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Calculating Lattice Thermal Conductivity via Compressive Sensing Lattice Dynamics WESTON NIELSON, University of California Los Angeles, FEI ZHOU COLLABORATION, VIDVUDS OZOLINS COLLABORATION — Calculating the lattice contribution to thermal conductivity (TC) is of great importance in a range of materials applications, including thermoelectrics. Common simulation-based methods for calculating the TC typically require either very long simulation times, large system size, or both. These constraints make it difficult or impractical to use DFT-based methods for calculating the TC. Classical molecular dynamics (MD), however, is typically unburdened by these constraints but is instead limited by the accuracy of the interatomic potentials. We have developed a method that uses DTF, combined with compressive sensing, to calculate the higher-order force constants from the theory of lattice dynamics. These force constants are then used to calculate interatomic potentials in a classical MD program. We present our findings from applying this method to a variety of materials.

Weston Nielson
University of California Los Angeles

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