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First principles lattice thermal conductivity of Li_2Se, Li_2Te and alloys: phase space guidelines for thermal transport[1] LUCAS LINDSAY, SAIKAT MUKHOPADHYAY, DAVID PARKER, Oak Ridge National Laboratory — The lattice thermal conductivities (k) of Li_2Se, Li_2Te and alloys are examined using a first-principles Peierls-Boltzmann transport methodology. The dominant resistance to heat-carrying acoustic phonons in Li_2Se and Li_2Te comes from the interactions of these modes with two optic phonons, aoo scattering. In typical cubic and hexagonal materials (*e.g.*, Si, GaAs, AlN) aoo scattering does not play a considerable role in determining k, as it requires significant bandwidth and dispersion of the optic phonon branches, both present in Li_2Se and Li_2Te. We discuss how these properties and other features of the phonon dispersion (*e.g.*, bunching of the acoustic branches and an acoustic-optic frequency gap) combine to determine the overall conductivity of a material. Thus, microscopic scattering phase space arguments are generalized to give a more comprehensive view of intrinsic thermal transport in crystalline solids. We note that these general considerations are important for the discovery and design of new 'high$k$' and 'low k' materials for thermal management applications.

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