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Approximate models for the lattice thermal conductivity of alloy thermoelectrics: Supporting information

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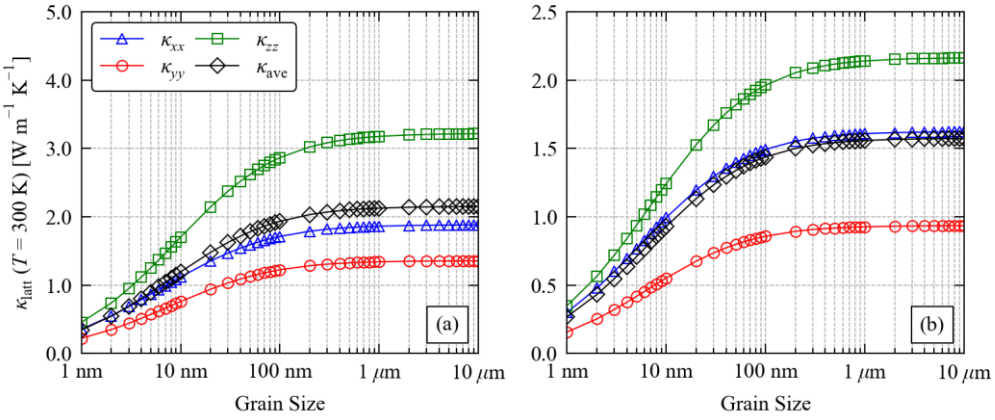

Figure S1 Calculated thermal conductivity κ_{latt} of SnS (a) and SnSe (b) at T = 300 K as a function of the crystal grain size, modelled using a boundary-scattering model to limit the phonon mean free paths. Each plot shows the principal κ_{xx}, κ_{yy} and κ_{zz} components of the κ_{latt} tensor, corresponding to transport along the crystallographic *a*, *b* and *c* axes, together with the diagonal average $\kappa_{\mathrm{ave}} = \frac{1}{3}\mathrm{Tr}[\boldsymbol{\kappa}_{\mathrm{latt}}] = \frac{1}{3}(\kappa_{xx} + \kappa_{yy} + \kappa_{zz})$.

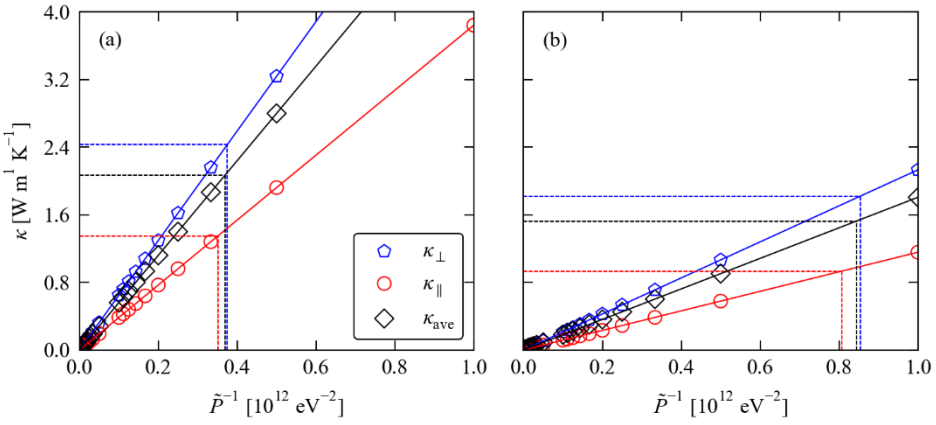

Figure S2 Dependence of the in-plane ($\kappa_{\perp}$, blue), out-of-plane ($\kappa_{\parallel}$, red) and average thermal conductivity ($\kappa_{\mathrm{ave}} = \frac{1}{3}[2\kappa_{\perp} + \kappa_{\parallel}]$, black) of SnS (a) and SnSe (b) at T = 300 K, computed in 32-atom alloy supercells, on the averaged phonon-phonon interaction strength $\tilde{P}$. The values of $\tilde{P}$ that reproduce the calculated $\kappa_{\perp}$, $\kappa_{\parallel}$ and κ_{ave} are indicated by dashed lines.

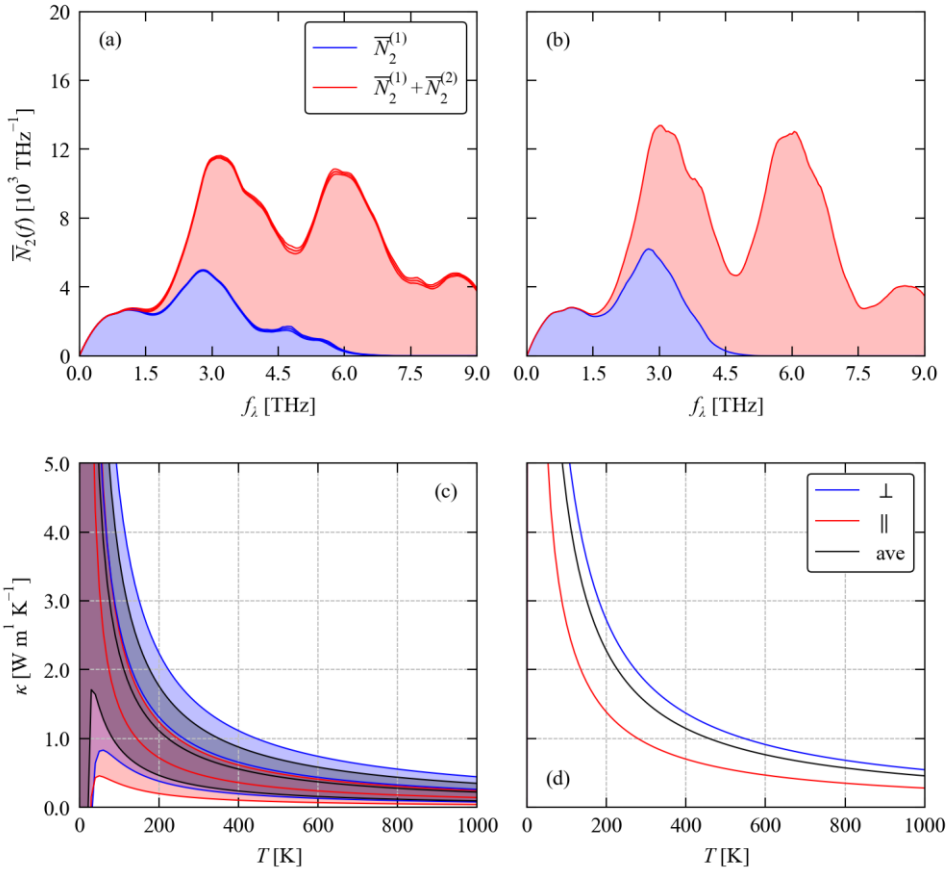

Figure S3 Thermal conductivity of $Sn(S_{0.1875}Se_{0.8125})$ predicted using the model defined in **Eq. 8** in the text with the phonon-phonon interaction strengths replaced by a constant value $\tilde{P}$ = 1.469 x 10^{-12} eV^2. (a)/(b) Two-phonon weighted join density-of-states functions $\overline{N}_2(\omega)$ defined in **Eq. 13** in the text. (c)/(d) Predicted in-plane ($\kappa_\perp$, blue), out-of-plane ($\kappa_\parallel$, red) and average thermal conductivity (κ_{ave}, black). Plots (a) and (c) show calculations on the $Sn(S_{0.1875}Se_{0.8125})$ alloy model, and the shaded areas indicate $\pm$ one standard deviation. Plots (b) and (d) show calculations on SnSe for comparison. This plot is identical to **Fig. 9** in the text but includes the two alloy structures for which the κ_{latt} was deemed unphysically large.