PURDUE UNIVERSITY | School of Nuclear Engineering

Nuclear Engineering Seminar

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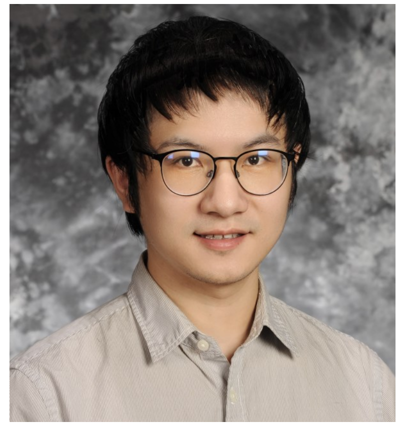

Wednesday, February 18, 2026

3:30 pm | PHYS 114

Thermal Transport in Nuclear Materials: Bridging Atomic-Scale Insights to Engineering Models

Abstract

Understanding thermal transport in nuclear materials is central to predicting fuel performance and ensuring reactor safety. Experimental measurements of thermal transport are often difficult and costly, particularly under irradiation or extreme operating conditions, making computational approaches an efficient alternative. Here, a multiscale modeling strategy is presented that connects atomic-scale transport information to predictive engineering-scale simulations. Obtaining reliable atomistic data for nuclear fuel materials, especially actinide compounds, remains challenging due to strong 5f-electron correlations; these challenges are addressed using advanced first-principles techniques, as demonstrated by accurate modeling of finite-temperature thermal conductivity in uranium dioxide. At the mesoscale, the predictive capability of molecular dynamics simulations depends critically on the quality of interatomic interactions. Improved interatomic potentials trained on irreducible derivatives from first-principles are developed to enable phonon-sensitive simulations with thermophysical fidelity. Finally, atomic-scale transport information is incorporated into engineering-scale frameworks through spatial Boltzmann transport methods, enabling physics-informed thermal property predictions across scales.

Dr. Shuxiang Zhou is a computational materials scientist in the Computational Mechanics and Materials Department at Idaho National Laboratory. He received his Ph.D. in Materials Science and Engineering from the University of Wisconsin–Madison and his Bachelor's degree in Physics from Peking University, China.

Dr. Zhou's research focuses on ab initio computational methods and multiscale simulations to understand and predict the behavior of nuclear materials. His interests include thermal transport, phonon scattering, electron correlation, and irradiation effects, with an emphasis on linking atomic-scale methods to mesoscale and engineering-scale modeling through physics-informed and data-driven approaches.