Synergistic effect by Na doping and S substitution to high thermoelectric performance of p-type MnTe

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**Fig. S1** (a) high magnification FSEM fractographs of the Na$_2$S-doped MnTe sample; (b) Low magnification TEM image of the Na$_2$S-doped MnTe sample; (c) A magnified nanoparticle image of the yellow rectangle; (d-h) corresponding EDS mapping of Mn, O, Te, Na and S elements, respectively. A whiter colour in the element maps corresponds to higher concentrations.
Fig. S2 Low magnification TEM image for all the samples (a) $x=0$, (b) $x=0.25$, (c) $x=0.5$, (d) $x=1$

Fig. S3 Temperature dependence of thermoelectric properties for the samples, (a)
electrical resistivity; (b) Seebeck coefficient; (c) power factor.

**Fig. S4** Vickers micro indentation of (a) MnTe and (b) 0.5 at% Na$_2$S-doped MnTe, respectively.

**S15:** the calculation of Lorenz number of all the samples

Assuming a single parabolic band model with acoustic phonon scattering[1], the Lorenz number ($L$) is estimated by the following equation:

$$L = \left(\frac{k_B}{e}\right)^2 \left(\frac{(r + 7/2)F_{r + 5/2}(\varphi)}{(r + 3/2)F_{r + 1/2}(\varphi)} - \left(\frac{(r + 7/2)F_{r + 3/2}(\varphi)}{(r + 3/2)F_{r + 1/2}(\varphi)}\right)^2\right)$$

Here, $F_n(\varphi)$ is the Fermi integration:

$$F_n(\varphi) = \int_0^\infty \frac{x^n}{1 + e^{x - \varphi}} dx$$

$r$ is the scattering parameter typical $r=-1/2$ for acoustic phonon scattering near room temperature) and $\varphi$ is the reduced Fermi energy $\varphi = E_F/k_B T$ and which can be derived from the measured $S$ on the basis of single band approximation:

$$S = \pm \frac{k_B}{e} \left(\frac{(r + 5/2)F_{r + 3/2}(\varphi)}{(r + 3/2)F_{r + 1/2}(\varphi)} - \varphi\right)$$

Finally, the temperature dependent calculated $L$ for pristine MnTe and Na$_2$S-doped samples ($x = 0-1$).
Fig. S6 Temperature dependence of the calculated Lorenz number.

Reference