PHYSICS COLLOQUIUM:

Atomistic Simulations of Matter Under Extreme Conditions

Dr. Margaret Berrens

Staff Scientist in the Materials Science Division
Lawrence Livermore National Laboratory

Date:
10/23/2026

Time:
10:30 AM – 11:50 AM

Location:
SSB 130

About The Speaker:

Maggie Berrens is a staff scientist at Lawrence Livermore National Laboratory in the Quantum Simulations Group in the Materials Science Division. She earned her Ph.D. in Physical Chemistry from the University of California, Davis, under the guidance of Prof. Davide Donadio, where her work centered on machine learning-enhanced atomistic simulations to investigate the fundamental properties of water and ice, particularly in the context of solvation and environmental chemical processes. In 2024 she joined LLNL as a postdoctoral scholar in the Quantum Simulations Group within the Physics Division. Her current research applies a range of atomistic simulation techniques to study matter under extreme conditions, with an emphasis on understanding structural and dynamical behavior in confined systems, as well as transport in high energy density environments.

Abstract:

Matter under extreme conditions exhibits unusual structural and transport behavior relevant to technologies ranging from selective membranes to fusion energy. However, accurately simulating these systems is challenging because quantum-mechanical methods are often limited to length and time scales much smaller than those probed experimentally. In this talk, I will discuss how machine-learning-accelerated atomistic simulations help overcome this limitation through two examples: water under extreme spatial confinement and matter under extreme temperatures and pressures.First, I will focus on water confined within subnanometer carbon nanotubes, where interactions with channel walls strongly influence molecular transport. Our simulations reveal how defect-induced chemical functionalization at nanotube openings produces experimentally observed pH-responsive gating. They also show how nanoscale confinement amplifies nuclear quantum effects and how the rate-limiting step in proton transport governs hydrogen-isotope selectivity. I will then turn to warm dense matter, an intermediate regime between condensed matter and plasma that occurs in planetary interiors, fusion experiments, and stellar environments. Using spectral-partitioned density functional theory and machine-learning accelerated molecular dynamics, we efficiently simulate warm dense D_2O while retaining Kohn-Sham-level accuracy. These simulations enable direct evaluation of equation-of-state and transport models used in high-energy-density physics and white dwarf evolution. Together, this work demonstrates how atomistic simulations can uncover molecular mechanisms and improve predictive models across extremes ranging from subnanometer confinement to the temperatures and pressures found in stars.

For more information contact: Aurora Pribram-Jones
apj@ucmerced.edu