A major challenge facing the world today involves exploiting clean, abundant energy sources, and reducing our overall consumption. A significant untapped energy source is waste heat, accounting for ~60% of the energy humans produce. Thermoelectrics are materials that can convert heat into useful electrical power, and hence have the potential to impact our energy future. The goal is to increase the thermoelectric conversion efficiency for this technology to become widespread, which requires exploring and discovering new materials with enhanced electronic and thermal (phonon) transport properties.

In this talk, I will give a brief overview of thermoelectrics, and present our recent efforts towards predictive theoretical modeling of electro-thermal transport. Our approach, based on first-principles, provides new insights into the scattering and transport physics as I will illustrate with two examples (time permitting): electron transport in quasi-2D GeTe, and thermal transport across a Si/Ge interface. This research will help accelerate experimental discovery by evaluating and optimizing the performance of materials before they are made.