Abstract Submitted
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First-principles investigations of phonon anharmonicity and electronic instability in thermoelectric SnSe[1] 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.[2] 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.

[1]Computations were performed using the OLCF at ORNL. Modeling of neutron data was performed in CAMM, measurements were funded by the US DOE, BES, Materials Science and Engineering Division.
[2]C.W. Li*, J. Hong*, A.F. May, D. Bansal, S. Chi, T. Hong, G. Ehlers, and O. Delaire, Orbitally driven giant phonon anharmonicity in SnSe, Nature Physics, (2015)

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