

Mechanism for the Soft-mode driven lattice instability in SnSe

Mariano Trigo^{1,2}, David Reis^{1,3}, Samuel Teitelbaum^{1,3}, Yijing Huang^{1,3}, Gilberto De la Pena⁵, Olivier Delaire⁴, Jennifer L. Niedziela⁴, Bansal Dipanshu⁴

¹ PULSE Institute, SLAC National Accelerator Laboratory, CA

²Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, CA

³Department of Applied Physics, Stanford University, CA

⁴Materials Science and Technology Division Oak Ridge National Laboratory, Oak Ridge, Tennessee

⁵Department of Physics, University of Illinois Urbana Champaign, Urbana, IL

SnSe holds the current record for the thermoelectric conversion efficiency, largely due to its high phonon anharmonicity. Recent work showed the contribution of electronic structure to phonon anharmonicity in SnSe based on DFT calculation. Using FT-IXS technique at LCLS, which photoexcites SnSe electronic states and probe the lattice dynamics with X ray, we were able to trace the nonequilibrium lattice dynamics right after photodoping. This provided more insight on how the valence electronic states got involved with phonon softening and anharmonicity.