

# **Engineering Non-Volatile Memory Materials: From Defect Discovery to Device Optimization**

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The rapid evolution of artificial intelligence and data-centric applications is driving unprecedented demands on semiconductor memory technologies. Emerging non-volatile memories such as Resistive RAM (RRAM), Ferroelectric RAM (FeRAM), and Phase-Change Memory (PCM) offer promising alternatives to conventional memory architectures, but their development hinges on deep material understanding and precise engineering.

We will provide a comprehensive overview of how atomic-scale simulations and advanced characterization techniques are revolutionizing material engineering for next-generation memory devices. We explore the critical role of defect spectroscopy in correlating electrical behavior with material properties, enabling sub-nanometer resolution insights into defect distributions and their impact on device performance and reliability.

For RRAM, we detail the forming, set, and reset operations, emphasizing the influence of oxygen vacancy dynamics and conductive filament evolution. In FeRAM, we discuss the interplay between ferroelectric switching, defect trapping, and endurance limitations, supported by calibrated atomistic models. PCM development is addressed through phase-field and kinetic Monte Carlo simulations that capture phase segregation and crystallization dynamics under electrical stress.

By integrating multi-scale Ginestra™ modeling with experimental validation, this work demonstrates how we can accelerate R&D, optimizes process-device co-design, and enhances reliability forecasting. The talk underscores the necessity of simulation-driven approaches to meet the stringent requirements of future memory technologies in the AI era.