Tuesday Evening, January 27, 2026

PCSI
Room Ballroom South - Session PCSI-TuE

Is AI a Bubble?
Moderator: Alping Chen, Los Alamos National Laboratory

7:00pm **PCSI-TuE-1 AI-Accelerated Discovery of Emergent Properties in 2D Materials and Moiré Superlattices***, Ting Cao,* University of Washington **INVITED**

Moiré superlattices formed in twisted and stacked 2D materials offer a powerful platform for engineering interfacial electronic and optical properties. Their vast supercells and complex reconstructions, however, challenge the limits of conventional first-principles methods. In this talk, I will present machine-learning assisted first-principles calculations that enable large-scale simulations of moiré structures, capable of handling twisted multilayer homo and heterostructures with varying composition, twist angles, stacking, and layer numbers.

Demonstrated on twisted MoTe2, our calculations capture topology-driven band transitions and provide a scalable solution for studying correlated moiré phenomena in complex environment, predicting emergent electronic features such as flatter Chern bands. The emergent moiré potentials and band structures in turn govern the behavior of excitons with unusually large dipole moments and tunable spatial profiles. By incorporating spin–lattice descriptors, the same machine-learning assisted framework reveals pathways to coupled excitonic and magnetic responses.

Our AI-accelerated strategy extends the predictive reach of first-principles theory, providing new insights into how twist angle, stacking order, and electric control can be used to design moiré materials with tailored optical, electronic, and spin functionalities**.**

7:40pm **PCSI-TuE-9 Full-Field Structural Microscopy Reveals Dynamic Film–Substrate Interactions in VO_2 Neuromorphic Devices***, Alex Frano,* University of California San Diego **INVITED**

Understanding how structural transitions govern neuromorphic functionality in quantum materials requires characterization tools that can probe local transformations in operando and across multiple length scales. We combine dark-field X-ray microscopy (DFXM) with complementary X-ray and electron microscopies to reveal the structural evolution of voltagedriven filaments in VO_2 memristive devices and their unexpected coupling to the underlying substrate. DFXM provides high-resolution, full-field, structure-selective imaging, enabling us to visualize rutile filament formation without destructive specimen preparation or slow rastering. We find [1] that rutile channels contain residual monoclinic clusters, revealing internal nonuniformity, and that rutile nucleation beneath electrodes precedes the Figure 1: A schematic of DFXM growth of conductive pathways. Additionally, imaging filamentary domains in a VO2 repeated voltage cycling induces a medium-term (<30 neuromorphic device. min) memory effect: specific sites in the device gap switch at lower voltages even after a brief thermal reset. Strikingly, we show [2] that these electronic/structural transformations in the VO_2 film are not mechanically isolated: filament formation generates strong, highly asymmetric strain fields that imprint deep into the Al_2O_3 substrate. This strain feeds back into the film, guiding subsequent filament expansion and redefining local switching dynamics. The observed film–substrate feedback mechanism expands the conventional view of epitaxial strain from a static constraint to an active, reconfigurable parameter during device operation. These results position DFXM as a powerful platform for operando studies of correlated oxides and point toward substrate engineering as an emerging route to control and functionalize neuromorphic architectures.

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