SUPPORTING INFORMATION

Deep defect level engineering: a strategy of optimizing the carrier concentration for high thermoelectric performance

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Thermoelectric properties of I-doped PbTe

Figure S1. Thermoelectric properties of PbTe$_{1-x}$I$_x$ ($x = 0.003, 0.0035, 0.004,$ and 0.005). (a) Electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) thermal diffusivity, (e) thermal conductivity, and (f) $ZT$. 
Figure S2. Pisarenko plot for the $n$-type PbTe-based materials.
Hall mobility

Figure S3. Relationship between the Hall carrier concentration and Hall carrier mobility of $n$-type PbTe.
Specific heat and diffusivity of In/I co-doped PbTe

Figure S4. (a) Specific heat and (b) thermal diffusivity of In$_x$Pb$_{1-x}$Te$_{0.996}$I$_{0.004}$ ($x = 0, 0.0025, 0.0035,$ and $0.0050$).
Lattice thermal conductivity of In/I co-doped PbTe

The lattice thermal conductivity of the In/I co-doped PbTe is calculated as shown in Fig. S5. The lattice thermal conductivity shows a non-monotonic dependence on the indium concentration, which can be partially ascribed to the uncertainty in the estimation of the Lorenz number.

Figure S5. Temperature-dependent lattice thermal conductivity of In/I co-doped PbTe
Figure S6. XRD patterns of PbTe$_{1-x}$I$_x$ ($x = 0.003, 0.0035, 0.004, \text{and} 0.005$).
Figure S7. The structures of the supercell used in the calculation (a) $\text{Pb}_{31}\text{InTe}_{32}$, and (b) $\text{Pb}_{31}\text{InTe}_{31}\text{I}$