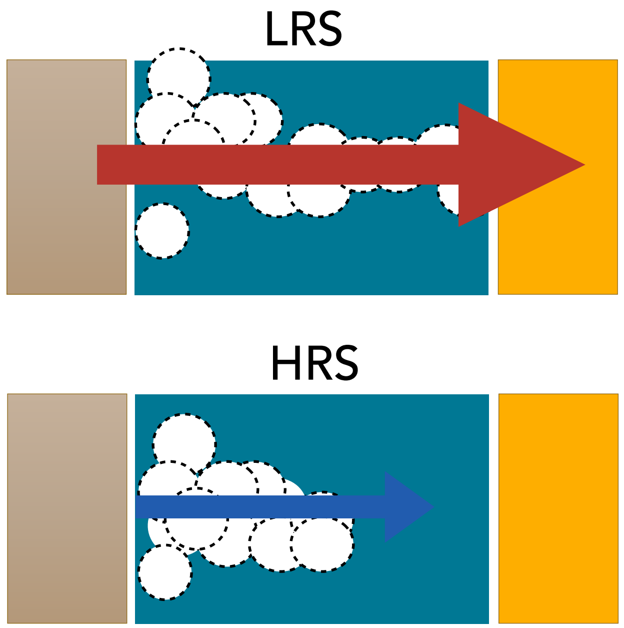

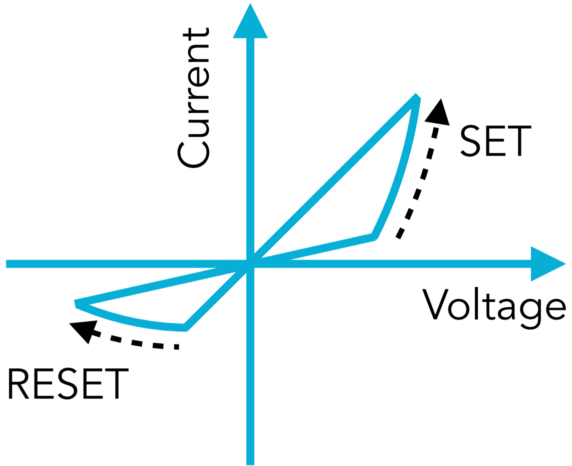

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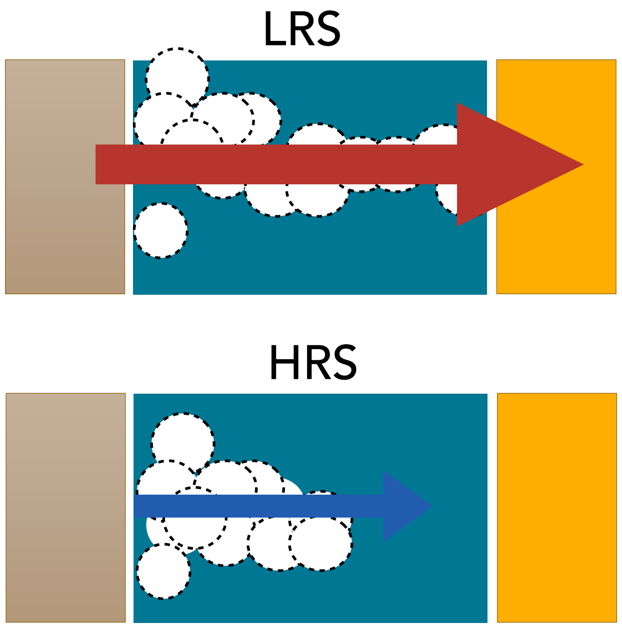

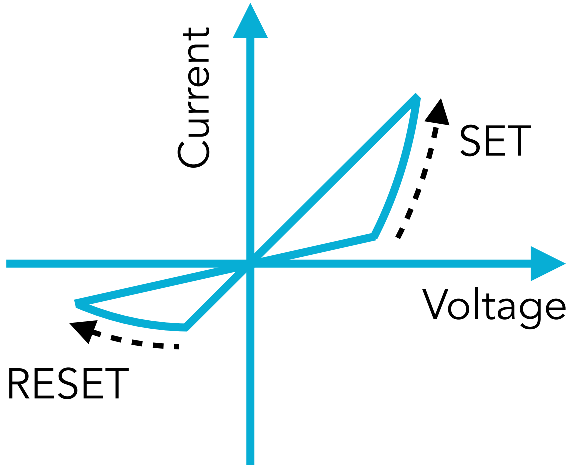

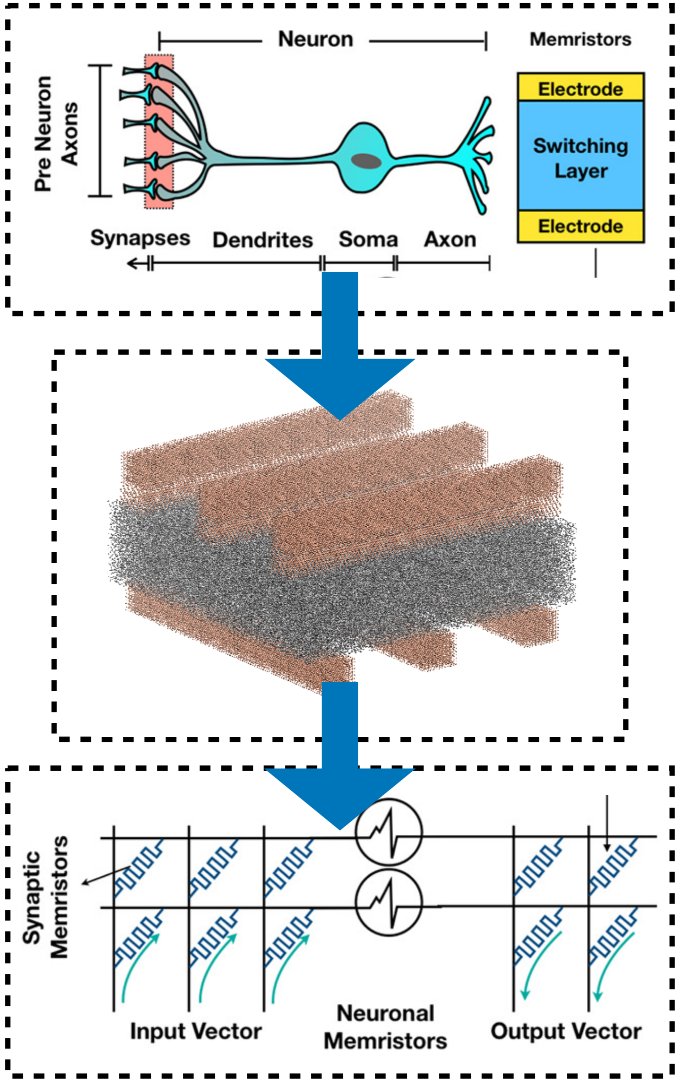

Zhang et al, *Phys. Status Solidi A*, 2018

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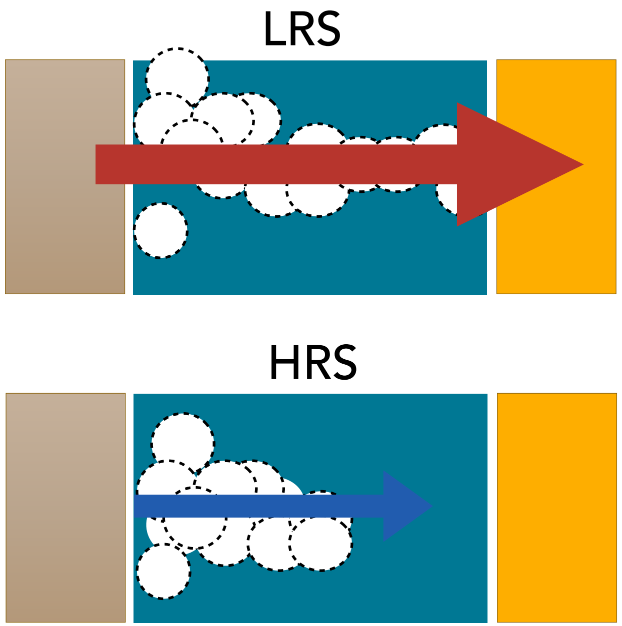
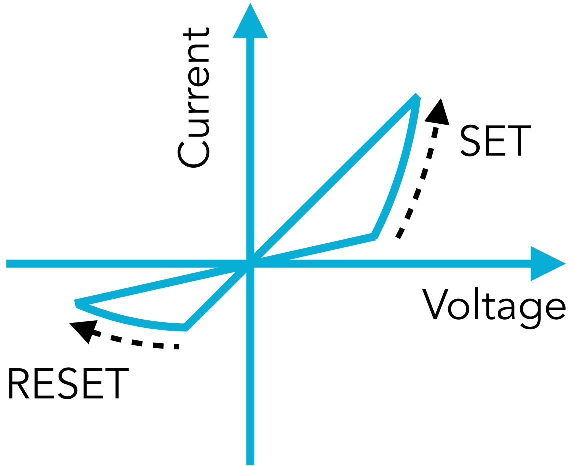
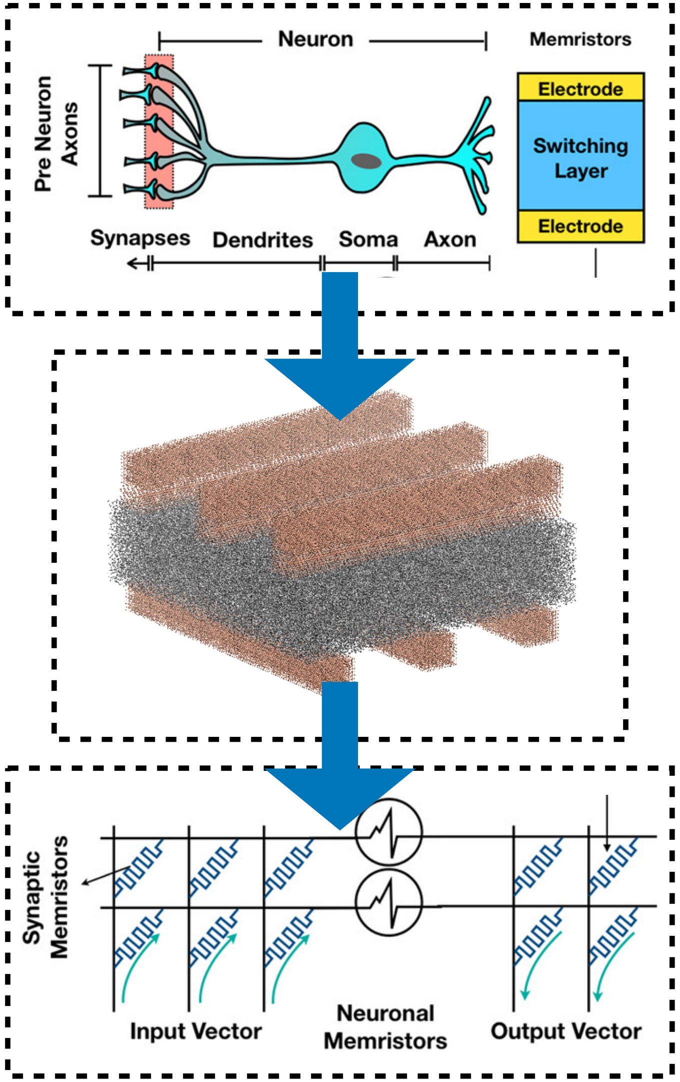






Zhang et al, *Phys. Status Solidi A*, 2018

Advantages:

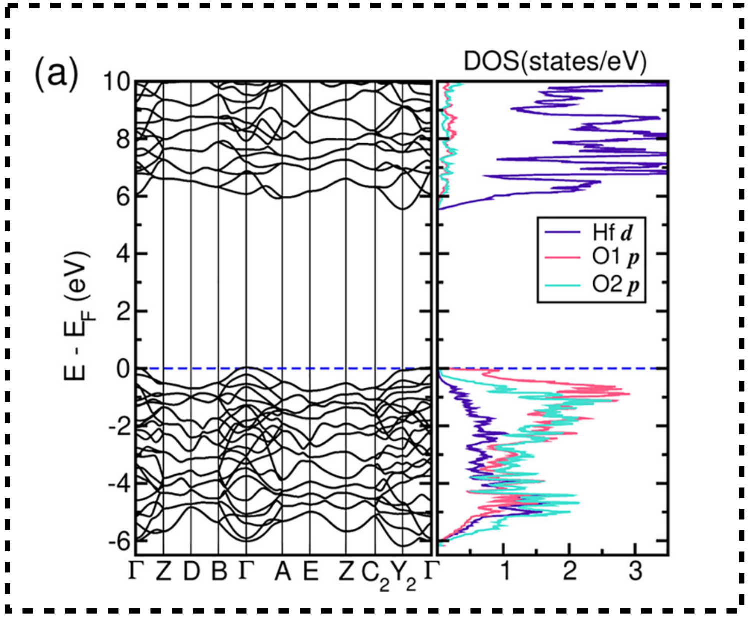
- High ON-OFF ratio
- Ease of fabrications
- Scalability

Disadvantages:

- Variability
- Failure

Atomistic Simulations: Overview of Different Methods

- **Density Functional Theory (DFT)**
- Molecular Dynamics (MD)
- Nudged Elastic Band (NEB)
- Kinetic Monte Carlo (KMC)
- Quantum Transport (QT)



N. Kaiser et al, *ACS Appl. Elec. Mater.* 2023

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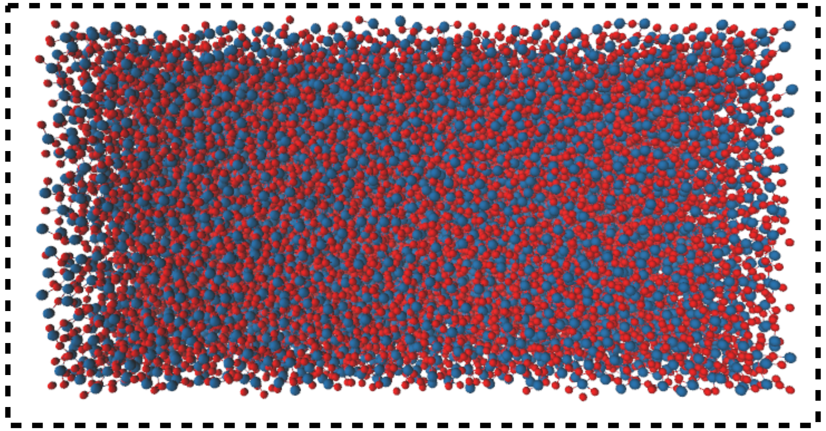

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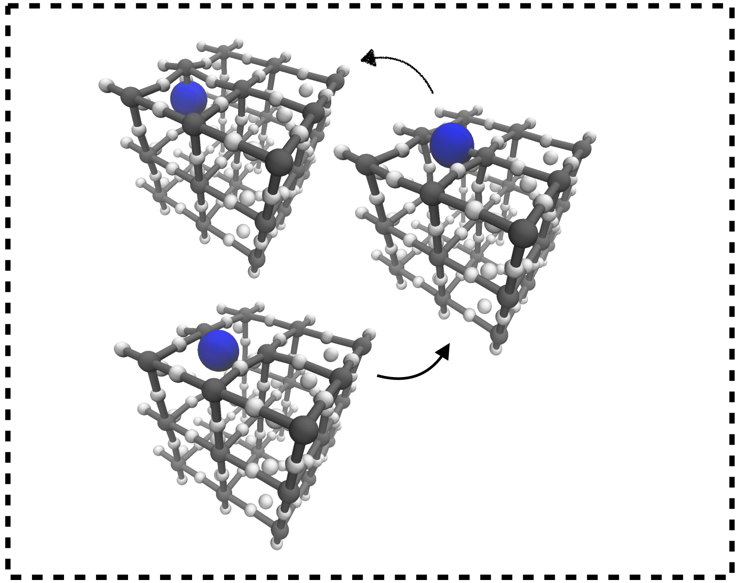

M. Mladenović, et al, *ACS Appl. Electron. Mater.*, 2025

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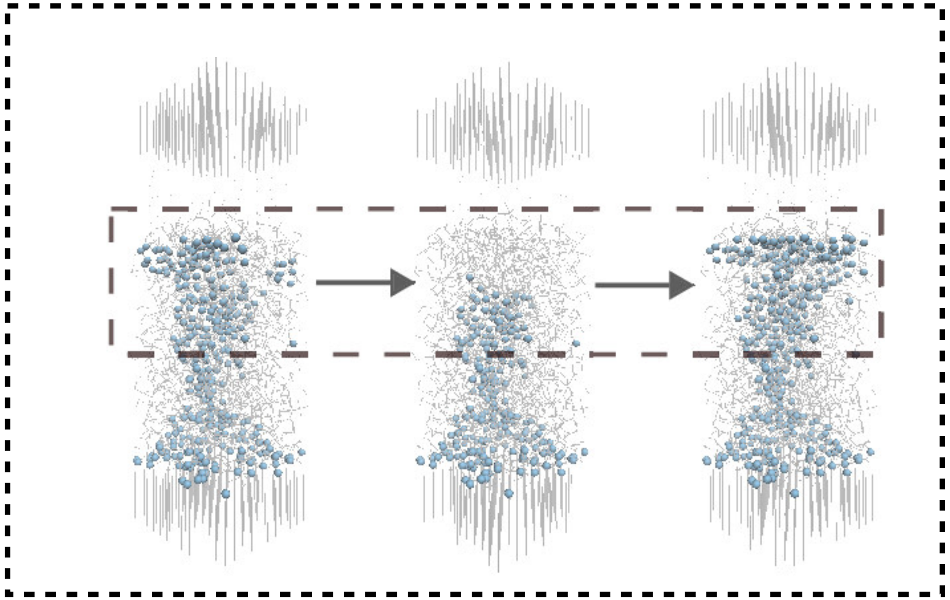

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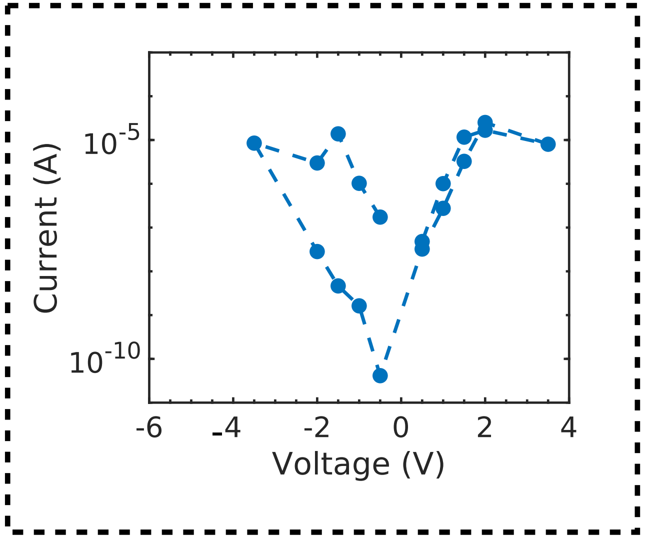

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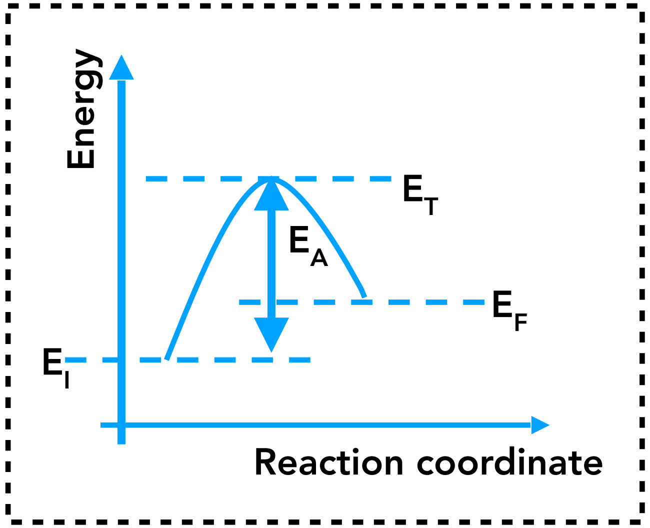
Atomistic Simulations: Overview of Different Methods

NEB



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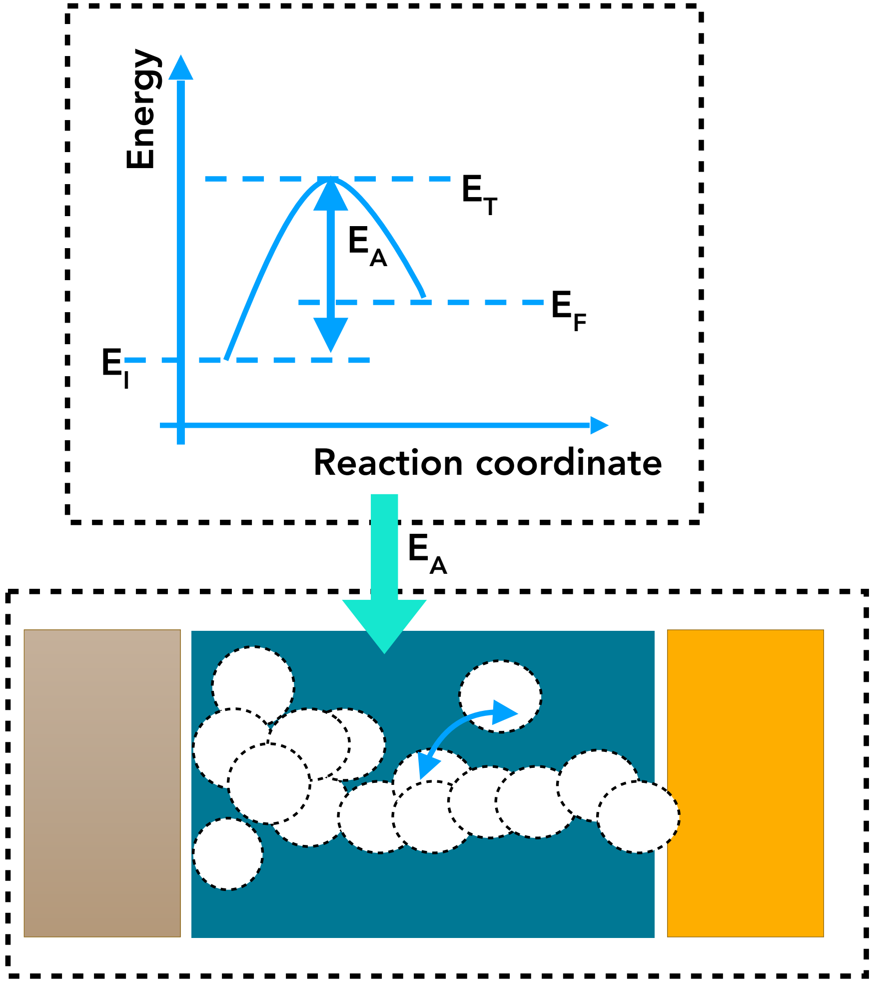
NEB

KMC



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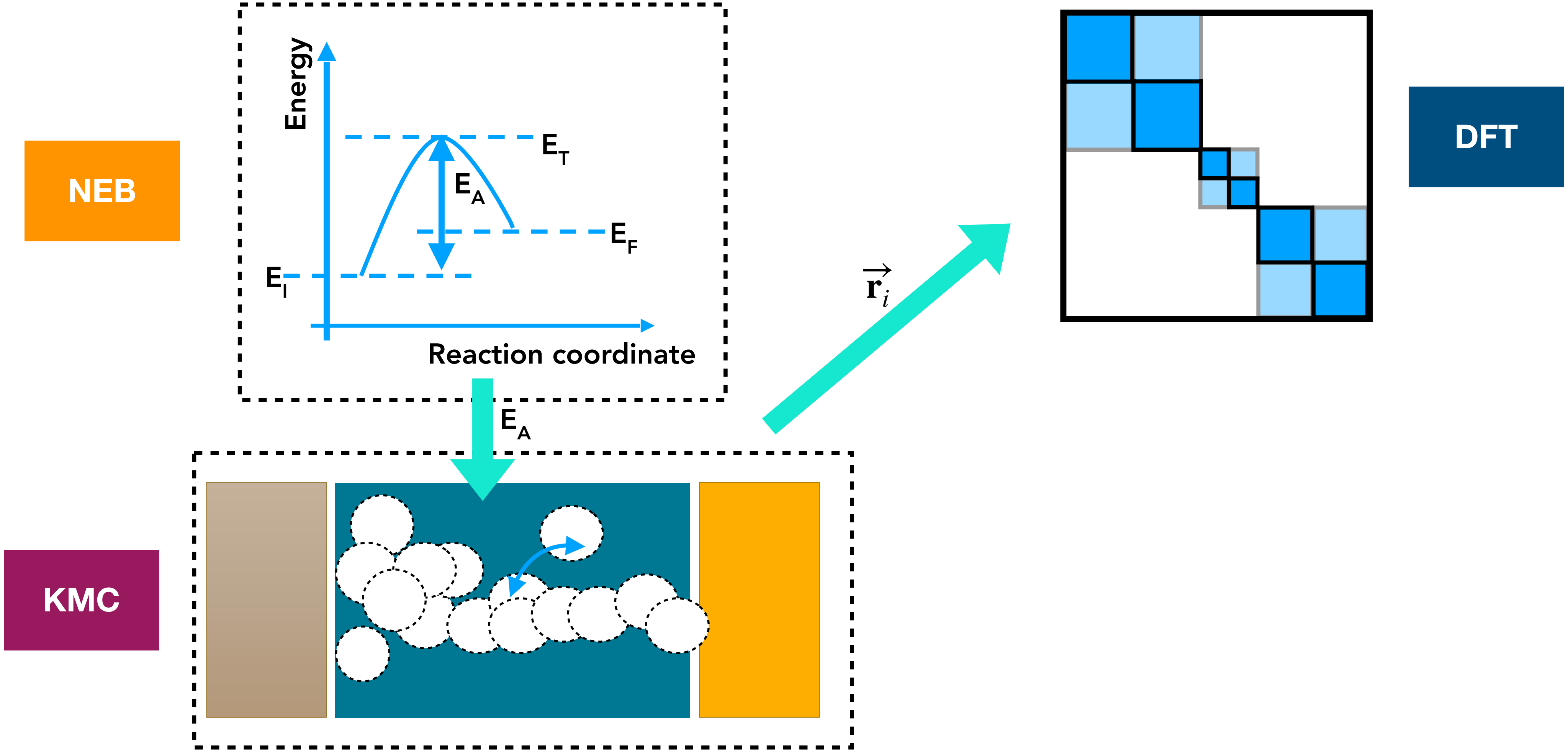

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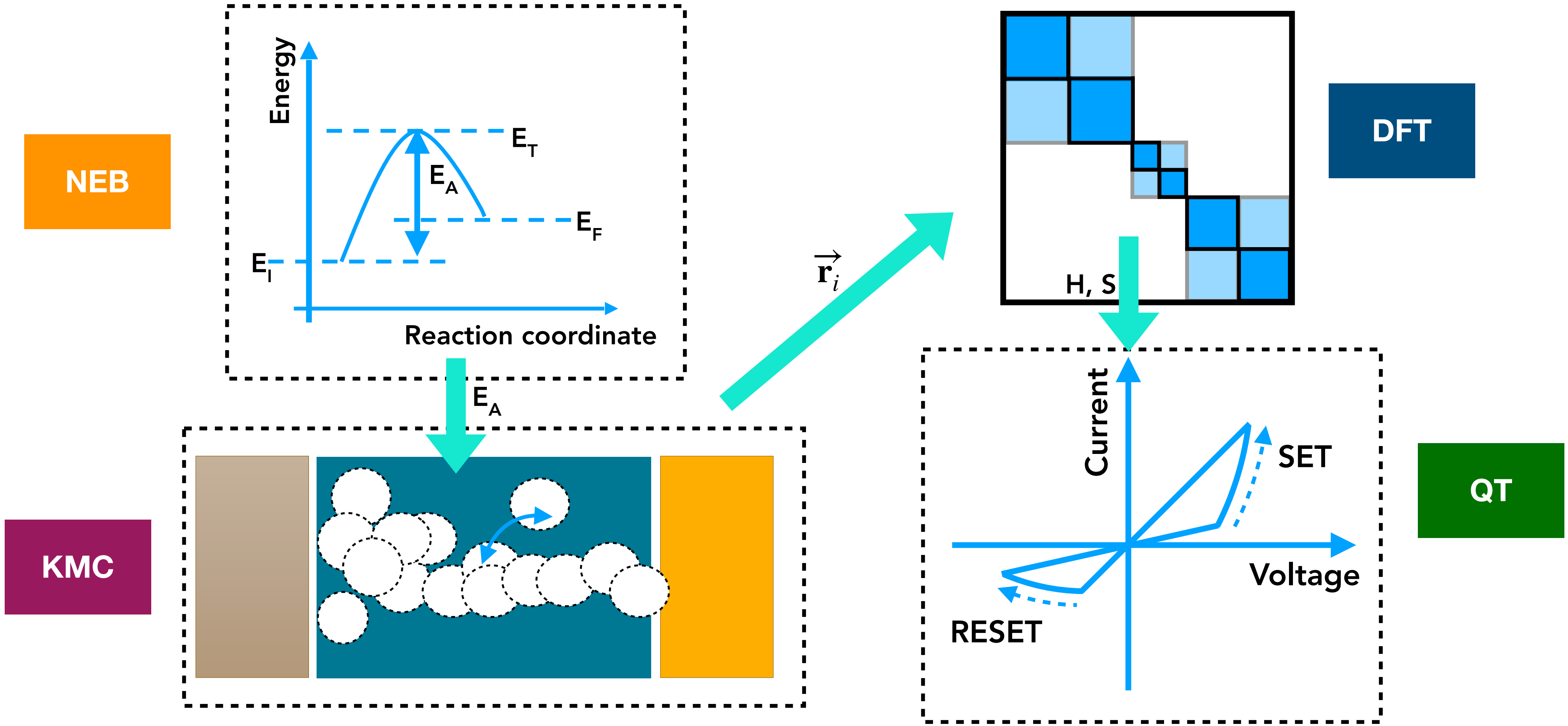
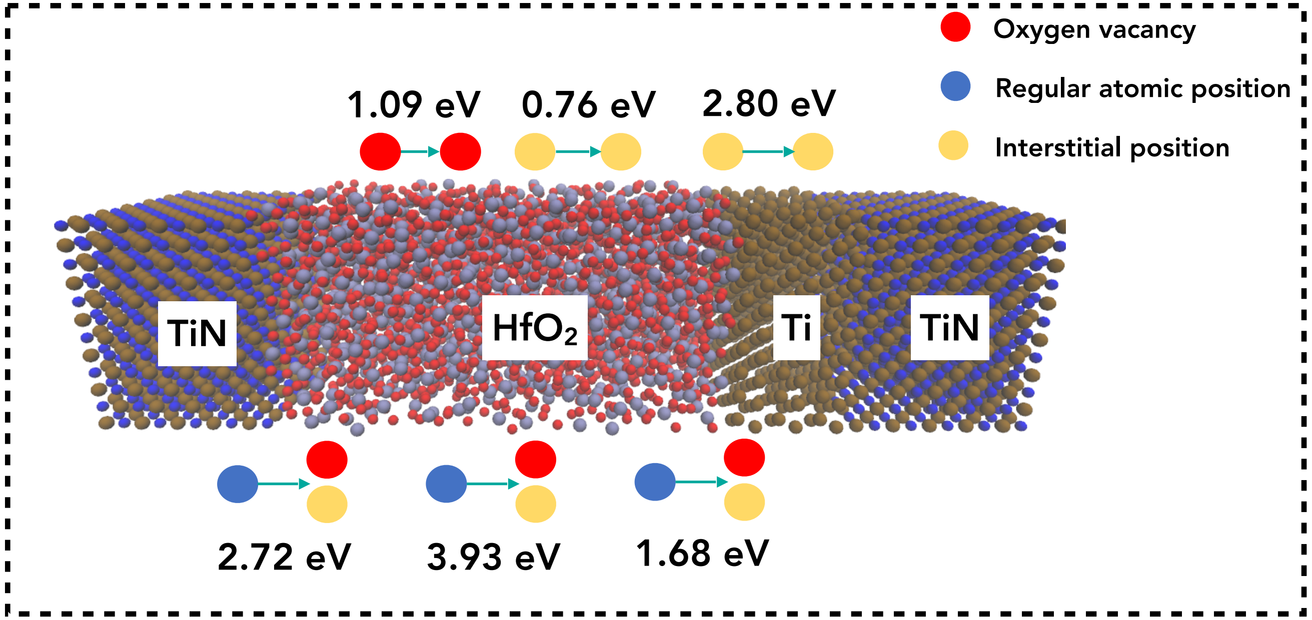


Example 1: Modeling of Resistive Switching in HfO_2



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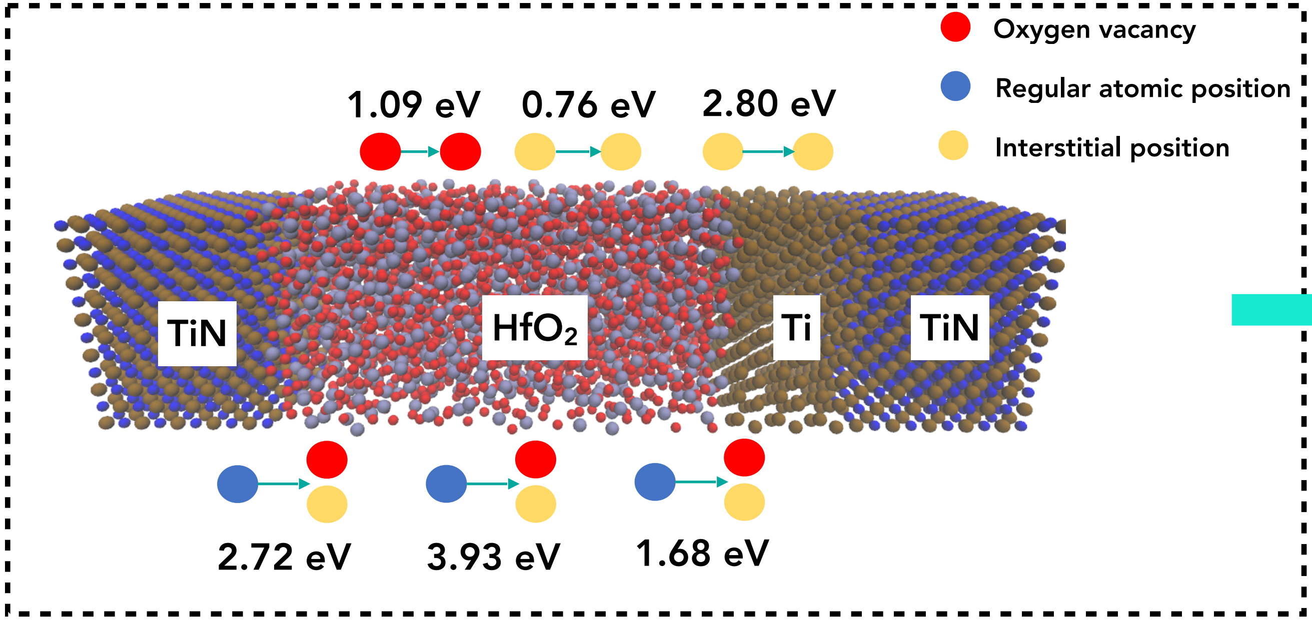

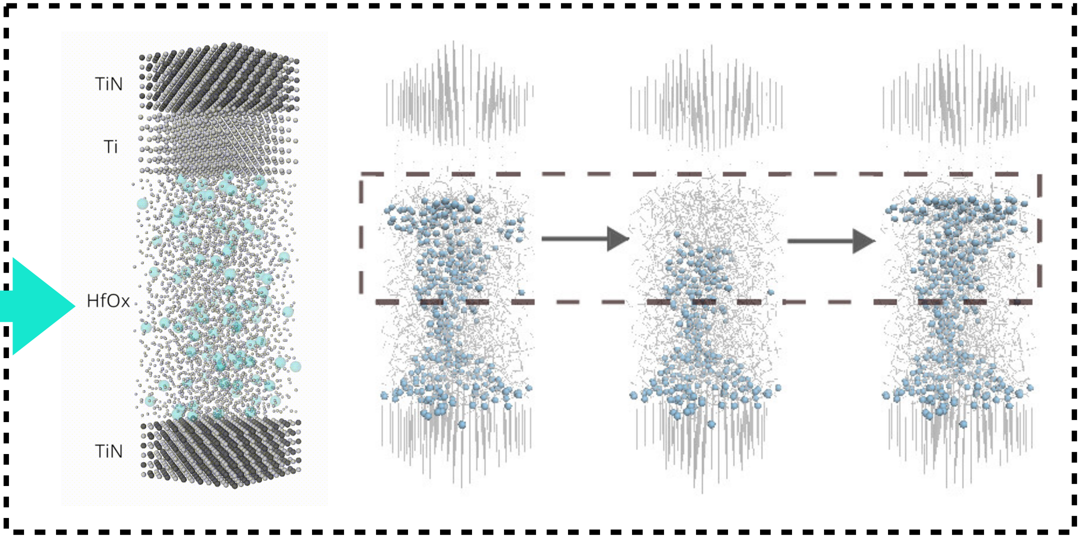

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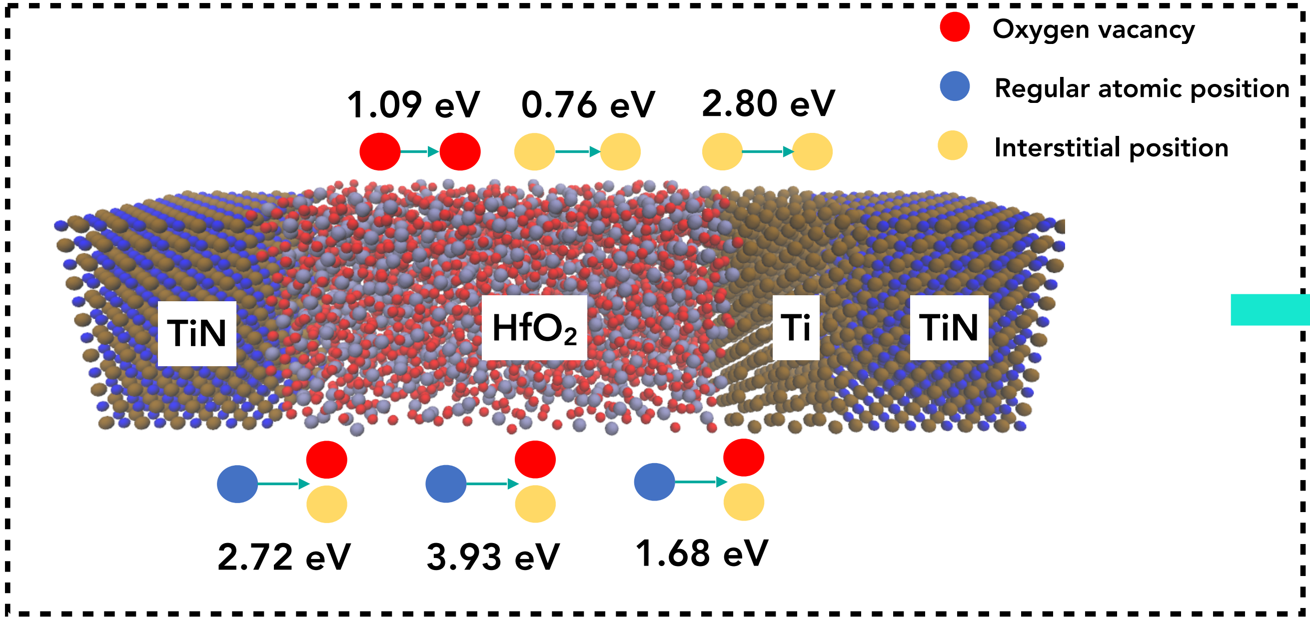

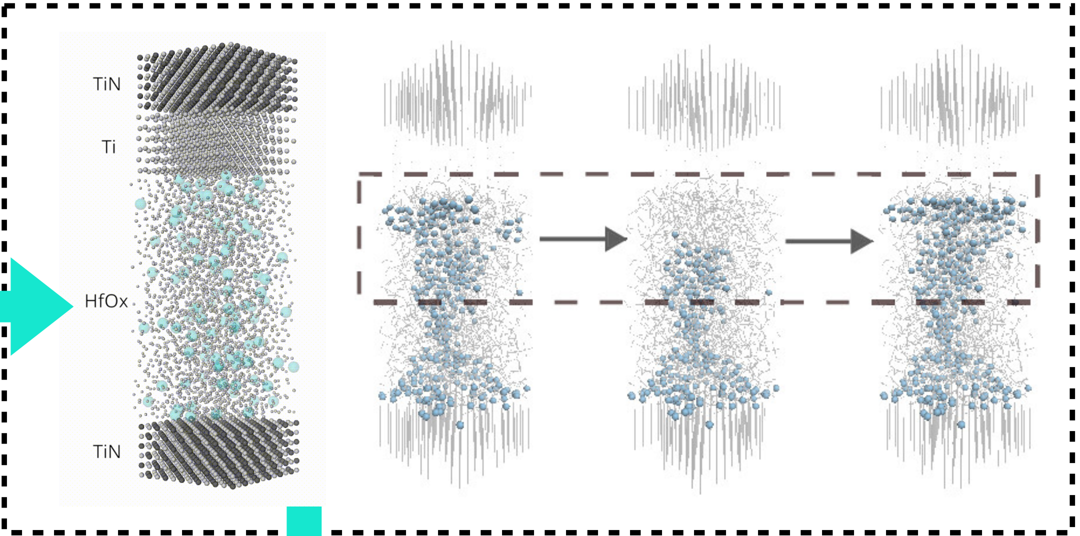

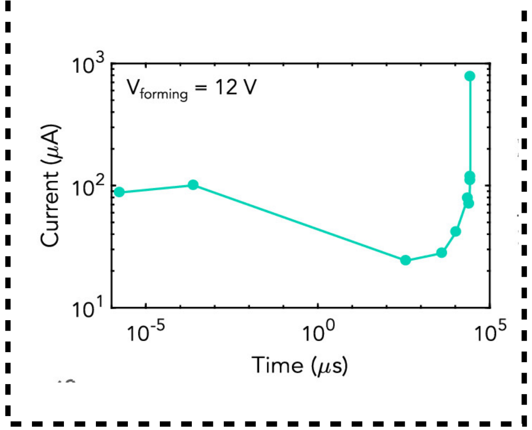

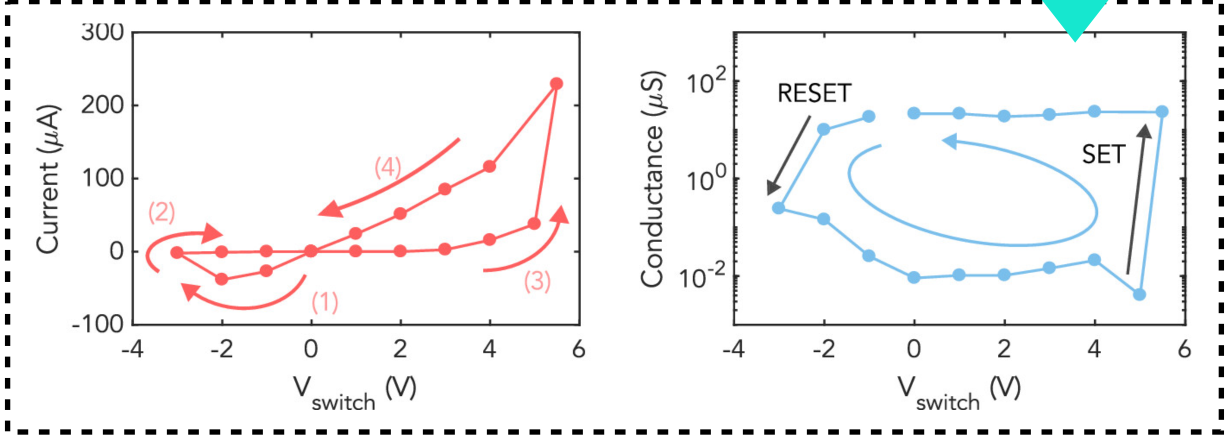

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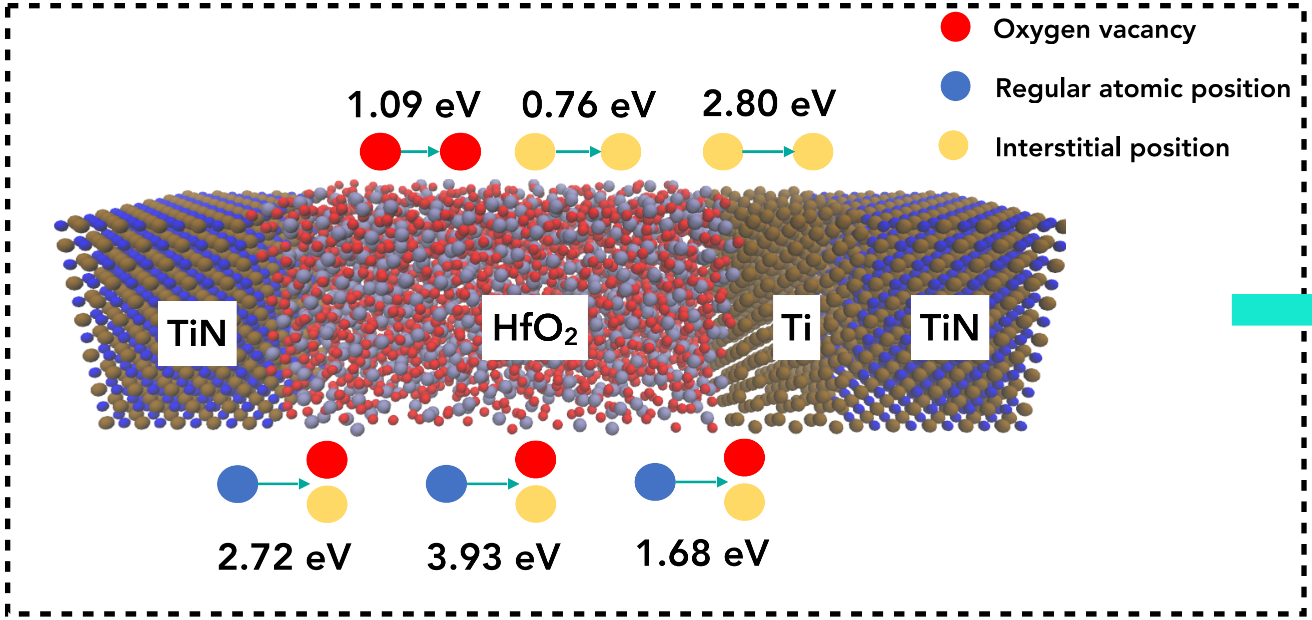

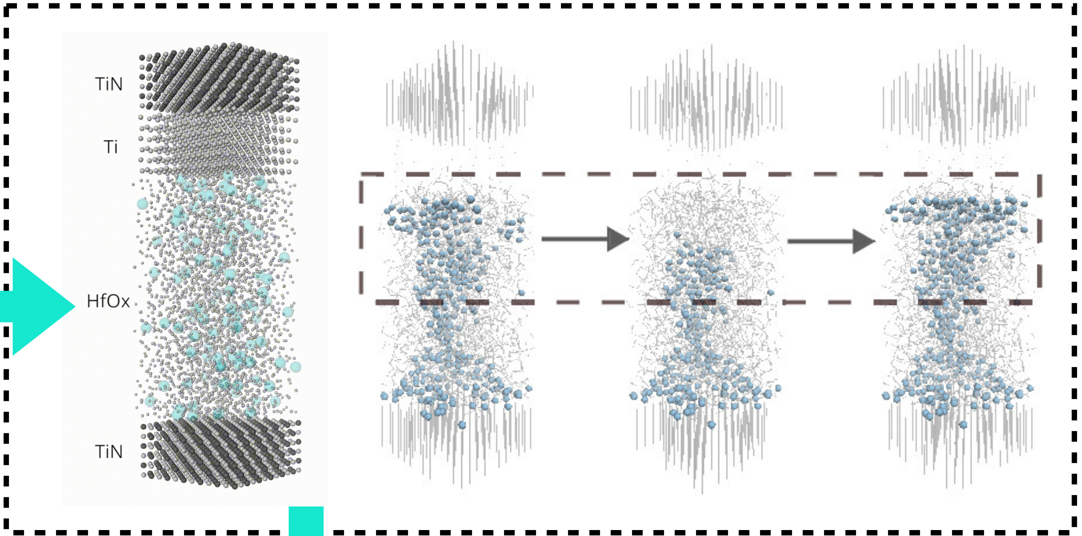

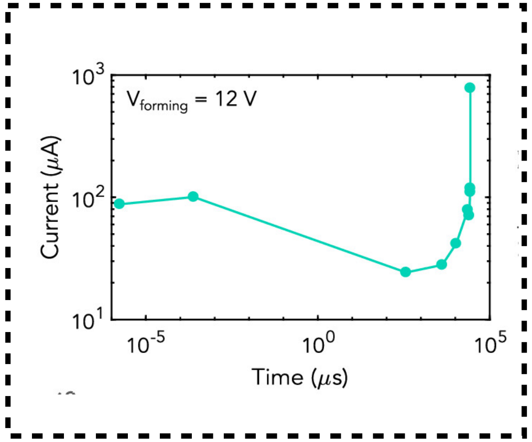

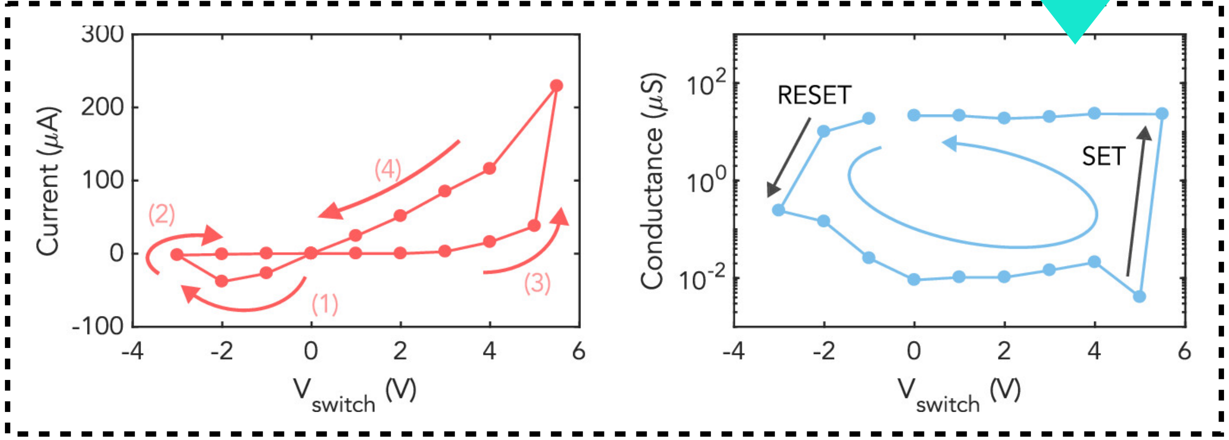

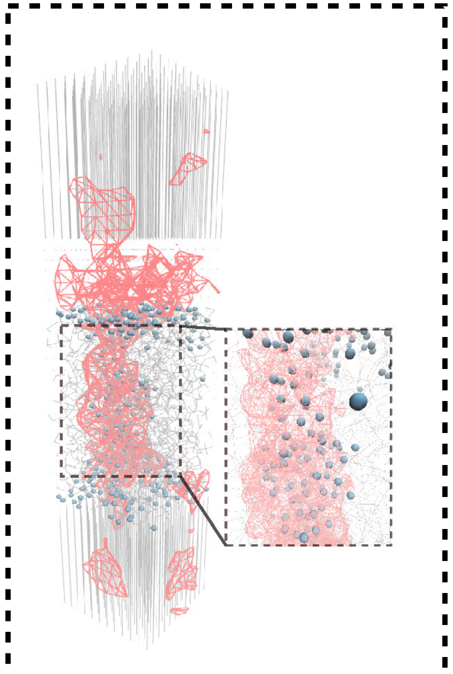

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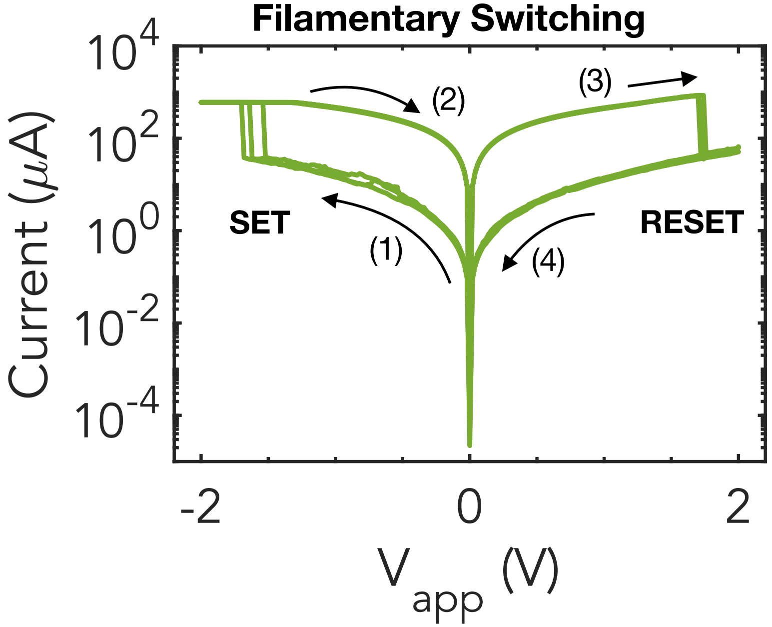
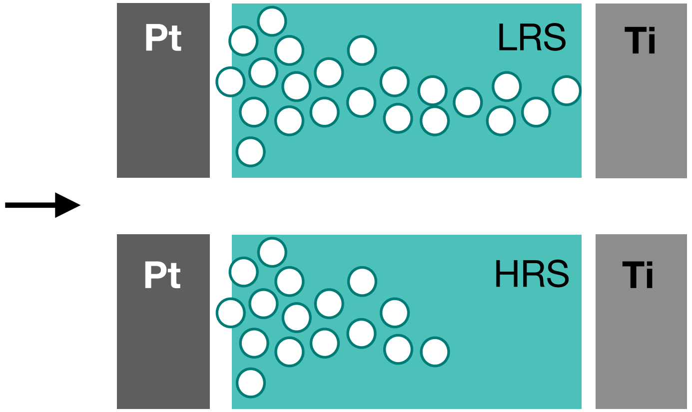
Example 2: Termination-Dependent Resistive Switching in $SrTiO_3$





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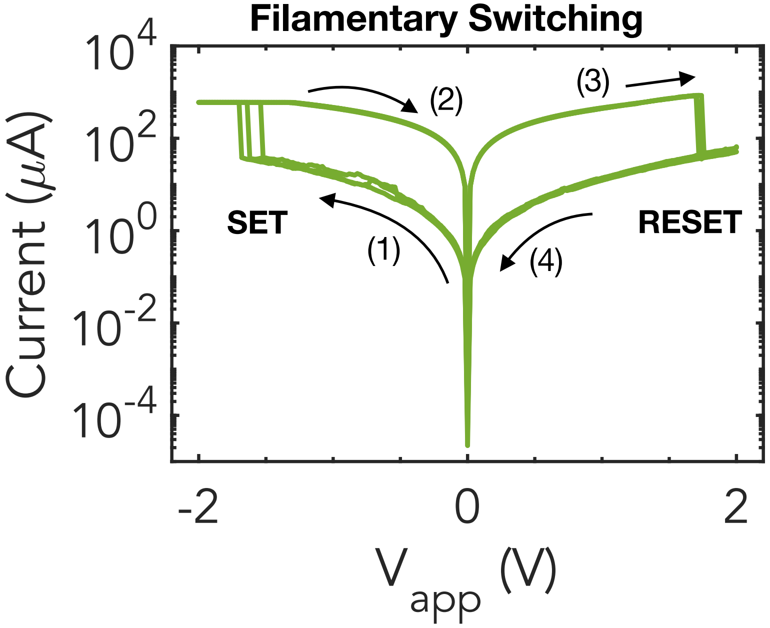

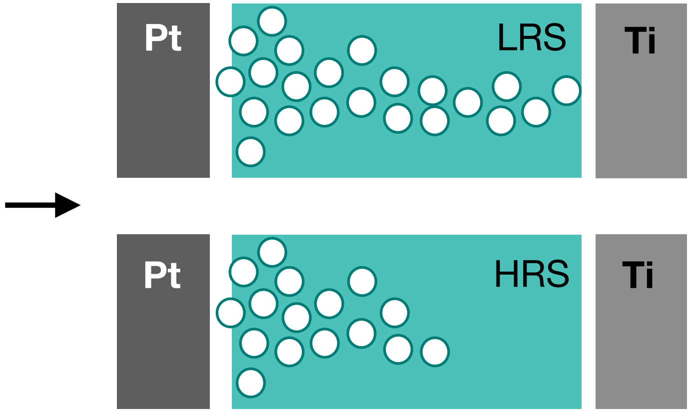

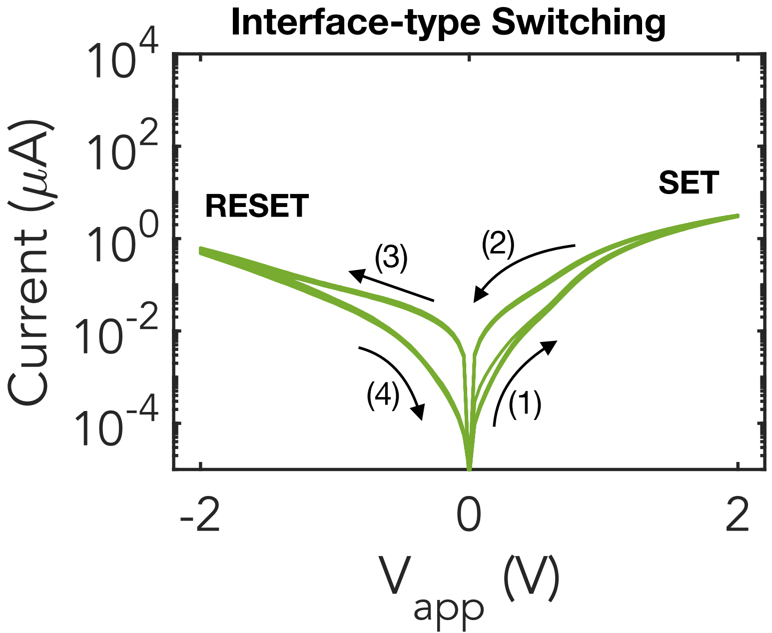

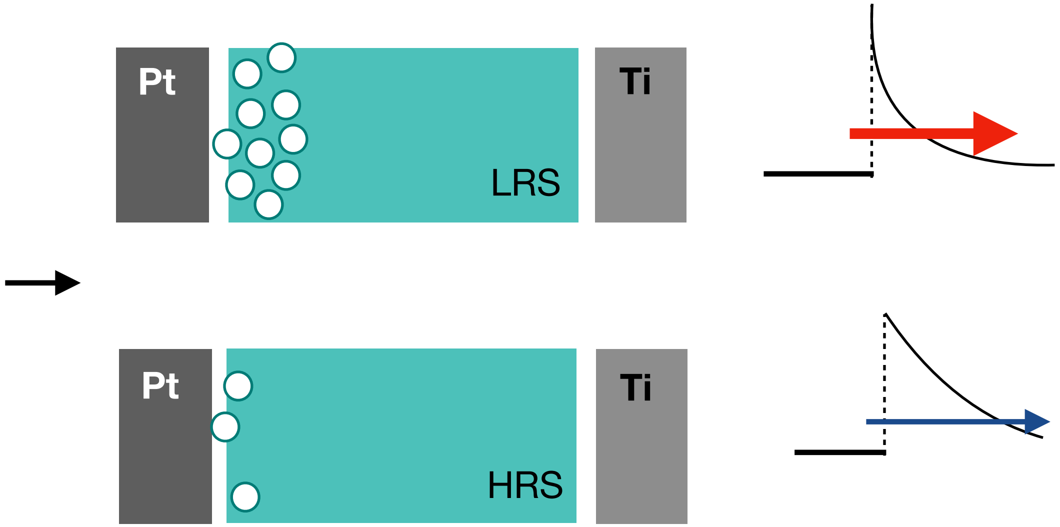

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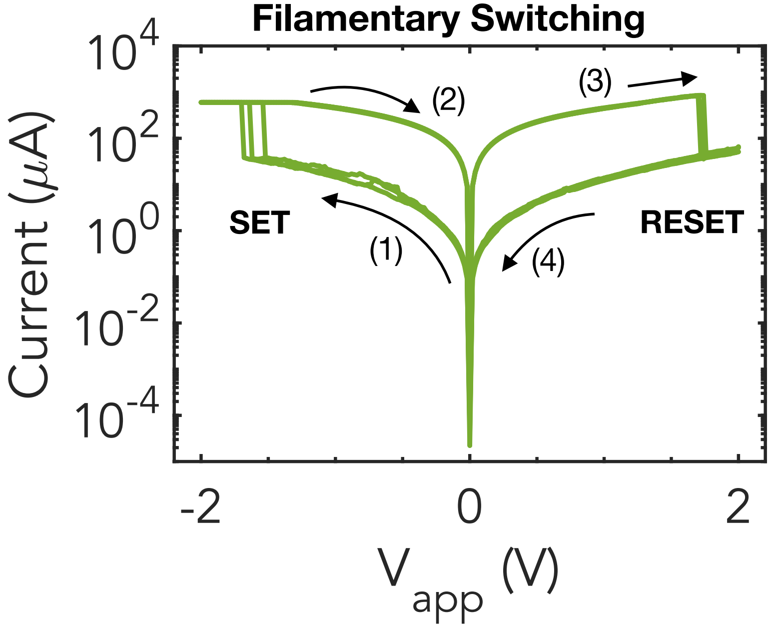
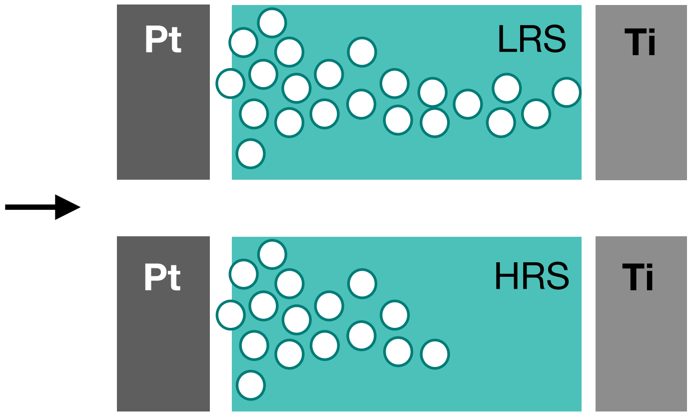
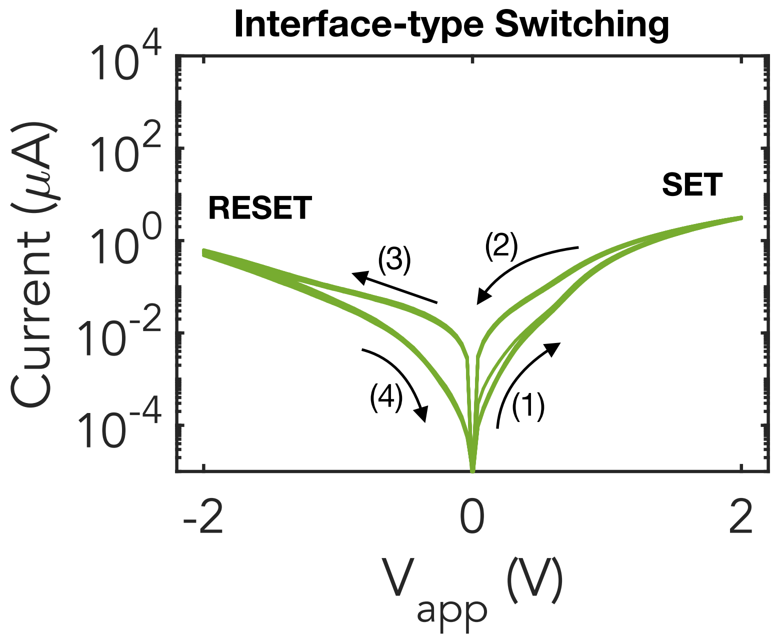
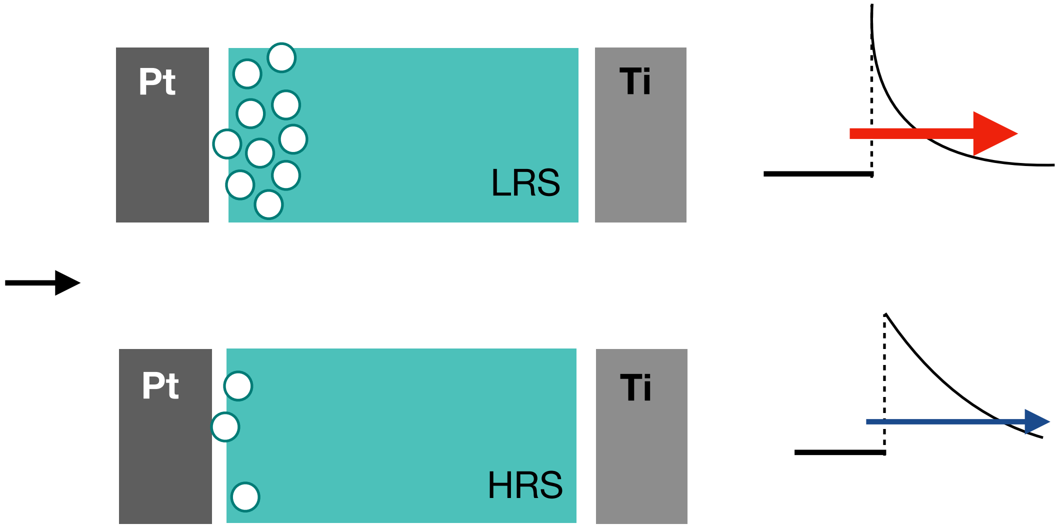




The Schottky barrier modulationcan be achieved via:

- Oxygen vacancy migration
- Charge trapping/detrapping
- Vacancy-ion pair generation/ recombination





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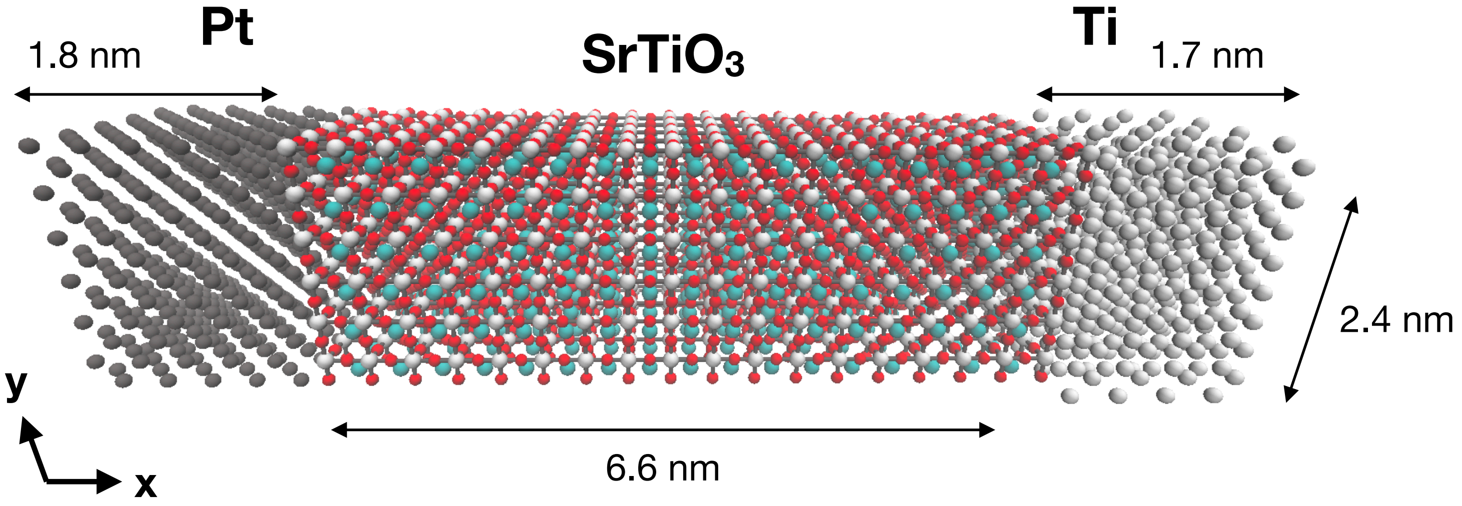

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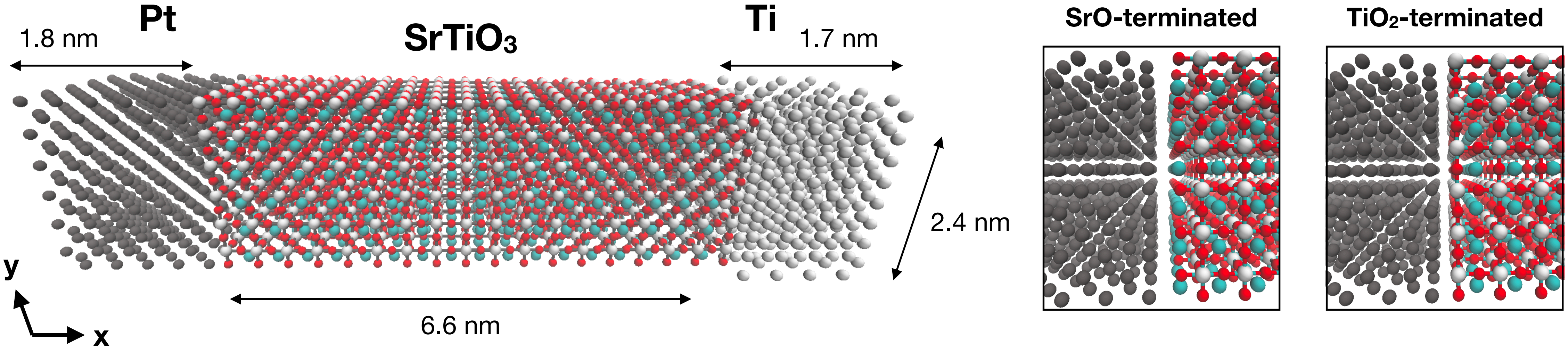

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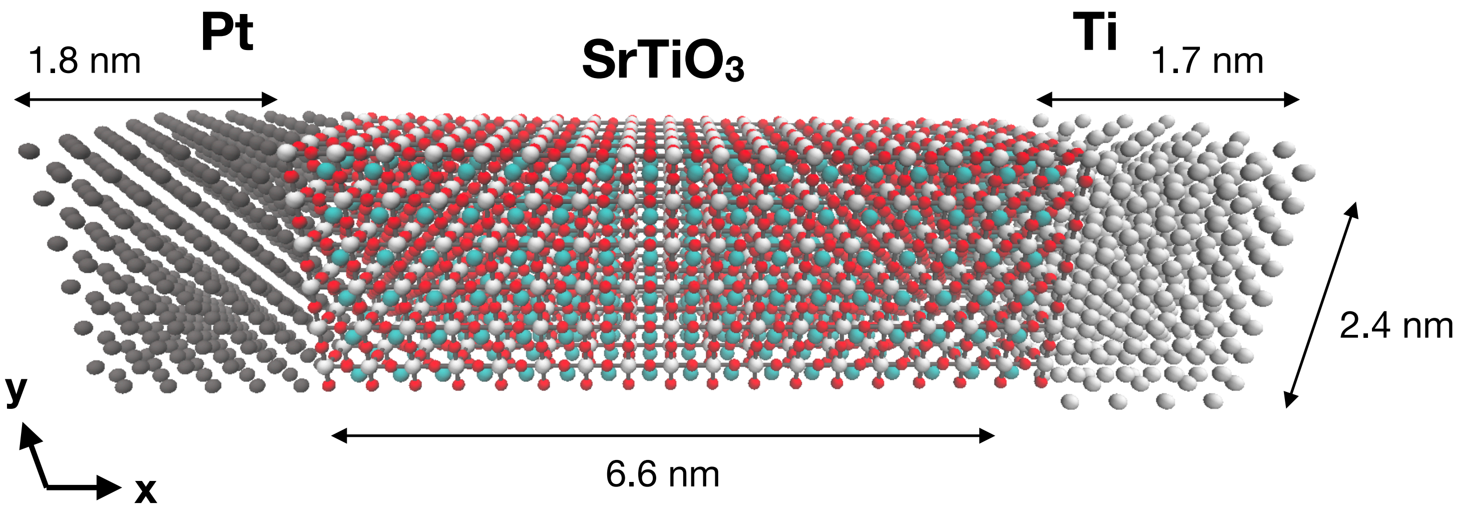
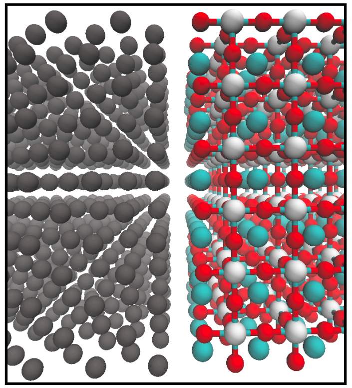
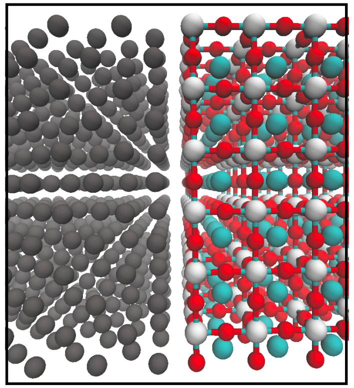


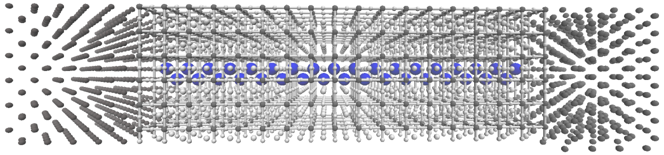
SrO-terminated



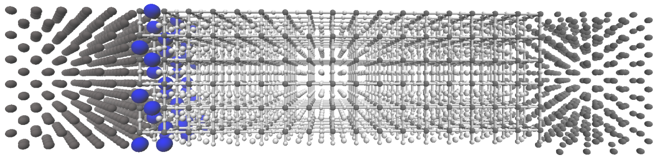
TiO_2-terminated



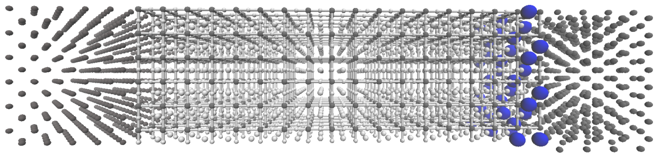
Uniform



Pt-end



Ti-end



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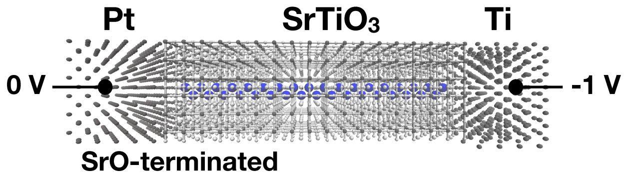

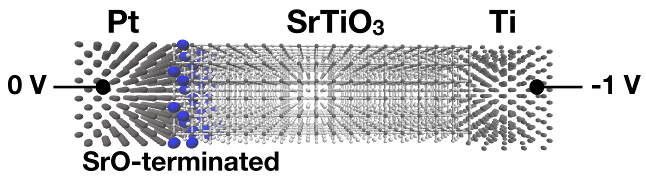

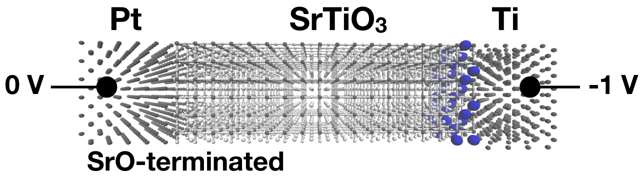

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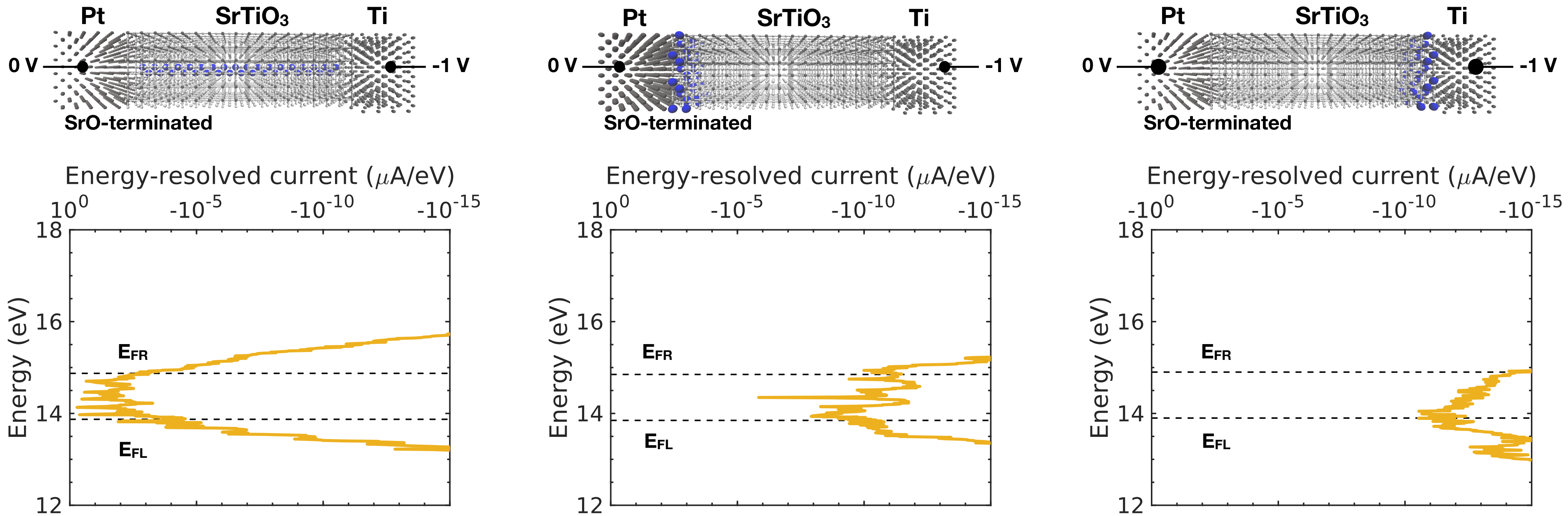

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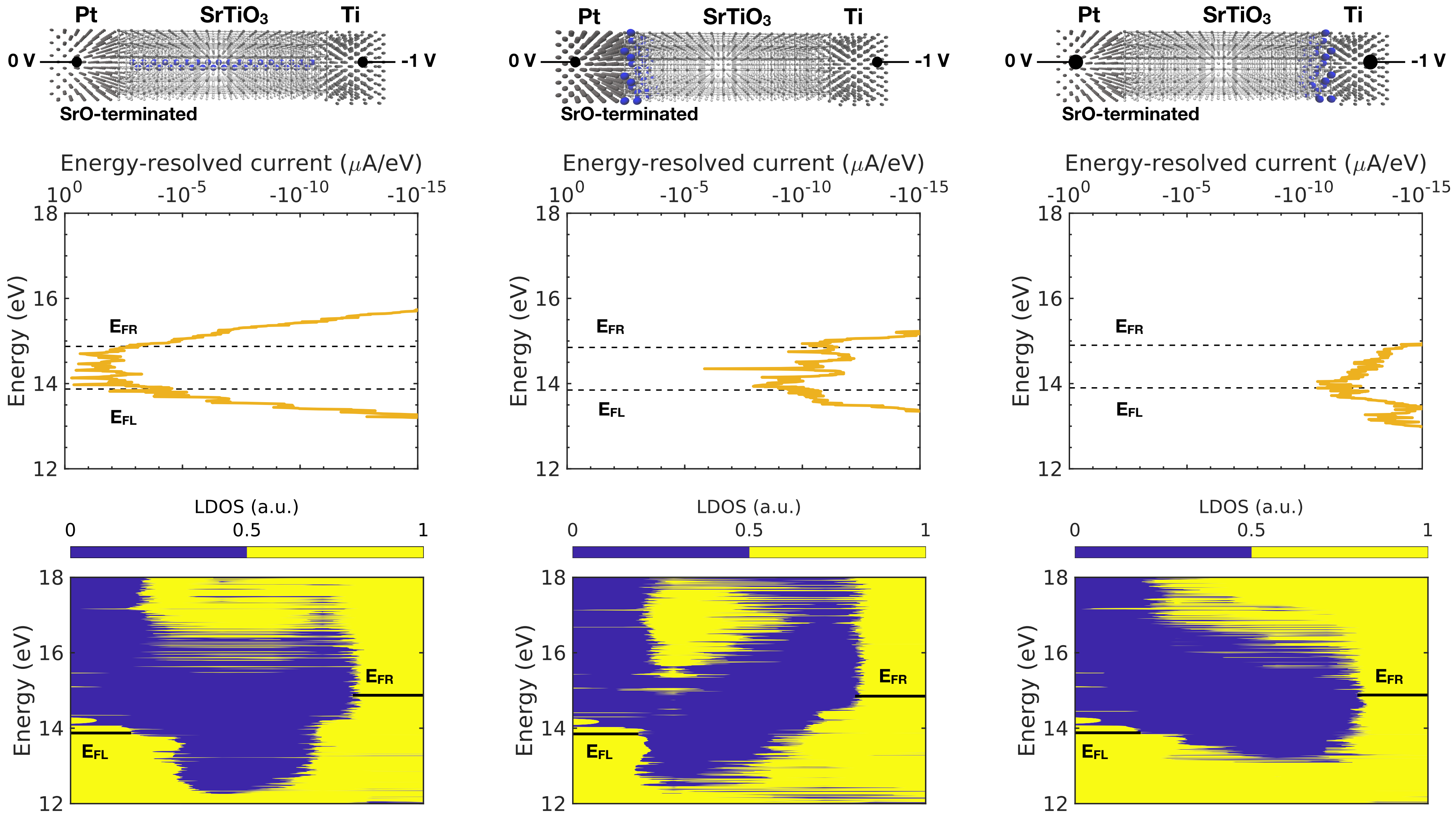

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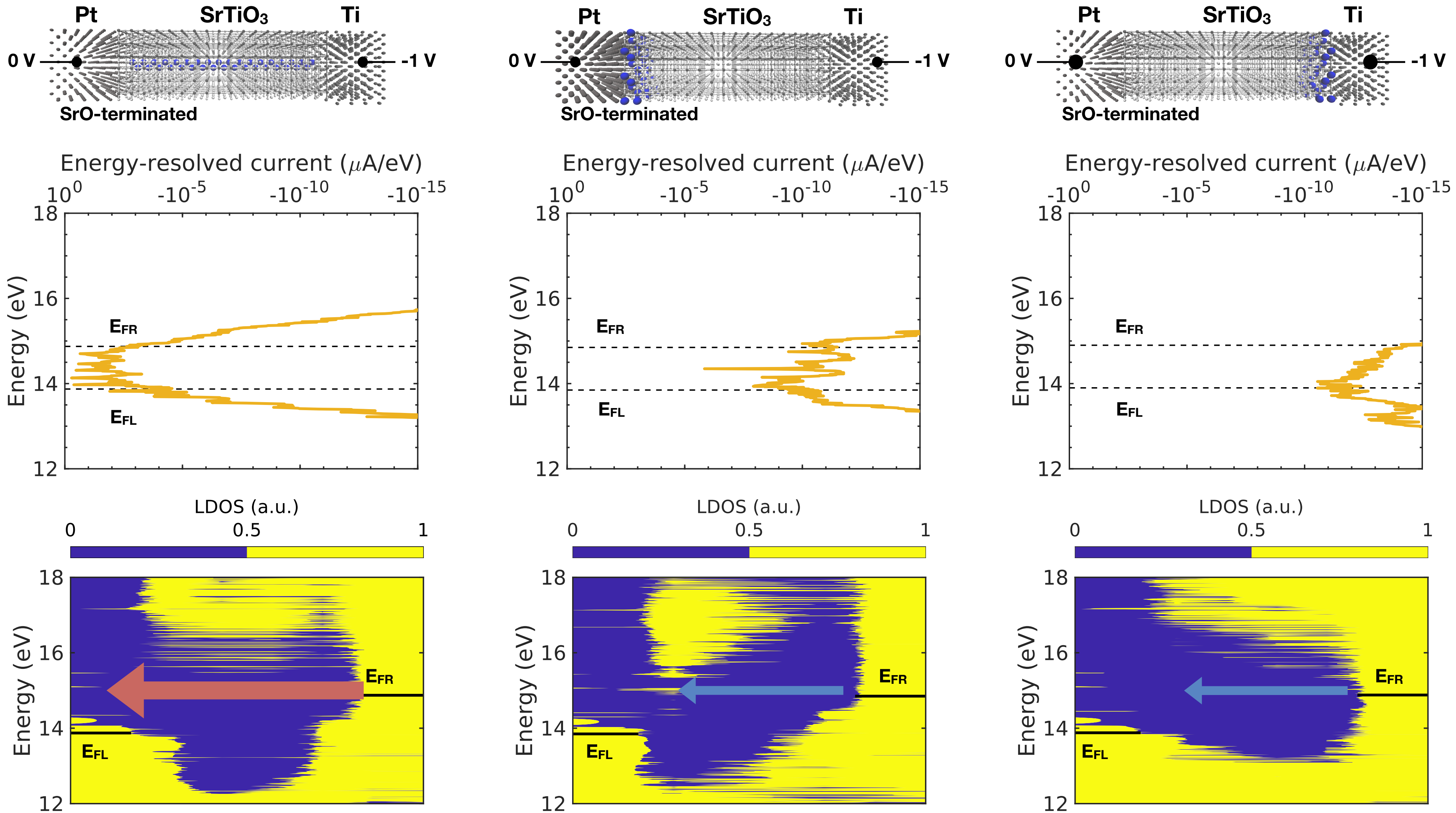

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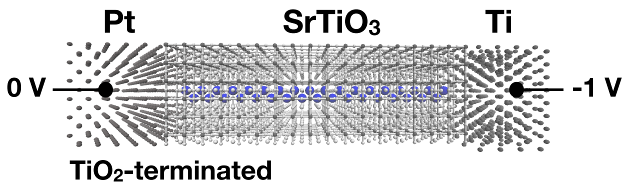

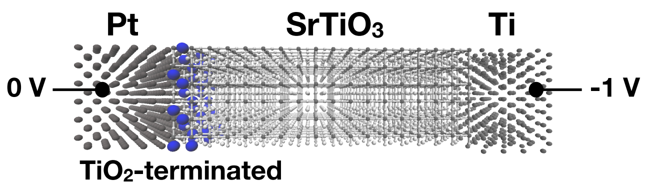

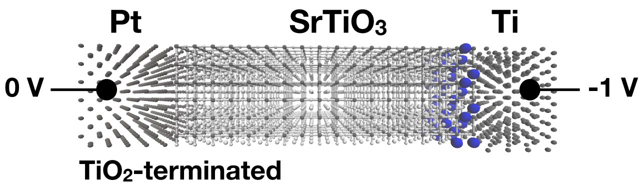

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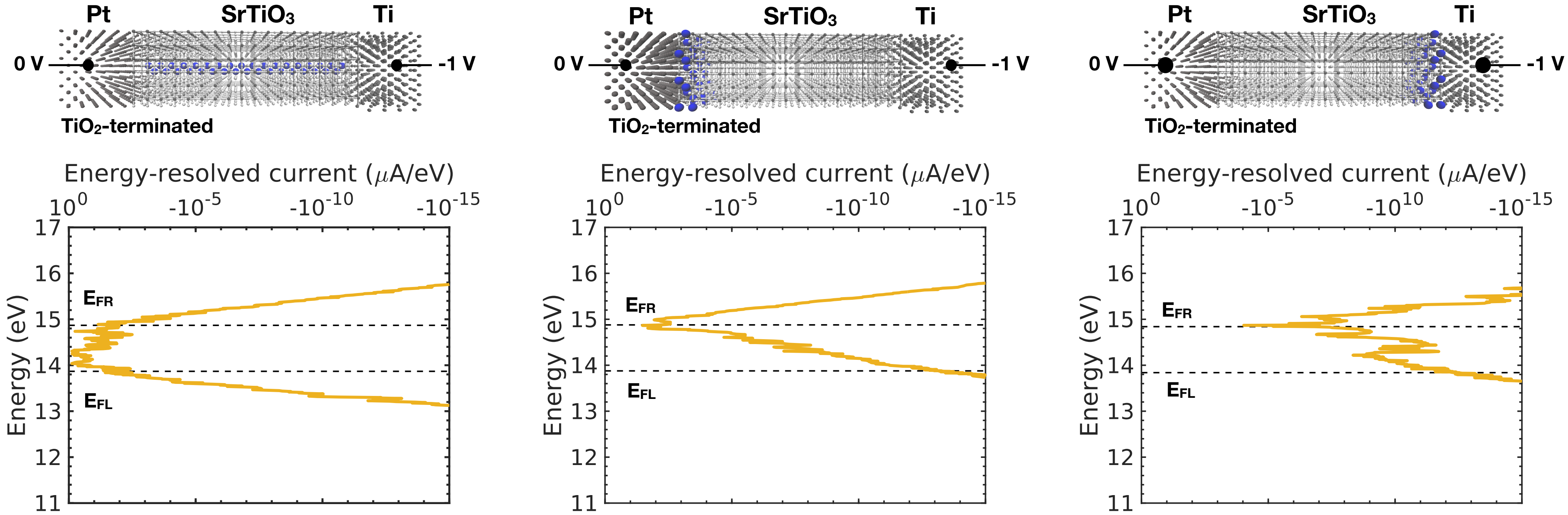

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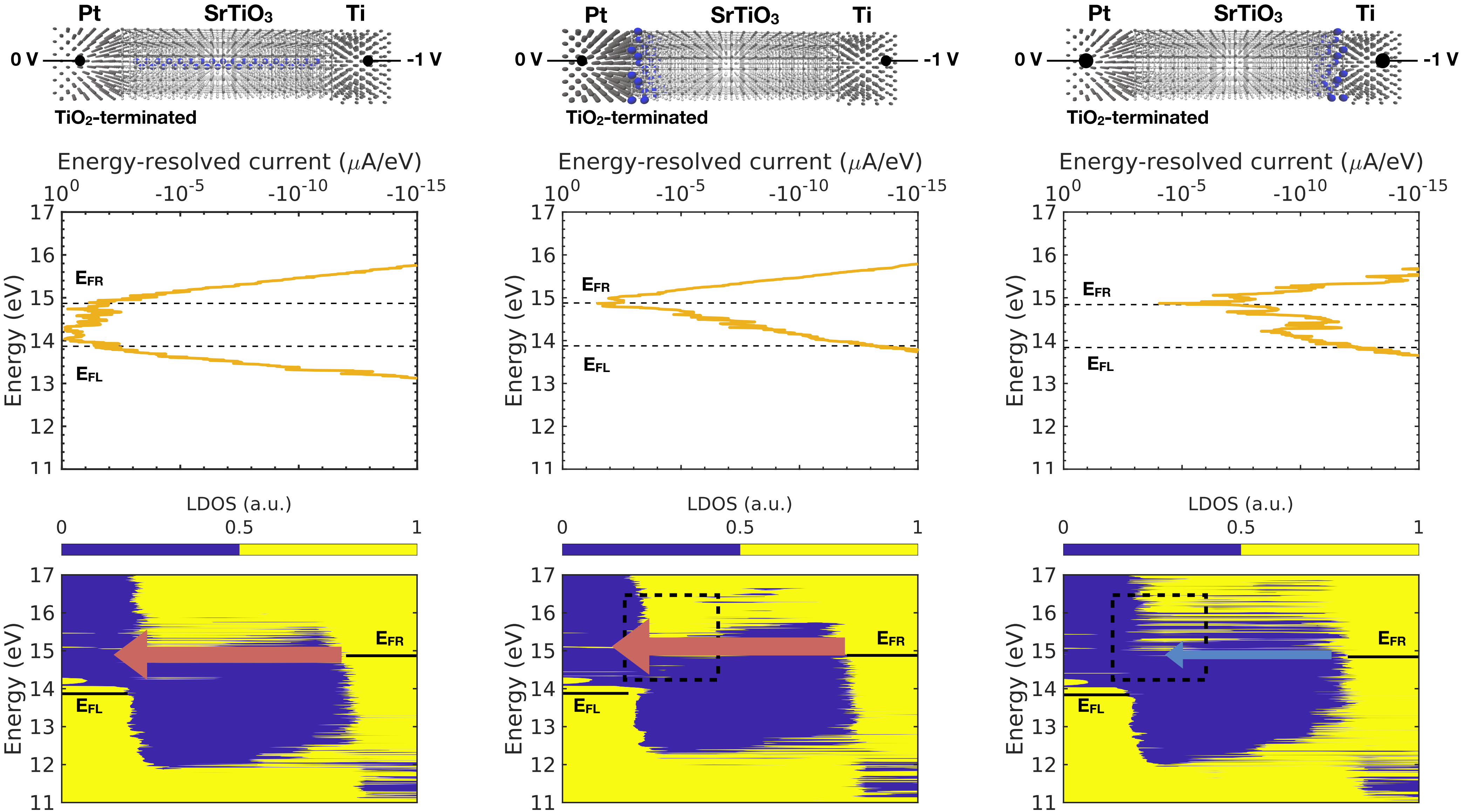
Example 2: Termination-Dependent Resistive Switching in $SrTiO_3$



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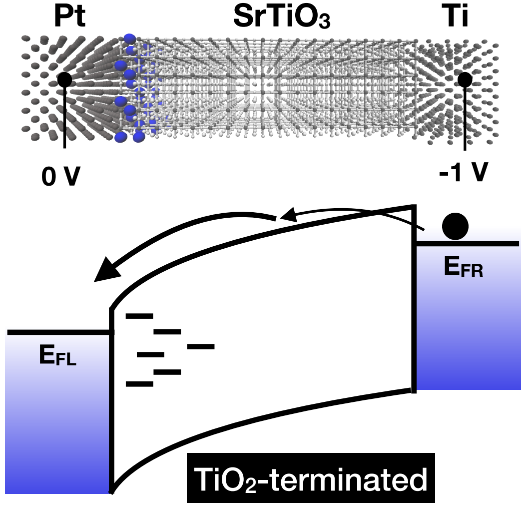
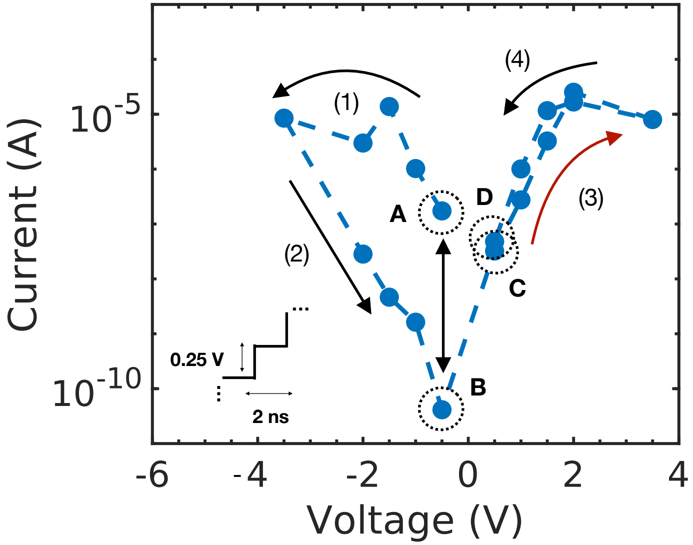
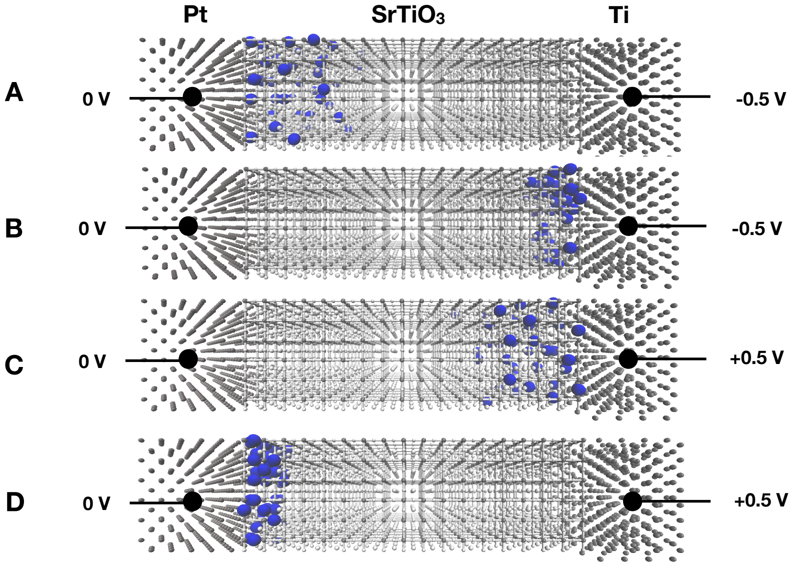
Example 2: Termination-Dependent Resistive Switching in $SrTiO_3$

Interface-type





Vacancy migration



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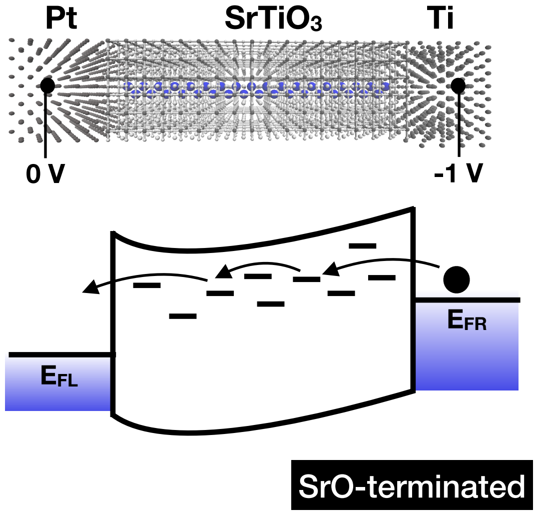
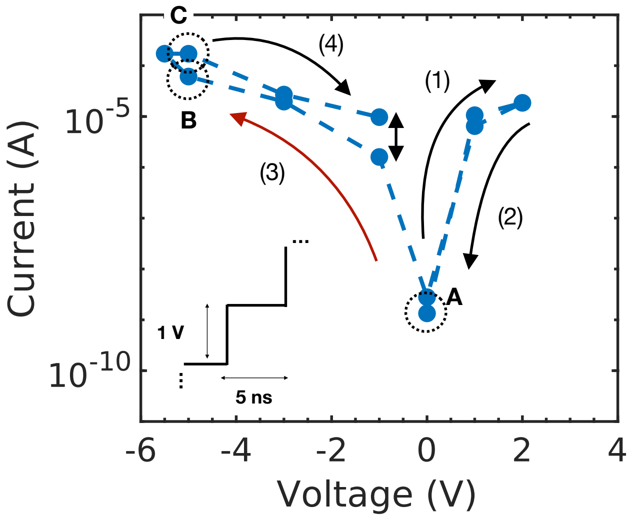
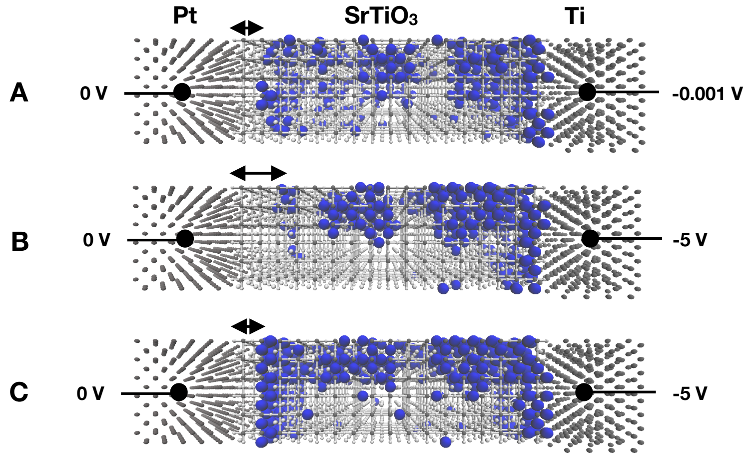
Example 2: Termination-Dependent Resistive Switching in $SrTiO_3$

Filamentary-type





Filament formation/rupture



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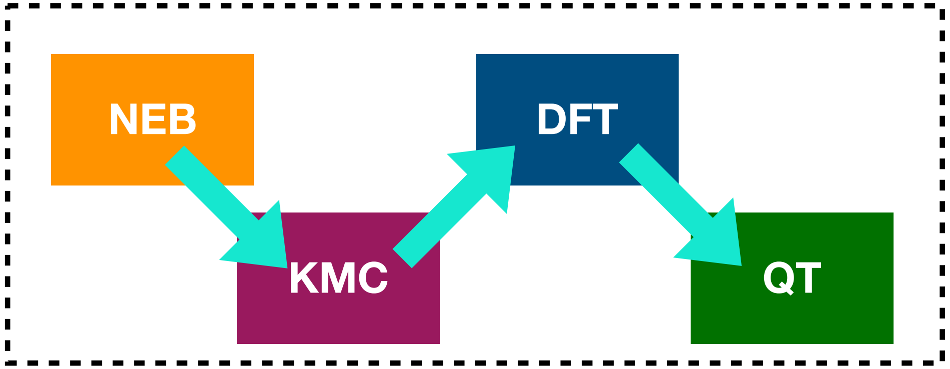
Summary



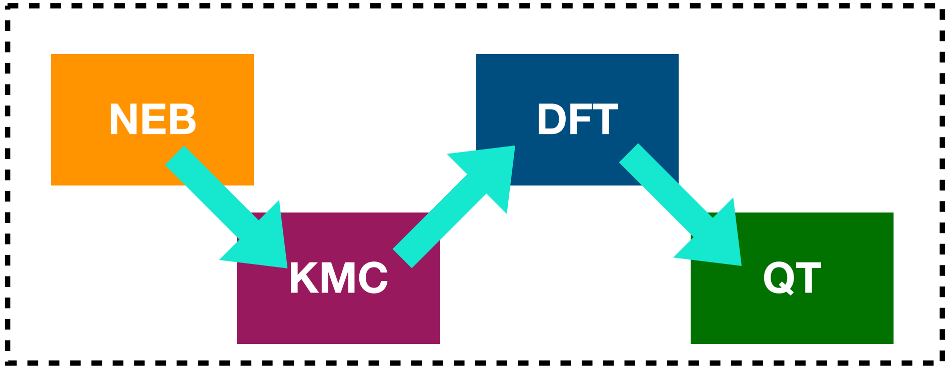
NEB

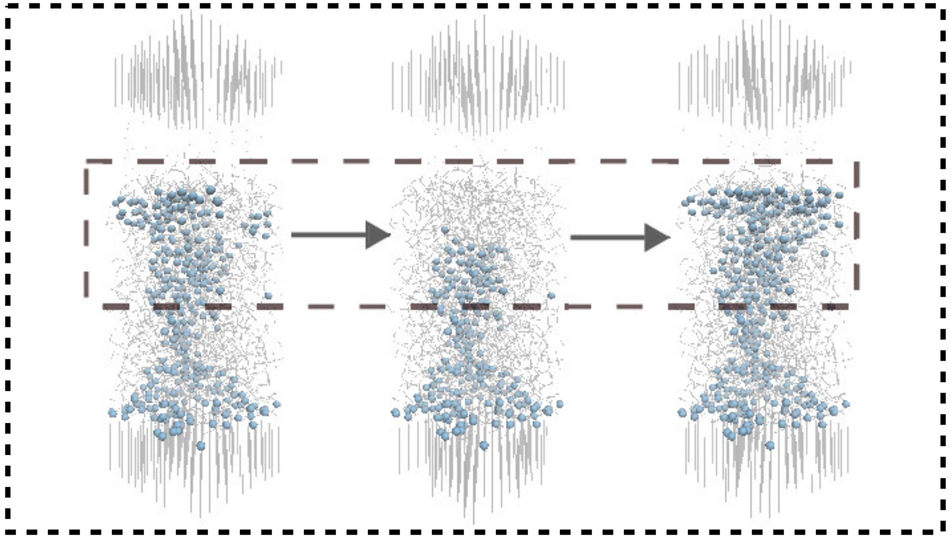
KMC

DFT

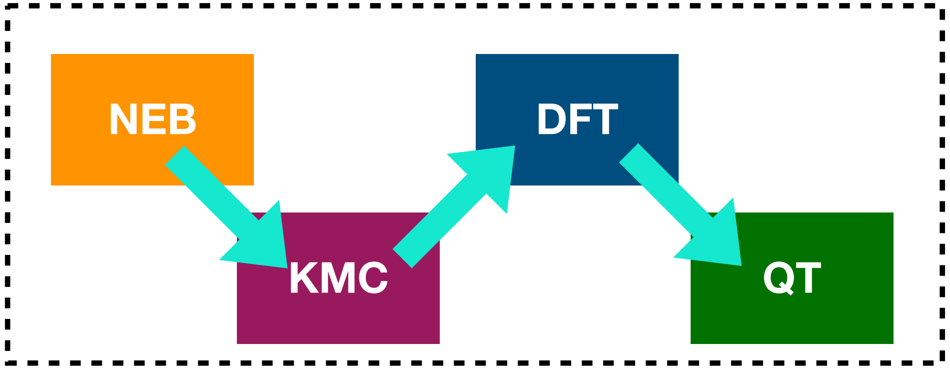
QT

Summary





Summary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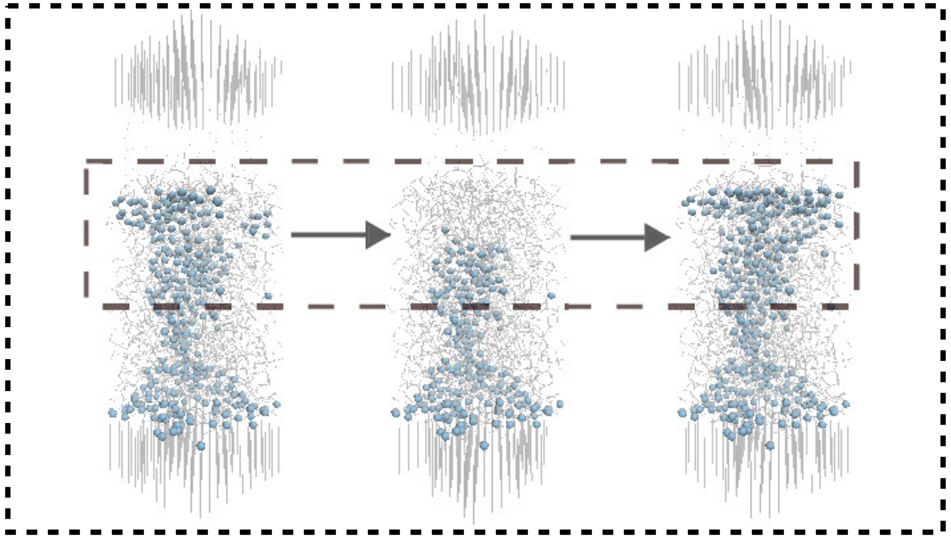

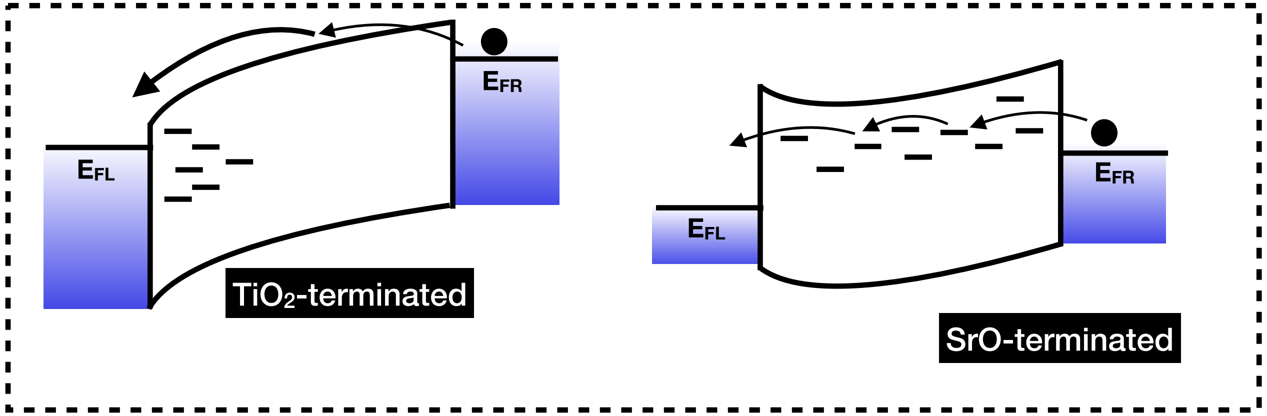

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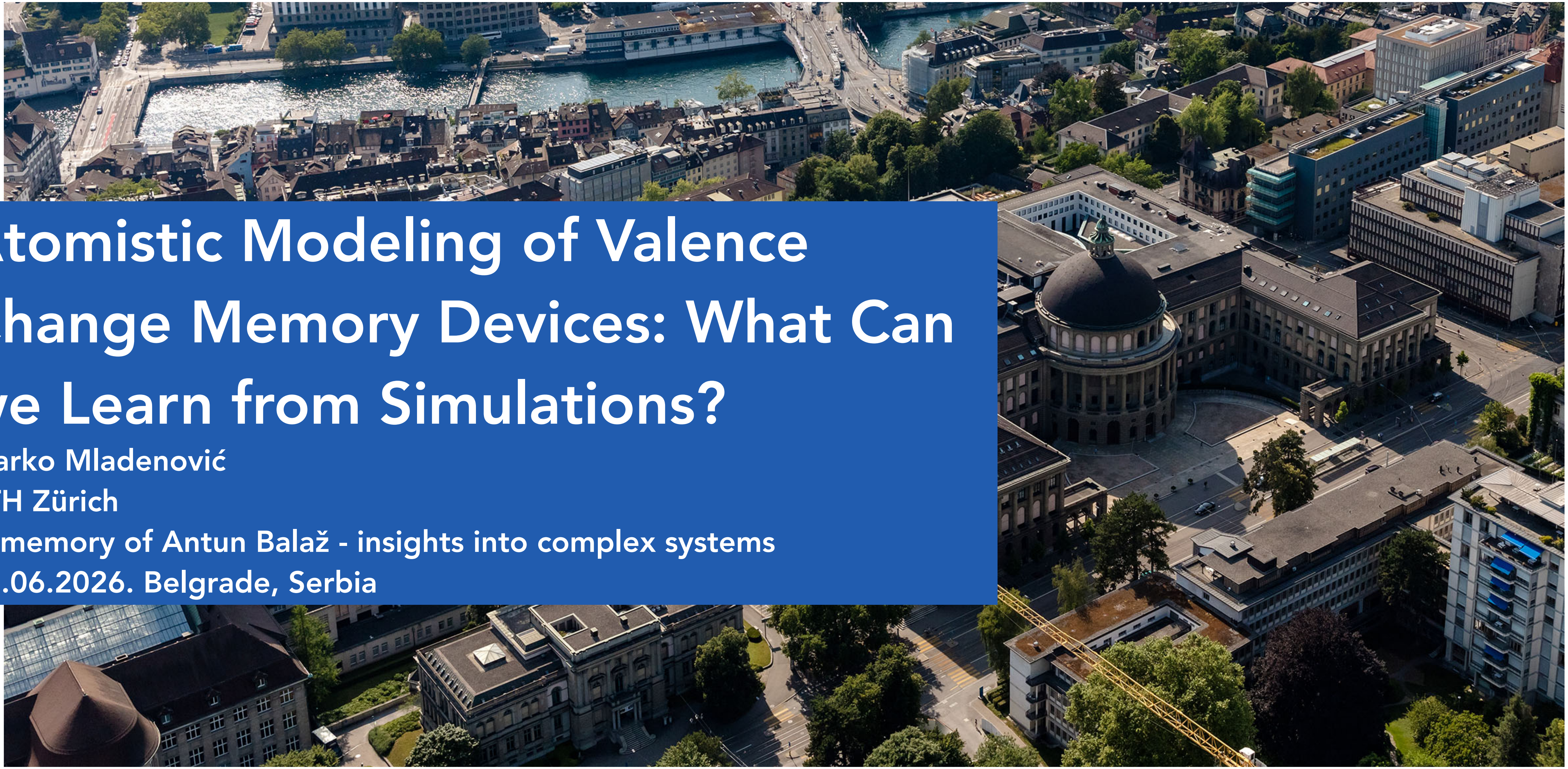

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Marko Mladenović
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In memory of Antun Balaž - insights into complex systems
12.06.2026. Belgrade, Serbia