

# DEPARTMENT OF MECHANICAL ENGINEERING

## WILLIAM MAXWELL REED SEMINAR SERIES

### “Pushing the Frontiers of Energy Transport by Predictive Simulations”

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**Abstract:** Energy transport is a key issue in many emerging applications such as the thermal insulation for buildings, thermal management of electronic devices, thermal protections in hypersonic vehicles, nuclear materials, and thermoelectric energy harvesting. Often these applications have been pushing extreme thermal performance of materials to an unprecedented level. Predictive simulation methods of thermal transport in various systems, temperature ranges, and scales can provide valuable guidance of the design and characterizations of materials and structures, to fulfil these extreme requirements. In this talk, I will demonstrate the advances we have made towards this goal, by showing how we have developed fully predictive atomistic simulation methods and used them to guide materials development and understanding. The talk consists of three parts. The first part will establish multiple-heat-carrier scattering, specifically, four-phonon scattering, as an important intrinsic heat carrier scattering mechanism. For half a century, four-phonon scattering had been persistently unclear and hence ignored. However, we have developed a rigorous first-principles perturbation method to predict four-phonon scattering rates and found its broad impact on the thermal transport in general solids. Our four-phonon scattering theory in BAs has recently been confirmed by experimental breakthroughs of achieving 1,300 W/m-K thermal conductivity in boron arsenide. I will also demonstrate that this predictive method has promising applications in thermal barrier coatings, power electronics, hypersonic vehicles, nuclear reactor materials, and radiative cooling. In the second part, I will discuss the developments of novel phonon spectroscopy based on molecular dynamics simulations to resolve mode-level phonon transport. These methods can guide the multi-scale engineering of thermal transport in various systems, and they are expected to pave the foundation for future phonon technologies revolution, analogous to the photon technologies revolution we have experienced in the past century. In the third part, I will briefly talk about our most recent advances in the development of predictive models for thermal engineering by using machine learning and experimental methods.

**Bio:** Dr. Tianli Feng is a postdoctoral fellow at Oak Ridge National Laboratory. He received his M.S. and Ph.D. degrees from the School of Mechanical Engineering at Purdue University in 2013 and 2017, respectively. Before that, he received a B.S. in Physics at the University of Science and Technology of China in 2011. His research is focused on the engineering of thermal energy transport by predictive multi-scale multi-physics simulations for various emerging applications.

**Date:** Thursday, Mar. 12<sup>th</sup>

**Place:** CB 122

**Time:** 3:00PM

**Contact:** Dr. Alexandre Martin 257-4462

Meet the speaker and have refreshments  
Attendance open to all interested persons