Modeling of switching and gate control in 2D memristive devices and memtransistors

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Memristive devices based on two-dimensional (2D) materials are emerging as potential candidates for next-generation neuromorphic computing hardware [1,2]. In particular, multi-terminal devices known as memtransistors combine nonvolatile memristive behavior with the volatile gate tunability of transistors, enabling desired features such as high linearity, adjustable learning rates, and ultra-low switching energies and voltages [3]. Building on these early achievements, further progress is expected through exploration of the vast 2D material space and development of a detailed understanding of the microscopic origins of memristive switching and gate tunability.

Here, we discuss the potential mechanisms contributing to memristive switching in memristive devices based on 2D materials focusing on lateral device structures. A finite volume model is presented to link atomistic defect dynamics to mesoscopic charge transport processes and macroscopic device behavior [4,5]. It is validated on lateral MoS_2-based memristive devices and memtransistors by reproducing experimental current-voltage characteristics, synaptic weight update curves, and temperature profiles under varying bias conditions. Based on simulations and experiments, we discuss memristive switching and gate tunability, including, e.g., the influence of Joule heating, trap states, and interface effects. The role of vacancy dynamics and grain boundaries is analyzed in detail by combining atomistic simulations [6] with the semiclassical transport approach, providing detailed physical insight into defect migration and switching mechanisms.

Finally, we discuss current limitations and the prospects of AI-driven model acceleration to support physics-guided investigations and device design in the future [6,7,8]. With an initial surrogate approach [8], tasks that require days to months with the full transport model, such as inverse parameter extraction, global sensitivity analysis, and multiobjective optimization, can be completed within seconds or minutes. This acceleration makes it possible to address complex iterative problems that are otherwise computationally prohibitive. The modeling framework provides a practical and physically motivated approach for the analysis and optimization of 2D memristive devices in neuromorphic applications.

Funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-Project-ID 434434223–SFB 1461, the Carl-Zeiss Foundation via the Project MemWerk, the Leibniz competition, and the German Academic Exchange Service (DAAD) is gratefully acknowledged, as well as by the National Science Foundation Neuroplane Program under award number NSF CCF-2106964 and the National Science Foundation EFRI BRAID Program under award number NSF EFMA-2317974.

[1] M.-K. Song, et al., *ACS Nano*, 17 (13), 11994–12039, 2023.
[2] A. Wali; et al., *Adv. Funct. Mater.*, 34 (15), 2308129, 2023.
[3] S. Hadke, et al., *Chem. Rev.,* 125 (2), 2025.
[4] B. Spetzler, et al., *Adv. Electron. Mater*., 10 (1), 2024.
[5] B. Spetzler, et al., *npj 2D Mater. Appl.*, 9 (1), 2025.
[6] A. Flötotto, et al., *Small*, e10679, 2026.
[7] B. Spetzler, et al., *APL Mach. Learn*., 3, 2025.
[8] B. Spetzler, et al., arXiv preprint arXiv:2505.13882, 2025