First-principles investigations of phonon anharmonicity and electronic instability in thermoelectric SnSe

JIAWANG HONG, CHEN W. LI, A. F. MAY, D. BANSAL, S. CHI, T. HONG, G. EHLERS, OLIVIER DELAIRE, Oak Ridge National Laboratory — The promising thermoelectric material SnSe exhibits ultra-low and strongly anisotropic thermal conductivity. By combining first-principles calculations and inelastic neutron scattering measurements, we have investigated the phonon dispersions and phonon scattering mechanisms, and probed the origin of the large anharmonicity in SnSe. We will discuss the connection between the phonon properties and the high-temperature structural phase transition, and how the electronic structure leads to large anharmonic phonon interactions in SnSe. The present results provide a microscopic picture connecting electronic structure and phonon anharmonicity in SnSe, which could help design materials with ultralow thermal conductivity.

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