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

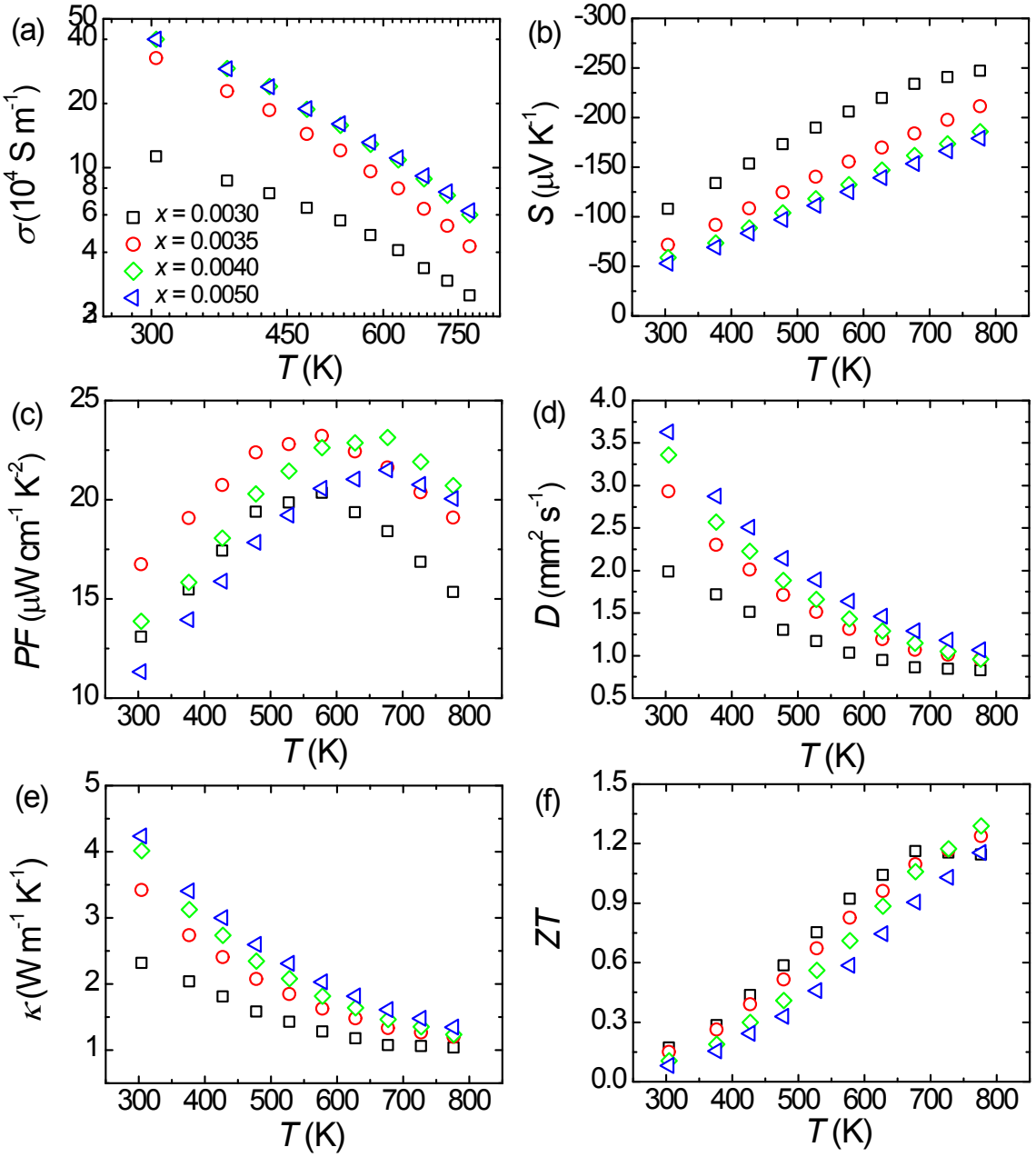

Figure S1. Thermoelectric properties of $PbTe_{1-x}I_x$ (x = 0.003, 0.0035, 0.004, and 0.005). (a) Electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) thermal diffusivity, (e) thermal conductivity, and (f) *ZT*.

Pisarenko plot

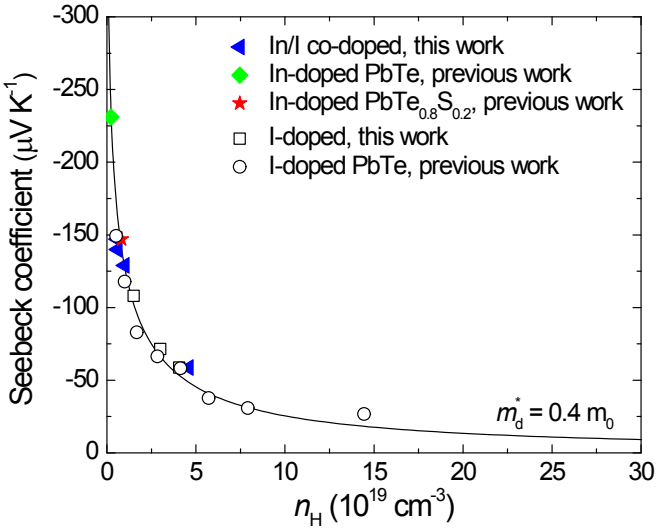

Figure S2. Pisarenko plot for the *n*-type PbTe-based materials.

Hall mobility

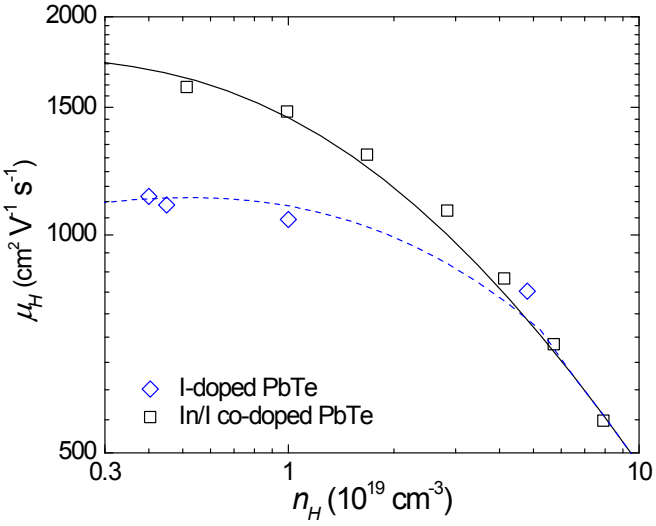

Figure S3. Relationship between the Hall carrier concentration and Hall carrier mobility of *n*-type PbTe.

Specific heat and diffusivity of In/I co-doped PbTe

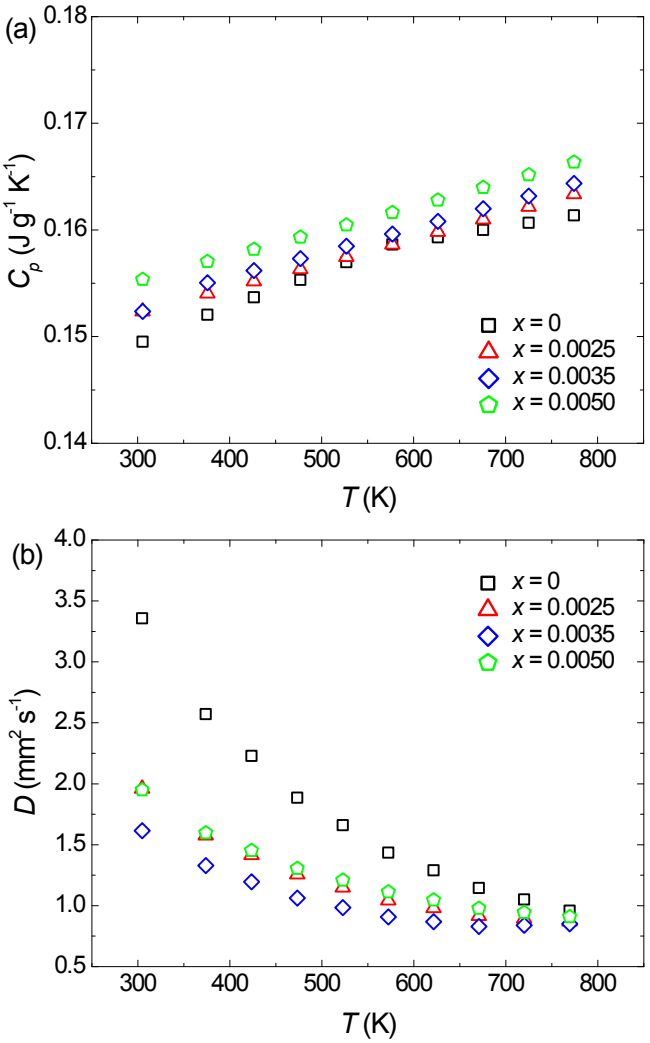

Figure S4. (a) Specific heat and (b) thermal diffusivity of $In_xPb_{1-x}Te_{0.996}I_{0.004}$ (x = 0, 0.0025, 0.0035, and 0.0050).

Lattice thermal conductivity of In/I co-doped PbTe

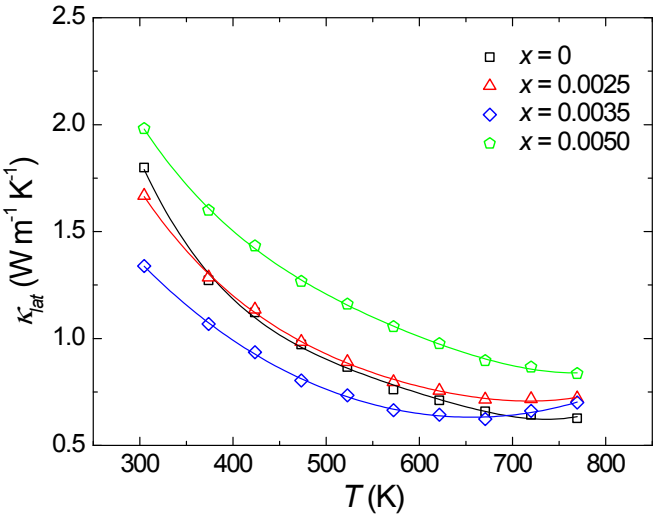

Figure S5. Temperature-dependent lattice thermal conductivity of In/I co-doped PbTe

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.

XRD

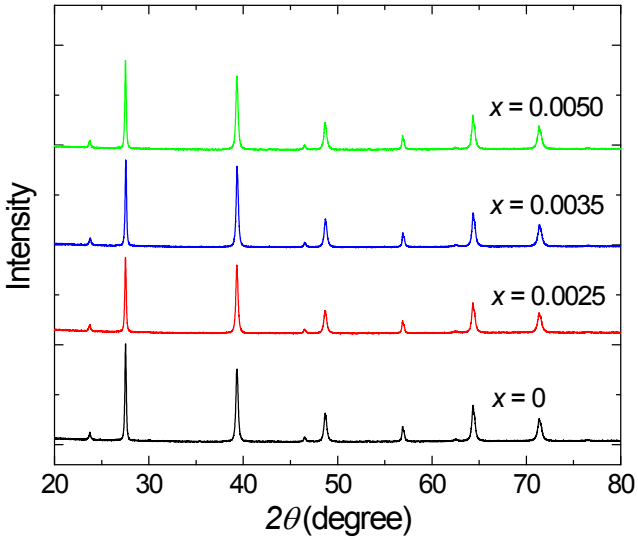

Figure S6. XRD patterns of $PbTe_{1-x}I_x$ (x = 0.003, 0.0035, 0.004, and 0.005).

Details for calculation

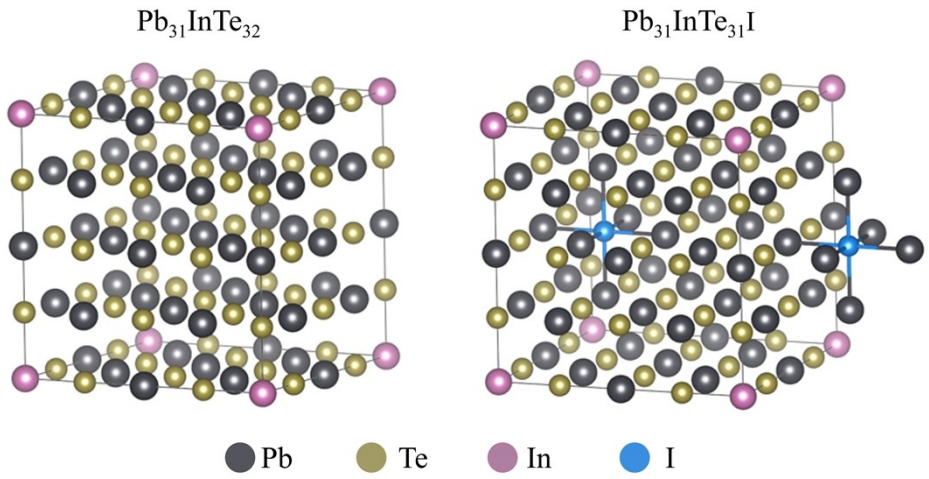

Figure S7. The structures of the supercell used in the calculation (a) $Pb_{31}InTe_{32}$, and (b) $Pb_{31}InTe_{31}I$