

**DEPARTMENT OF MECHANICAL ENGINEERING****SEMINAR****Online**

**Title:** A Simulation Study of Defect Engineering on the Lattice Thermal Conductivity of Thermoelectric Materials

**Speaker:** Mr. Cheng Ruihuan (PhD candidate)  
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**Date:** 28 April, 2022 (Thursday)

**Time:** 2:30 p.m. (Hong Kong Time)

**Zoom meeting:** 1) Link to join the meeting:

<https://hku.zoom.us/j/96252281952?pwd=dXpCQUlxdVNWVkxaZXU2dkZUNTZoUT09>

2) Meeting ID: 962 5228 1952

3) Password: 915298

**Abstract:**

Reducing the lattice thermal conductivity ( $\kappa_L$ ) is one of the effective means to improve the figure of merit (ZT) of thermoelectric materials. Defect engineering, including point defects (0D), dislocations (1D), interfaces (2D), inclusions, and pores (3D) in terms of dimensions, gives the avenue to achieve this intervention strategy by introducing additional phonon scattering. In this seminar, brief concepts of phonon scattering mechanisms of different defects based on the Debye–Callaway model are first summarized.

To further reveal the phonon scattering mechanisms from a microscopic perspective, we perform large scale molecular dynamic simulations, based on machine learning potential and GPU-acceleration. Preliminary results of thermal transport in PbSe-doped PbTe will be discussed.

**ALL INTERESTED ARE WELCOME**

For further information, please contact Dr. Y. Chen at 3917 7095.

**Research area: Advanced Materials**