Thermal transport in crystals and glasses

Improving our ability to manipulate thermal energy or heat is key to enhancing the performance of a wide range of technologies, from tiny integrated circuits to giant spacecraft and power plants. For example, better thermoelectric materials that block thermal energy more effectively could help recover some of the wasted heat dumped into the environment. Predictive modeling methods can play an important role in the design and prediction of novel materials for thermal management applications. Recently, first-principles computational methods have been developed to calculate vibrational thermal transport in infinite defect-free crystals by solving linearized Boltzmann transport equation for the phonon populations. Within this project the student will focus on exploring thermal transport in strongly anharmonic materials. A prior knowledge of quantum mechanics and condensed matter physics, along with basic knowledge of python is recommended.