

## **ACSESS 2026 - Keynote Speaker**

**Title:** Engineering Nanostructured Materials for Novel Quantum Functionality: Research Stories Bridging Experiment, Theory, and AI

### **Abstract:**

The most transformative discoveries in quantum materials rarely emerge from a single discipline working in isolation. Instead, they arise from a virtuous cycle where experimental observation demands theoretical interpretation, and theory in turn inspires new experimental directions. Together they generate deeper understanding than either could achieve alone. This cycle, long practiced in the physical sciences, is now entering a new era as artificial intelligence offers powerful tools to augment and accelerate each of its stages.

In this keynote, Dr. Archana Raja will share research stories from her team's work on multimodal photon- and electron-based characterization techniques, illustrating how the interplay between experiment and computation has driven discovery in nanostructured quantum materials. From optical spectroscopy and microscopy to ultrafast electron diffraction and electron energy loss spectroscopy, these complementary probes illuminate the rich physics emerging at the atomically sharp interfaces of two-dimensional (2D) semiconductors. By capturing how electrons and other quasiparticles behave in these systems, they reveal new pathways for manipulating energy, charge, and information from the atomic scale to the application scale. These pathways can be tailored by design in 2D heterostructures, that are built by stacking different van der Waals crystals whose weak interlayer forces impose none of the constraints of conventional epitaxy. The resulting datasets are rich and complex, demanding sophisticated theoretical frameworks for meaningful interpretation, while theory simultaneously opens new experimental frontiers to explore.

In the second part of her talk, Dr. Raja will introduce LEAP: Low-Energy, AI-Informed Phase Transitions — a recently awarded University of California AI Science at Scale initiative on which she is a co-investigator. LEAP brings together theory, experiment, and simulation to train specialized large language models that can accelerate the discovery of topological materials with unconventional electron behavior, targeting the next generation of energy-efficient chip design. She will then discuss how the team is extending this virtuous cycle into the age of AI, including the development of benchmarks that rigorously evaluate AI research agents on real experimental data, a gap that existing benchmarks have yet to address. These efforts are laying the groundwork for agentic research assistants that support scientific workflows end to end, and context-aware AI tools that make complex domain knowledge more accessible and queryable.

This keynote will offer ACSESS students and researchers a compelling vision of how interdisciplinary collaboration spanning experiments, theory, and artificial intelligence is reshaping the frontier of quantum materials science, and how the next generation of scientists can find their place within it.

Key topics will include:

- How multimodal photon- and electron-based characterization techniques reveal quantum behavior in nanostructured 2D materials and heterostructures
- The virtuous cycle of experiment and theory as a model for interdisciplinary collaboration
- Benchmarking AI agents on authentic experimental data and closing the gap between domain knowledge and real-world research workflows
- How autonomous agentic tools and context-aware AI will redefine the PhD experience for the next generation of scientists across the physical sciences, placing powerful new research capabilities directly in their hands



Bio: Dr. Archana Raja is a Staff Scientist in the Imaging and Manipulation of Nanostructures Facility at the Molecular Foundry, and a faculty member at the Kavli Energy NanoScience Institute, Lawrence Berkeley National Laboratory. Her research focuses on how energy, charge, and information can be manipulated in nanoscale quantum materials and their heterostructures for device functionality. Using multimodal photon- and electron-based characterization techniques, she bridges fundamental understanding of optoelectronic phenomena from the application scale to the atomic scale. She is the recipient of the Berkeley Lab Director's Award for Exceptional Early Scientific Career Achievement, the Kavli ENSI Heising-Simons Junior Fellowship, the Blanche R. and David Kasindorf Fellowship in Physical Chemistry at Columbia University, and the Institute Silver Medal at the Indian Institute of Technology Bombay.