Supplementary Information:

Modification of the Intermediate Band and Thermoelectric Properties in Se-Doped CoSbS_{1-x}Se_x Compounds

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The calculated mass fluctuation scattering parameter \( \Gamma_M \) and the strain field fluctuation scattering parameter \( \Gamma_S \) are presented in Table S1. Assuming that Umklapp processes and point defects are the dominant scattering mechanisms during the heat transport, the lattice thermal conductivity of alloyed CoSbS_{1-x}Se_x (\( \kappa_L^P \)) and of pure CoSbS (\( \kappa_L^P \)) compounds can be expressed as:

\[
\frac{\kappa_L^P}{\kappa_L} = \tan^{-1} \frac{u}{u^2}
\]

(1)

\[
u^2 = \frac{\pi^2 \Theta D \Omega}{h v^3} \kappa_L^P \Gamma
\]

(2)

where \( u, \Theta, D, h, v, \Gamma \) are the disorder scaling parameter, Debye temperature, average atomic volume, Planck constant, average sound velocity and scaling parameter, respectively. \( \Gamma \) can be calculated by the model of Abeles\(^{39}\) and Slack\(^{40}\) as \( \Gamma = \Gamma_M + \Gamma_S \):

\[
\Gamma_M = \frac{\sum_{i=1}^n c_i \left( \frac{\bar{M}_i}{M} \right)^2 f_i^1 f_i^2 \left( \frac{M_i^1 - M_i^2}{\bar{M}_i} \right)^2}{\sum_{i=1}^n c_i}
\]

(3)

\[
\Gamma_S = \frac{\sum_{i=1}^n c_i \left( \frac{\bar{M}_i}{M} \right)^2 f_i^1 f_i^2 c_i \left( \frac{r_i^1 - r_i^2}{r_i^1} \right)^2}{\sum_{i=1}^n c_i}
\]

(4)

where \( n \) is the number of different crystallographic sublattice types in the lattice and \( c_i \) are the relative degeneracies of the respective sites. In pure CoSbS, \( n = 3, c_1 = c_2 = c_3 = 1, \bar{M} \) is the average atomic mass, \( M_i \) and \( r_i \) are the average atomic mass and radius on the \( i \)-th sublattice, respectively. \( f_i^k \) is the fractional occupation of the \( k \)-th atom on the \( i \)-th sublattice. The atomic mass and radius are \( M_i^k \) and \( r_i^k \), respectively. The relations discussed above can be expressed as:

\[
\bar{M}_i = \sum_k f_i^k M_i^k
\]

(5)
\[
\bar{r}_i = \sum_k f_i^k r_i^k \tag{6}
\]

\[
\bar{M} = \frac{\sum_{i=1}^n c_i \bar{M}_i}{\sum_{i=1}^n c_i} \tag{7}
\]

The results is listed in Table S1.

<table>
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<th>Compound</th>
<th>(\kappa_L) (Wm(^{-1})K(^{-1}))</th>
<th>(u)</th>
<th>(\Gamma_M)</th>
<th>(\Gamma_S)</th>
<th>(\Gamma)</th>
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