AB-INITIO SIMULATIONS OF RERAMS: FROM ATOMS TO CURRENT VS. VOLTAGE CHARACTERISTICS

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The functionality of resistive random access memories (ReRAMs) often depends on the relocation of few atoms, e.g. metallic cations in conductive bridging RAMs or oxygen vacancies in valence change memory (VCM) cells. To accurately model the behaviour of these memristive nano-devices, it is therefore important to capture the interplay between atomic positions and electrical current trajectories. An *ab-initio* quantum transport approach is ideally suited for that purpose as it can take any structure that was created, for example, through molecular dynamics (MD) or kinetic Monte Carlo (KMC) simulations as input and compute the electrical current that flows through it. Quantum mechanical tunnelling, boundary resistances, and disorder are automatically accounted for, while complex phenomena such as heat dissipation via electron relaxations and phonon emissions can also be included, but typically at high computational cost.
In this presentation I will briefly introduce the simulation framework that we developed to model ReRAM-type memristors [1] and illustrate it with two applications, namely the switching of an atomic-scale CBRAM [2] and the influence of self-heating on these devices [3]. I will also present our vision on how to integrate such computationally intensive simulations into the design flow of future ReRAMs by combining modelling tools operating at different scales.

Keywords
ReRAM, *ab-initio* modelling, quantum transport, multi-scale approach.

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