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A Robust Approach to Lattice Thermal Conductivity WESTON NIELSON, Univ of California - Los Angeles, FEI ZHOU TEAM, YI XIA TEAM, VIDVUDS OZOLINS TEAM — Thermal conductivity is a key parameter in designing high performance thermoelectric materials. A multitude of computational methods have been developed to calculate lattice thermal conductivity. Molecular dynamics (MD) based techniques, including equilibrium and non-equilibrium methods, in addition to non MD-based solutions, such as the Boltzmann Transport Equation (BTE), are all capable of calculating thermal conductivity, but each comes with different sets of limitations and difficulties. After extensive use of these different methods, we have developed a robust set of tools for obtaining high-quality lattice thermal conductivity values of crystalline solids. The crux of our method involves a novel compressive sensing (CS) based approach for efficiently calculating high quality force constants for crystalline materials. The result is a technique for building lattice dynamical models that can treat compounds with large, complex unit cells and strong anharmonicity, including those with harmonically unstable phonon modes.

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