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Giant phonon anharmonicity and thermal resistance from topological dispersion nesting in CuCl. SAIKAT MUKHOPADHYAY, DIPANSHU BANSAL, Oak Ridge National Laboratory , OLIVIER DELAIRE, Duke University, DIDIER PERRODIN, EDITH BOURRET-COURCHESNE, Lawrence Berkeley National Laboratory, DAVID SINGH , University of Missouri, LUCAS LINDSAY, Oak Ridge National Laboratory — We report the phonon properties of zincblende CuCl, a very simple system with surprisingly rich anharmonic phonon physics, combining first principles calculations with inelastic neutron scattering measurements. We find a new quasiparticle peak in the phonon density of states emerging with increasing temperature. This peak arises from nesting of numerous off-resonance modes with highly asymmetric line shapes providing large phase space for both coalescence and decay processes involving longitudinal acoustic, transverse acoustic and transverse optic modes throughout the Brillouin zone. We further correlate this strong anharmonicity in CuCl to its non-monotonic pressure dependent thermal conductivity behavior via a balance of increasing group velocities and scattering rates of longitudinal acoustic modes, challenging the existing theory.

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