Contribution ID: **59** Type: **Poster Only**

Tuning the Memristive Behavior in Single-Crystal Transition Metal Dichalcogenides

Memristors based on two-dimensional transition metal dichalcogenides (TMDs) are emerging as key components for future memory and neuromorphic computing technologies. In single-crystal TMDs such as $MoSe_2$ and WSe_2, we attributed that memristive switching to an electrode-facilitated 1H to 1T′ phase transition, stabilized by defect binding [1]. Expanding on this, we present a data-driven framework for the rational design of TMD memristors through interface engineering. Using high-throughput calculations within the density functional theory (DFT) and utilizing machine learning regression models, we systematically investigate how different transition metal electrodes affect the stability of the 1T′ phase across a range of group-VI TMDs (MoS_2, WS_2, $MoSe_2$, WSe_2, $MoTe_2$). We analyze means to control phase stability such as the dielectric environment, electrode defect energetics, and TMD thickness. Our results reveal that electrodes from groups 10–12 (e.g., Cu, Ag, Zn) may improve the memristive performance of the TMDs, as they both decrease phase energy barriers and favor the 1T'phase upon absorption. Additionally, we find that due to the low energy difference between 1H and 1T'phases in $MoTe_2$, bilayer or thicker systems are required to achieve stable switching behavior. These structure-property relationships assist the selection of optimal electrode/TMD combinations and offer valuable design principles to guide experimental development of tunable, high-performance TMD-based memristors. This work is supported by NSF Grant No. 1848344 and is part of a user project at the CNMS.

[1] Kirk et al., ACS Appl. Mater. Interfaces, 17, 23, 34717 (2025).

Topical Area

Hard matter: quantum, electronic, semiconducting materials

Authors: KIRK, Dakotah (Auburn University); KURODA, Marcelo (Auburn University)

Presenter: KIRK, Dakotah (Auburn University)