From First Principles to Devices: Modeling Filamentary Switching in va-TMD Memristors

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Memristors are a new class of components that mimic the operation of nerve cells. They can be used to form neural networks that imitate the structure of the brain, enabling operations that are up to a hundred times more energy-efficient than current ones by circumventing the von Neumann architecture of traditional computers. This offers enormous potential for machine learning applications, enabling faster, smaller, and more environmentally friendly devices. This is especially relevant today, as already $\sim 20\%$ of the electricity consumed by data centers is taken by AI. Its ongoing rapid adoption and massive investments are expected to substantially increase global energy consumption in a world where still $\sim 80\%$ of energy is produced by burning fossil fuels. A commercially viable memristor has yet to be realized, and the search is therefore ongoing across different device types and operating mechanisms. Our research group investigates electrochemical metallization cell (ECM) type memristors based on filamentary resistance switching, with vertically grown transition metal dichalcogenides (va-TMDs) acting as the ion-conduction layer. The working principle is to form a metallic filament during device operation inside the ion-conducting layer, which significantly lowers the device resistance (by multiple orders of magnitude).Our research group not only fabricates these devices but also employs theoretical investigations to unveil the atomic-level operating mechanisms. The guiding principle in our theoretical inquiry is to begin from first principles at the atomic scale, distilling the most important physical properties and scaling them up in time and space.Using DFT, we have studied metallic defects in va-MoS_2 and translated their properties into macroscopically observable quantities such as diffusion constants and drift velocities [1]. This has yielded important insights to explain the experimental observations of volatile/non-volatile switching using different top metal electrodes in MoS_2 devices [2].A screening study of all vertically growable TMDs (MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2) and top electrodes (Ag, Cu) highlighted WS_2 with a Cu top electrode as an exceptionally promising ECM memristor candidate. This observation later led to the fabrication of the first va-WS_2 ECM device in the world. Experimental research on this new device is ongoing, and the results are promising. The theoretical part has yielded a research paper that is currently under review [3].Finally, further theoretical investigation of our most studied va-TMD memristor system, MoS_2 with a Cu top electrode, is underway. Fine-tuned machine-learning force fields (MLFFs) were used to search for and identify the most favorable Cu clustering structures in MoS_2 by enumerating and relaxing >13,000 cells. This led to the generation of a "dimer expansion" term to model Cu–Cu interactions. DFT was then used to verify these results and confirm the metallic nature of the Cu clusters. This information is now used to model the entirety of Cu filament formation in MoS_2 at device level of tens of nanometers, which could be considered the "holy grail" of the experimental side of the research project.

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