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First-principles Study of Lattice Thermal Conductivity of Cu_3SbS_4 and Cu_3SbSe_4 YI XIA, Department of Materials Science and Engineering, University of California, Los Angeles, CA 90095, USA, FEI ZHOU, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, California 94550, USA, WESTON NIELSON, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, CA 90095, USA — Linearized self-consistent Boltzmann transport equation (BTE), utilizing interatomic force constants (IFCs) obtained via compressive sensing lattice dynamics (CSLD), is used to study the lattice thermal conductivity (κ_l) of Cu_3SbS_4, Cu_3SbSe_4 and their solid solutions. With these IFCs we obtain bulk lattice thermal conductivity in good agreement with experimental measurements. We also compare Cu_3SbS_4 and Cu_3SbSe_4 with respect to Grüneisen parameter, group velocity, phonon lifetime, mean free path and cumulative κ_l. All the analysis indicates that (1) slightly larger group velocity and lifetime of acoustic modes found in Cu_3SbS_4 lead to larger κ_l compared with Cu_3SbSe_4 over the whole temperature range. Contributions from optical modes to κ_l for both compounds are about 25% at temperature higher than 300K. This large portion of κ_l can not be neglected if one aims to predict accurate κ_l; (2) Nanostructures with length less than 10nm can effectively reduce κ_l by about 80% for both of the compounds; (3) solid solution of two compounds can effectively reduce κ_l as much as 40% at room temperature.

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