Department of
Mechanical Engineering
The University of Hong Kong

DEPARTMENT OF
MECHANICAL ENGINEERING
THE UNIVERSITY OF HONG KONG

SEMINAR

Physics-Informed Graph Nerual Networks for Accelerated Prediction of Multi-Phonon Scattering and Lattice Thermal Conductivity

Date: 25 April, 2025 (Friday)
Time: 3:00 p.m.
Venue: Online via Zoom

Speaker: Mr. Zhiqiang Cui (PhD candidate)
Department of Mechanical Engineering
The University of Hong Kong

Join Zoom Meeting:
https://hku.zoom.us/j/91716106753?pwd=ZkIha9FsSqNWZeQc82fcoB5YAjNR2G.1

Meeting ID: 917 1610 6753
Password: 452773

Abstract:

Accurate prediction of lattice thermal conductivity (κ_L) through first-principles calculations of multi-phonon scattering processes remains computationally intensive. While machine learning approaches offer promising alternatives, conventional methods often fail to capture the intricate topological relationships in phonon interactions by reducing them to simple concatenated features. Here, we present a physics-informed graph neural network (GNN) framework that naturally encodes phonon scattering processes as directed graphs, where nodes represent phonon modes and edges capture interaction dynamics. Our model incorporates fundamental physical constraints by embedding momentum conservation, eigenvector projections, and energy conservation into graph-structured features. The architecture employs attention mechanisms to identify dominant scattering channels and utilizes residual connections to bridge local phonon properties with global conservation laws.Validated across diverse materials including Si, MgO, and $LiCoO_2$, our GNN demonstrates superior accuracy in predicting phonon scattering rates compared to conventional deep neural networks, while requiring 80% less training data. The model maintains κ_L prediction errors below 3% relative to first-principles calculations. Furthermore, we demonstrate effective transfer learning capabilities between different materials and phonon scattering orders, enhancing model generalizability. This physics-informed graph representation accelerates thermal conductivity calculations through accurate prediction of multi-phonon scattering rates, while providing a promising blueprint for developing generalizable models for phonon scattering rate prediction.

ALL INTERESTED ARE WELCOME
For further information, please contact Prof. Y. Chen at 3917 7095.