Microscopic insights to resistive switching mechanisms in heterojunctions with monolayer materials

Wenne Wang

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have recently been shown to demonstrate non-volatile resistive switching (NVRS), offering significant advantages such as high-density integration and low energy consumption due to their atomic-scale thinness. Previous experimental work indicate that MoS2/Au-based vertical heterojunctions show I-V hysteresis. This finding indicates that these junctions have potential application in memory devices such as memristors and advanced neuromorphic logic circuits. Understanding the separate electronic, ionic, and coupled contributions in resistive switching mechanisms using first-principles methods is an overarching goal. In this workshop, I will discuss our on-going work in computational characterization of defects in 2D materials in the monolayer and at the interface, understanding materials trends relating to switching energy, and elucidating the impact of an applied electric field on interfacial transport.