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Thermal Conductivity of Complex Crystals and Van der Waals Layered Materials

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ABSTRACT:

Thermal conductivity is a critical property for thermal management of devices and a key parameter for designing functional materials, especially for thermoelectrics and thermal barrier coatings. The nanoscale heat transfer community has developed first-principles methods for predicting and experimental methods for characterizing thermal conductivity of a wide range of materials. However, mostly simple and isotropic crystals are investigated at or below room temperature. This is because the first-principles calculation is limited to simple crystals at ground state and most experimental methods are only capable of measuring thermal conductivity along a single direction. In this talk, I will address these challenges in modeling and characterizing thermal conductivities. On the modeling side, an integrated density functional theory and molecular dynamics method is developed to model the thermal conductivity and phonon properties of hybrid organic-inorganic crystals, a special kind of complex crystals integrating both organic molecules and inorganic frameworks. Further, I will show that machine learning could be a promising tool for developing high-fidelity potential to investigate phonon and thermal properties at high temperatures. On the experimental side, I will develop an ultrafast laser based pump-probe thermoreflectance technique for characterizing anisotropic thermal transport by varying laser spot size and heating frequency. In addition, we discovered new phonon transport physics beyond local equilibrium regime under transient heating, which could be essential for electronic devices operating at high frequencies.

BIOGRAPHY:

Xin Qian is currently a postdoctoral associate in the mechanical engineering department at Massachusetts Institute of Technology (MIT). He receives his PhD in mechanical engineering at University of Colorado Boulder (CU Boulder) in May 2019, supervised by Prof. Ronggui Yang. His doctoral research focused on ab-initio modeling and ultrafast laser based characterization of thermal conductivity in complex crystals and anisotropic materials including wide bandgap semiconductors and layered van der Waals materials. His PhD thesis received the Outstanding Dissertation Award of the College of Engineering and Applied Science and the Woodward Outstanding Dissertation Award of the Mechanical Engineering Department at CU Boulder. Following this, Xin joined the nanoengineering group at MIT supervised by Prof. Gang Chen. His postdoctoral research focused on developing thermally regenerative flow battery systems for refrigeration and harvesting low-grade heat.