Phonons Near Lattice Instabilities in Thermoelectric SnSe, SnTe, and PbTe

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— A number of high-performance thermoelectric materials are found in the vicinity of lattice instabilities, including PbTe, SnTe, SnSe, tetrahedrites, Cu₂Se, among others. The large phonon anharmonicity found in such compounds suppresses the lattice thermal conductivity, a key aspect of their thermoelectric efficiency. In this presentation, we will discuss results from our recent investigations of phonons in these materials using inelastic neutron scattering and first-principles simulations, focusing on anharmonic effects near lattice instabilities. Commonalities will be highlighted, including connections between strong anharmonicity and the electronic structure and bonding.