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Compressed sensing approach for calculating lattice thermal conductivity of complex thermoelectric compounds VIDVUDS OZOLINS, YI XIA, WESTON NIELSON, Dept of Materials Science and Engineering, University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory
— Earth-abundant minerals such as tetrahedrite $Cu_{12}Sb_4S_{13}$ have recently received attention as promising thermoelectrics due to a combination of a relatively high figure of merit ($ZT > 1$ at $T = 700$ K in tetrahedrite), good mechanical properties and inexpensive bulk processing methods. Like many large unit-cell thermoelectrics, these compounds often have complex chemical formulas with very large unit cells that pose challenges to our ability to study their lattice dynamical properties theoretically. Here we show that a recently introduced approach, compressive sensing lattice dynamics (CSLD) [F. Zhou *et al.*, Phys. Rev. Lett. 113, 185501 (2014)] provides an accurate and computationally efficient platform for investigating anharmonic lattice dynamics in complex materials. We will discuss the basic ideas and illustrate the performance of CSLD for the lattice thermal conductivity κ_L of tetrahedrite, collusite, pyrite, and other earth-abundant mineral compounds.

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