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**Anharmonic phonon dynamics in superionic conductor $CuCrSe_2$**
JENNIFER NIEDZIELA, DIPANSHU BANSAL, ANDREW MAY, Oak Ridge National Laboratory - Materials Science and Technology Division, GEORG EHLERS, DOUGLAS ABERNATHY, Oak Ridge National Laboratory - Quantum Condensed Matter Division, AYMAN SAID, Argonne National Laboratory - Advanced Light Source, OLIVIER DELAIRE, Duke University Department of Mechanical Engineering and Materials Science Oak Ridge National Laboratory Materials Science and Technology Division — Efficient mechanisms to reduce thermal conductivity are critical in the search for new thermoelectric materials for energy applications. Here we investigate in detail the lattice dynamics of $CuCrSe_2$, a candidate thermoelectric material. $CuCrSe_2$ undergoes a superionic transition at 463 K, and exhibits extremely low lattice thermal conductivity. Using neutron and x-ray spectroscopy combined with first principles calculations, we show that the ultralow thermal conductivity arises from strongly anharmonic Cu vibrations, which broaden dramatically on heating and increase the scattering of heat carrying acoustic phonons. We find that these modes broaden at temperatures much below the superionic transition, signaling a dynamic precursor before the Cu sublattice melting at the superionic transition. The strongest anharmonic effects are confined to the quasi two dimensional lattice of copper ions, and the dynamics of the surrounding structure remain relatively intact, validating the physical picture of a part-liquid/part-solid system.

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