Supporting materials

Validity range of the SPB model

From the above data, the thermoelectric properties of the samples show that the minority carriers contribute at high temperature (see Fig. 1 and Fig. 2). However, the SPB model is only valid when the sample has a single carrier type and there is no significant contribution from the minority carriers. This temperature range depends on carrier concentration and on x as band gap and the mobility ration of holes and electrons depend on the x. For most thermoelectric with a simple band structure m_D^* varies only slowly with temperature. We therefore use the difference in η from S (eq. 1) and the η values from n and m_D^* (eq. 2) (assuming m_D^* to be constant with T) as a criterion for applicability of the SPB model. Specifically, we have used a maximum deviation of ≈20 % between these two values for Sn-rich samples ($x \geq 0.6$) to determine the validity range of the SPB model for each sample (see Fig. S 1 for an example). For further modeling, the density of states effective mass was averaged from all samples with the same Si/Sn ratio. As discussed previously (Fig. 4b), this is a simplification but the resulting error is acceptable. It furthermore keeps the number of model parameters to a minimum. The low dopant efficiency in the Si-rich samples prevents the carrier concentration to go high enough for the SPB to be valid. For all samples of this study with $x \geq 0.6$ the SPB is valid up to at least 500 K. At a given carrier concentration range the maximum temperature decreases with increasing x, mainly due to the decreasing band gap.

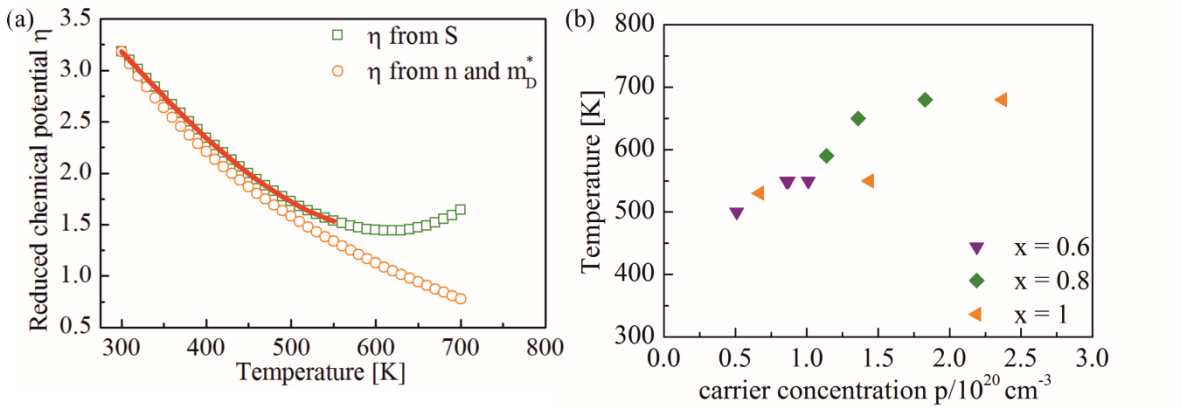
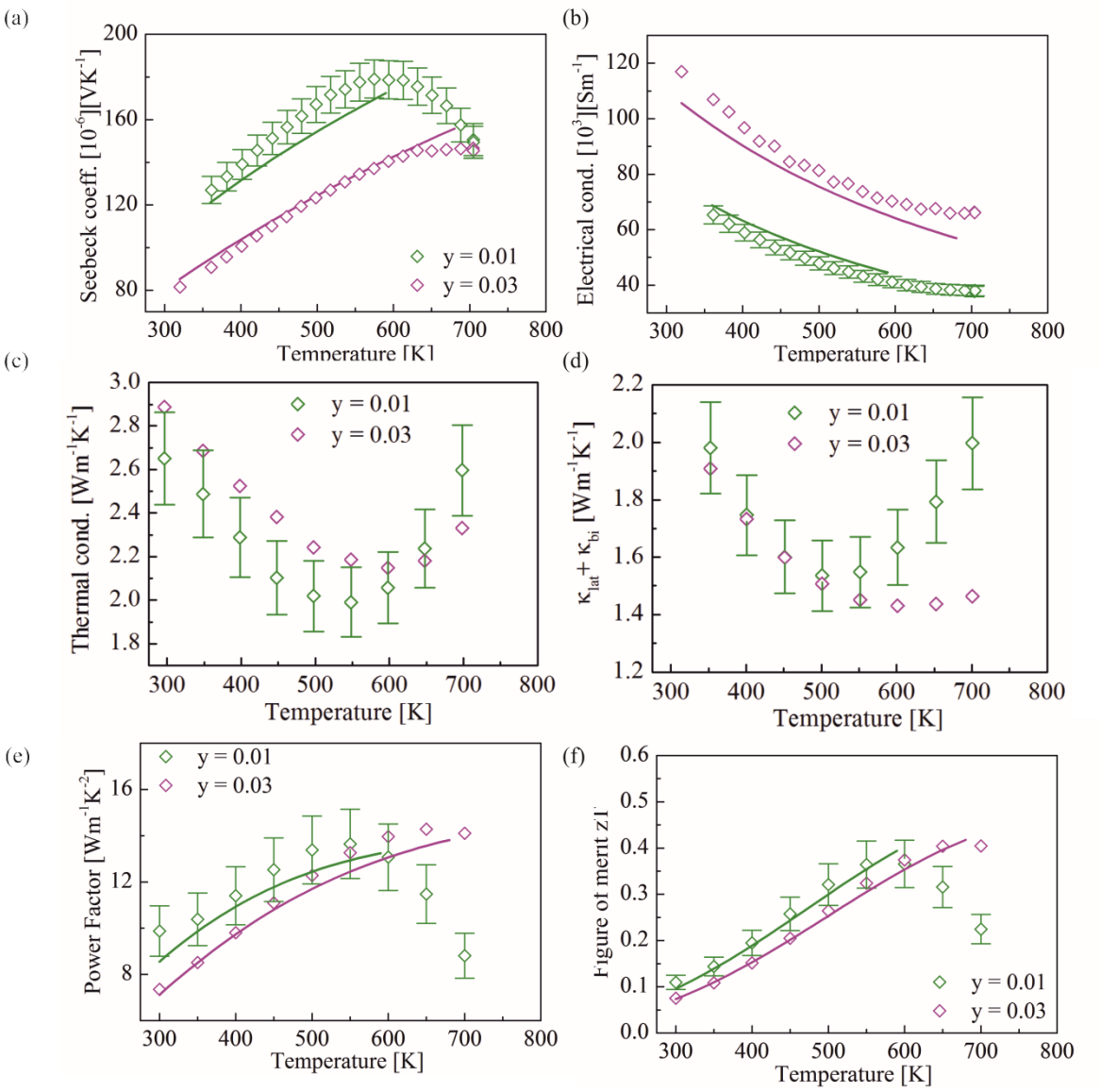


Fig. S 1 (a) Reduced chemical potential as determined from the Seebeck coefficient (green square) and from the carrier concentration and density of states effective mass (orange circle), the red line shows the temperature range where the SPB model is approximately valid using $Mg_{1.99}Li_{0.01}Sn$ as example and (b) Temperature up to which the SPB is valid vs. carrier concentration of that sample. profile for each compositions where SPB is valid.

Thermoelectric properties of $Mg_{2-y}Li_ySi_{0.2}Sn_{0.8}$



Thermoelectric properties of $Mg_{2-y}Li_ySi_{0.2}Sn_{0.8}$ with $\boldsymbol{y = 0.01, 0.03}$ (a) Temperature dependent Seebeck coefficient, (b) electrical conductivity, (c) thermal conductivity, (d) lattice thermal conductivity, (e) power factor, and (f) figure of merit $\boldsymbol{zT}$. Data points indicate experimental results and theoretical results are shown by lines based on single parabolic band (SPB) model.

Thermoelectric properties of $Mg_{2-y}Li_ySn$

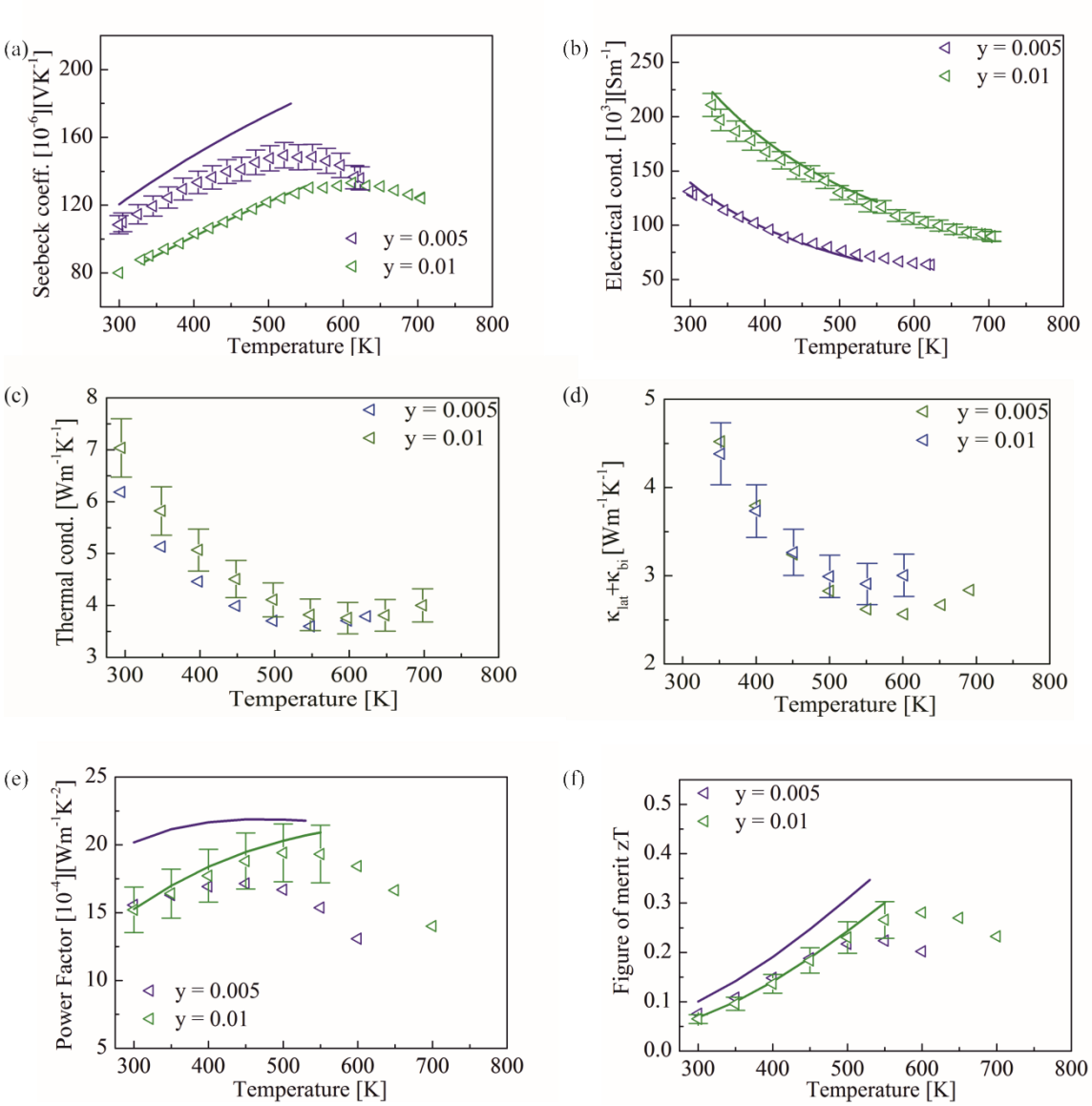


Fig. S 3 Thermoelectric properties of $Mg_{2-y}Li_ySn$ with $\boldsymbol{y = 0.005, 0.01}$ (a) Temperature dependent Seebeck coefficient, (b) electrical conductivity, (c) thermal conductivity, (d) lattice thermal conductivity, (e) power factor, and (f) figure of merit $\boldsymbol{zT}$. Data points indicate experimental results and theoretical results are shown by lines based on single parabolic band (SPB) model.