Physics-Informed Neural Networks as Fast Design AI Tool for Oxide Memristors

The semiconductor industry faces critical challenges in computational modeling that span nanometer to millimeter scales. Traditional finite-element methods struggle with multi-scale physics problems, particularly in oxide heterostructures where length scales span six orders of magnitude. This talk presents a novel Physics-Informed Neural Network (PINN) approach that achieves 100-1000x acceleration in semiconductor device modeling while maintaining physics-based accuracy critical for tape out decisions.

We demonstrate this methodology on Pt/$SrTiO_3$/Si memristors, where resistive switching arises from voltage-driven oxygen-vacancy drift-diffusion that modulates Schottky-barrier heights. Our cascaded four-stage PINN architecture decomposes the coupled drift-diffusion problem into sequential sub-networks for vacancy concentration, electrostatic potential, carrier densities, and device current. By operating in log-space and employing a custom RELCH V2 optimizer with Chebyshev polynomial acceleration, we overcome the extreme ill-conditioning (condition numbers ~10^{16}) that causes Newton-Raphson failures in conventional solvers.

Our approach delivers four key innovations: (1) differentiable end-to-end training enabling automatic extraction of physical parameters like ideality factors and series resistance; (2) continuous spatiotemporal representation avoiding mesh discretization; (3) hysteresis modeling as a learned latent variable capturing progressive vacancy redistribution; and (4) inference speedups from 25 minutes to 0.3 milliseconds per I-V curve. Experimental validation against conducting-AFM measurements on epitaxial $SrTiO_3$ films demonstrates that PINNs can serve as trustworthy surrogates for multi-physics materials modeling. This work opens pathways for AI-accelerated materials discovery, real-time device optimization, and integration of experimental test data with physics-based simulations—addressing the long tail of scientific problems not served by commercial AI.