ETH zürich

Bachelor / Master / Semester Thesis

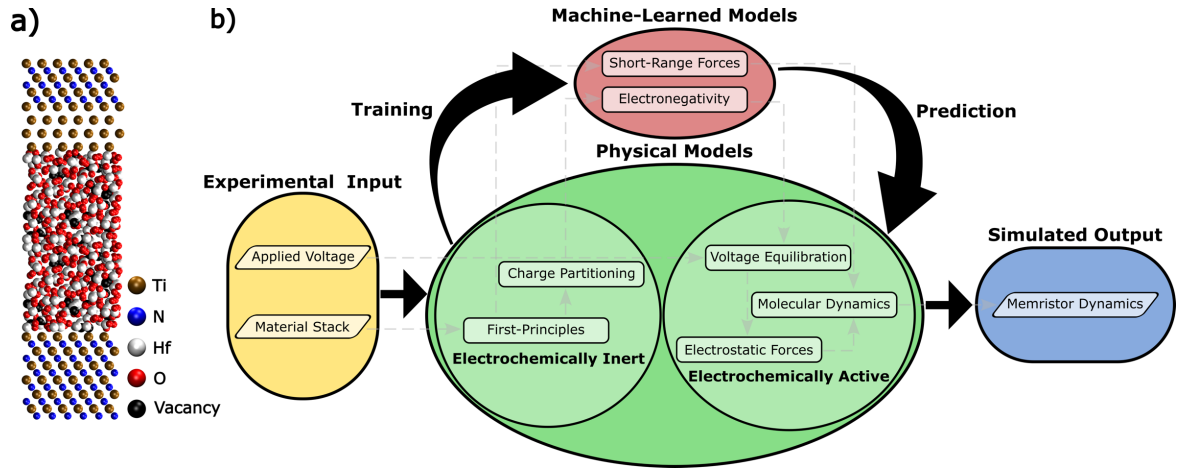
Algorithms for Machine-Learning Enhanced Simulation of Electrochemistry in Memristors

Short Description
We are looking for motivated students to develop and implement algorithms within a novel, machine-learning (ML) enhanced, atomistic simulation methodology for electrochemical phenomena in memristors. These algorithms include, but are not limited to: (1) calculation of the atomically-resolved electrostatic potential, (2) efficient integration of ML predictions with molecular dynamics (MD), or (3) high-throughput screening of material stacks.

The Big Picture
Memristors, an emerging class of electrical devices characterized by their tunable resistivity, show promise for future hardware applications, for example in brain-inspired computing. However, widespread adoption hinges on addressing key challenges, such as optimizing material stacks and mitigating noise. Atomistic modeling, powered by recent ML advances, efficiently addresses these issues while remaining independent of the chemical composition via training on first-principles calculations based on density functional theory (DFT). Despite this progress, certain memristors, like the TiN/Ti/HfO_2/TiN stack, involve the electrochemistry-driven motion of oxygen atoms and vacancies, which is beyond current ML capabilities. To address this, existing ML methods can be applied to enhance a physical modeling methodology, enabling the simulation of electrochemistry in memristors.

Type of Work
Computational Science and Engineering (algorithm development and implementation - 70%) & Machine Learning (data collection/model training – 30%)

Prerequisites
You have (1) an interest in nanoelectronics and/or solid-state physics, (2) basic experience with Python or C++ programming in a Linux environment. Previous experience with ML, memristors, DFT, or MD simulations is advantageous but not necessary.



a) Atomistic structure of TiN/Ti/HfO_2/TiN memristor. b) Workflow enabling the simulation of electrochemical processes in memristors.

Status: Available
Looking for 1-2 Bachelor/Master/Semester students
Interested candidates please contact: Dr. Luiz Felipe Aguinsky → laguinsky@iis.ee.ethz.ch
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Integrated Systems Laboratory (IIS)