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 Γ_M and the strain field fluctuation scattering parameter Γ_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 $CoSbS_{1-x}Se_x$ (κ_L) and of pure CoSbS (κ_L^P) compounds can be expressed as:

$$\frac{\kappa_L}{\kappa_L^P} = \frac{\tan^{-1} u}{u} \qquad (1)$$

$$u^2 = \frac{\pi^2 \theta_D \Omega}{h v^2} \kappa_L^P \Gamma \qquad (2)$$

where u, θ_D, Ω, h, v, Γ are the disorder scaling parameter, Debye temperature, average atomic volume, Planck constant, average sound velocity and scaling parameter, respectively. Γ can be calculated by the model of Abeles[39] and Slack[40] as $\Gamma = \Gamma_M + \Gamma_S$.

$$\Gamma_M = \frac{\sum_{i=1}^{n} c_i \left(\frac{\bar{M}_i}{\bar{\bar{M}}}\right)^2 f_i^1 f_i^2 \left(\frac{M_i^1 - M_i^2}{\bar{M}_i}\right)^2}{\sum_{i=1}^{n} c_i} \qquad (3)$$

$$\Gamma_S = \frac{\sum_{i=1}^{n} c_i \left(\frac{\bar{M}_i}{\bar{\bar{M}}}\right)^2 f_i^1 f_i^2 \varepsilon_i \left(\frac{r_i^1 - r_i^2}{\bar{r}_i}\right)^2}{\sum_{i=1}^{n} c_i} \qquad (4)$$

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, $c_1 = c_2 = c_i = 1$, $\bar{\bar{M}}$ is the average atomic mass, $\bar{M}_i$ and $\bar{r}_i$ 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:

$$\bar{M}_i = \sum_k f_i^k M_i^k \qquad (5)$$

$$\overline{r_i} = \sum_k f_i^k r_i^k \quad (6)$$

$$\overline{\overline{M}} = \frac{\sum_{i=1}^{n} c_i \overline{M}_i}{\sum_{i=1}^{n} c_i} \quad (7)$$

The results is listed in Table S1.

Table S1 Lattice thermal conductivity κ_L, disorder scaling parameter u, and disorder scattering parameters Γ_M , Γ_S and Γ of $CoSbS_{1-x}Se_x$ ($0 \le x \le 0.07$) compounds.

Compound	κ_L ($Wm^{-1}K^{-1}$)	u	Γ_M	Γ_S	Γ
0	9.36				
0.01	8.57	0.546	0.00144	0.00400	0.00544
0.03	8.51	0.572	0.00419	0.00607	0.01026
0.05	8.27	0.659	0.00677	0.00831	0.01508
0.07	7.23	1.046	0.00920	0.01071	0.01991