Supplementary

Near room temperature Thermoelectric performance improvement for Mg_2Sn

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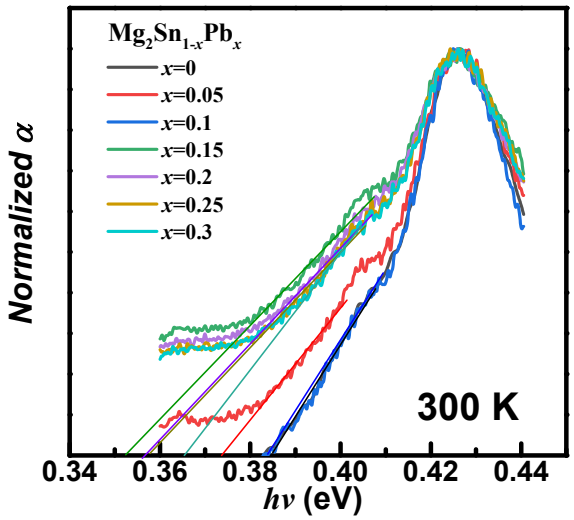

Fig. S1. The normalized inferred absorption peak of $Mg_2Sn_{1-x}Pb_x$ ($0 \le x \le 0.3$) samples at room temperature, indicating the decrease of band gap by Pb alloying.

The calculation process of Lorenze number:

$$L_e = \left(\frac{k_B}{e}\right)^2 \left[\frac{\left(r+\frac{7}{2}\right)F_{r+\frac{5}{2}}(\xi_e)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\xi_e)} - \left(\frac{\left(r+\frac{5}{2}\right)F_{r+\frac{3}{2}}(\xi_e)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\xi_e)} \right)^2 \right] \#(1-1)$$

$$L_h = \left(\frac{k_B}{e}\right)^2 \left(\frac{\left(r+\frac{7}{2}\right)F_{r+\frac{5}{2}}(\xi_h)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\xi_h)} - \left(\frac{\left(r+\frac{5}{2}\right)F_{r+\frac{3}{2}}(\xi_h)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\xi_h)} \right)^2 \right) \#(1-2)$$

$$S = \pm \left(\frac{\left(r+\frac{5}{2}\right)F_{r+\frac{3}{2}}(\xi_e)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\xi_e)} - \xi_e \right) h \#(1-3)$$

$$\xi_h = -\left(\frac{E_g}{k_B T} + \xi_e\right) \#(1-4)$$

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$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right) F_{\frac{1}{2}}(\xi_e) \#(1-5)$$

$$p = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right) F_{\frac{1}{2}}(\xi_h) \#(1-6)$$

$$\left(n_{300\,K} + \Delta\right)\left(p_{300\,K} + \Delta\right) = AT^3 \exp\left(-\frac{E_g}{k_B T}\right) \#(1-7)$$

Here, the r is the scattering parameter for the carrier transport based on the relaxation time approximation, where the acoustic phonon (r = -1/2) scattering dominants. The reduced Fermi energy ξ_e and ξ_h near room temperature could be estimated from the Seebeck coefficient on the basis of single band approximation formula Eq. (1-3 and 1-4). The reduced Fermi energy $\xi(T)$ at the higher temperature is obtained by Eq. (1-4~1-7) at a given temperature.

m_e^* was obtained from the measured carrier concentration and Seebeck coefficient of $Mg_{2.03}Sn_{1-x}Pb_x$ in this study, while $m_h^* = 1.3\ m_0$ was used.

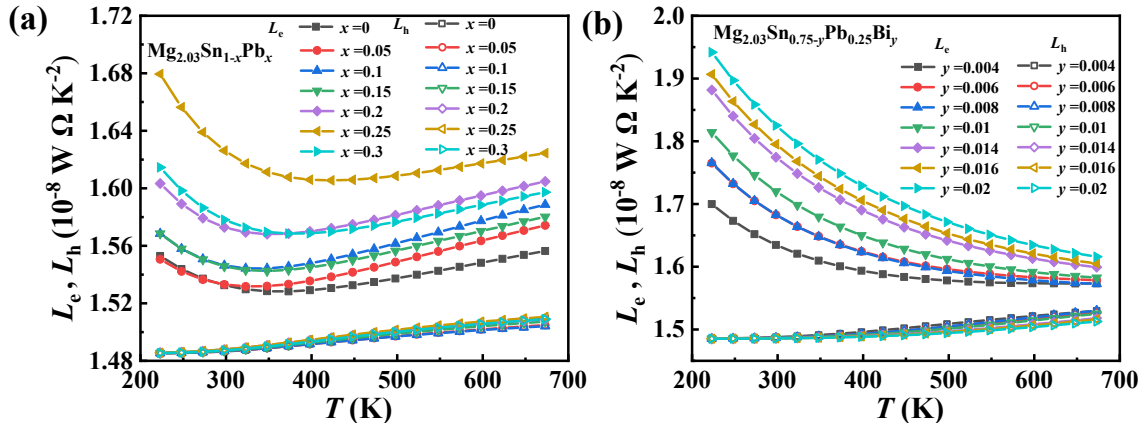

Fig. S2. The temperature dependent L_e、L_h of $Mg_2Sn_{1-x}Pb_x$ ($0 \le x \le 0.05$) (a) and $Mg_{2.03}Sn_{0.75-x}Pb_{0.25}Bi_y$ ($0 \leqslant y \leqslant 0.02$) (b) samples in this work.

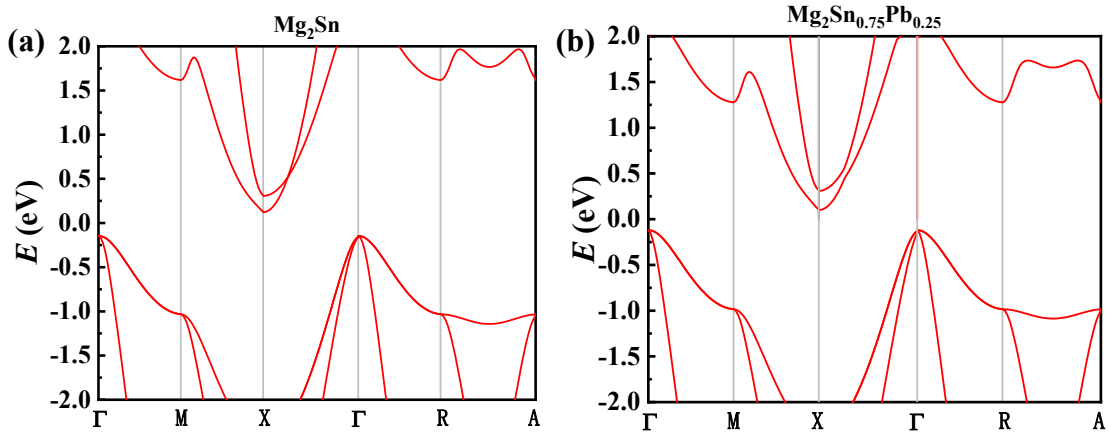

Fig. S3. The first-principle calculated band structure of Mg_2Sn(a) and $Mg_2Sn_{0.75}Pb_{0.25}$ (b) .