Origin of thermal conductivity changes in strained systems

The effects of strain on thermal transport are well-known from a macroscopic perspective but the nanoscopic origins are unknown. In semiconductors and insulators, thermal transport is dominated by phonons, which are vibrations of the atomic lattice. From a solution of the phonon Boltzmann transport equation obtained using the Fourier law, the contribution of a phonon to thermal conductivity is the related to its heat capacity, group velocity, and lifetime. What combination of changes to these properties is responsible for strain-related changes in thermal properties is unknown.

In this study, we use the Green-Kubo method in molecular dynamics simulayions to first predict the strain-dependence of the thermal conductivity of Lennard-Jones (LJ) argon between temperatures of 20 and 80 K. Simultaneously to this top-down approach, we apply the bottom-up technique of normal mode decomposition which, through a combination of lattice dynamics calculations and molecular dynamics simulations, predicts the values of the individual properties of each phonon mode in the system. These properties can then be used to predict thermal conductivity from the bottom-up, allowing us to elucidate the mechanisms responsible for the thermal conductivity change.