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Electron-phonon coupling and thermal transport in thermoelectric compound $Mo_3Sb_{7-x}Te_x$ DIPANSHU BANSAL, CHEN LI, Oak Ridge National Lab, AYMAN SAID, Argonne National Lab, DOUGLAS ABERNATHY, JIAQIANG YAN, OLIVIER DELAIRE, Oak Ridge National Lab — Complex interactions between solid-state excitations, such as phonon-phonon, phonon-electron, and phonon-magnon couplings are often responsible for unusual material properties. In this presentation, we report on our investigations of phonon propagation and thermal transport in thermoelectric $Mo_3Sb_{7-x}Te_x$. We have performed extensive inelastic neutron and x-ray scattering measurements of phonons in $Mo_3Sb_{7-x}Te_x$, mapping the phonon dispersions and density of states, as function of temperature and composition. Our first-principles density functional theory simulations, coupled with experimental measurements, reveal the importance of electron-phonon coupling, which dominates the scattering rates over alloy disorder scattering. Doping with Te shifts the Fermi surface near the top of the valence band, suppressing screening and causing phonons to stiffen markedly. Our measurements of acoustic dispersions and linewidths, coupled with DFT simulations and models of phonon scattering enable us to quantify the impact of the electron-phonon coupling on the thermal conductivity.

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