Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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

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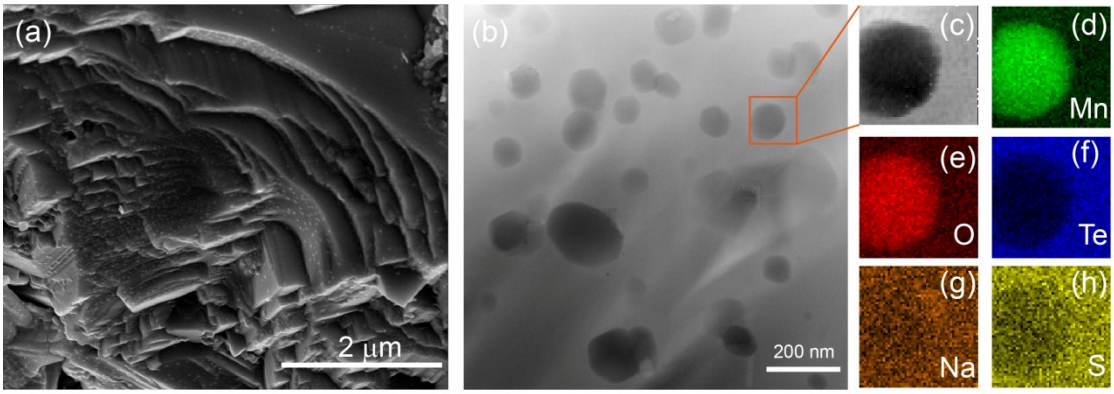

Fig. S1 (a) high magnification FSEM fractographs of the Na_2S-doped MnTe sample; (b) Low magnification TEM image of the Na_2S-doped MnTe sample; (c) A magnified nanoparticle image of the yellow rectangle; (d-h) corresponding EDS mapping of Mn, O, Te, Na and S elements, respectively. A whiter colour in the element maps corresponds to higher concentrations.

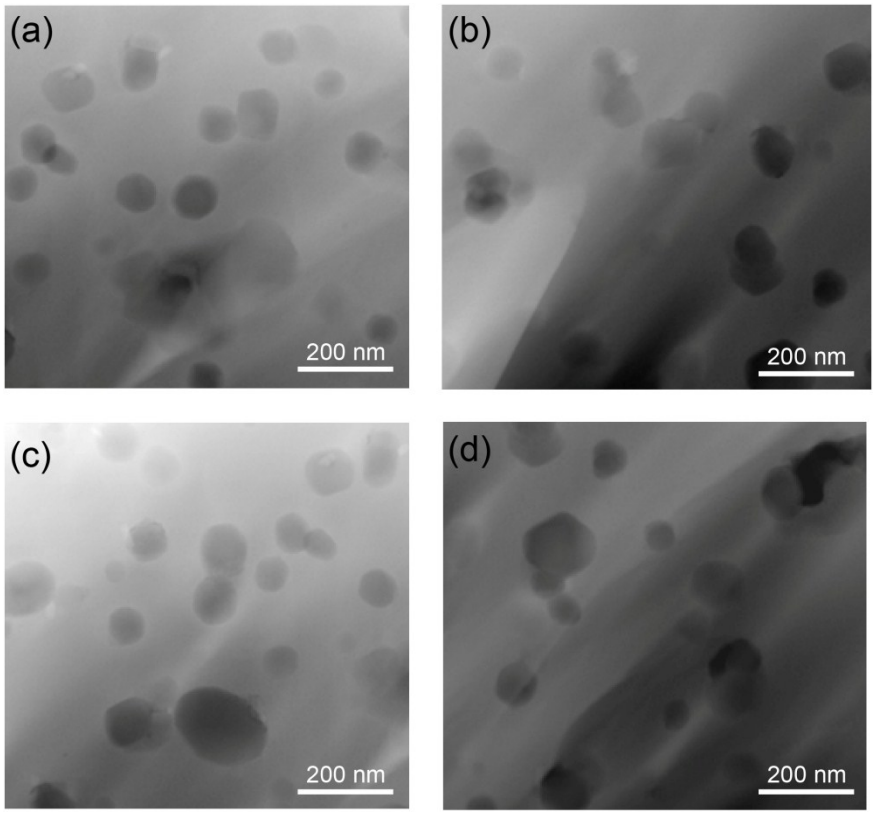

Fig. S2 Low magnification TEM image for all the samples (a) x=0, (b) x=0.25, (c) x=0.5, (d) x=1

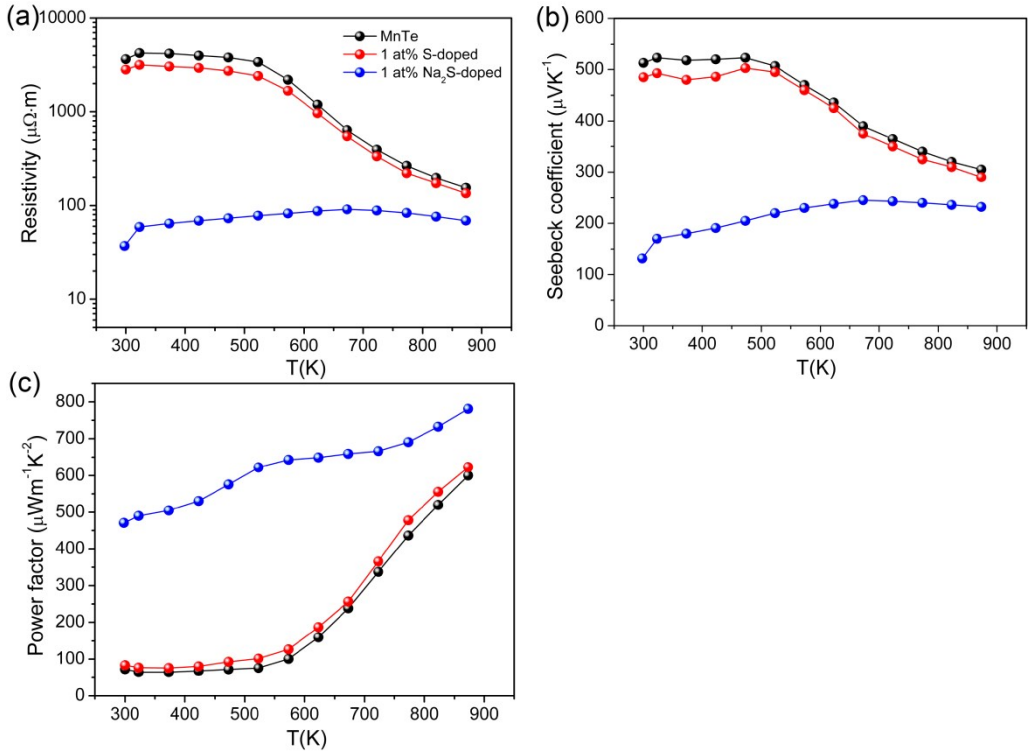

Fig. S3 Temperature dependence of thermoelectric properties for the samples, (a)

electrical resistivity; (b) Seebeck coefficient; (c) power factor.

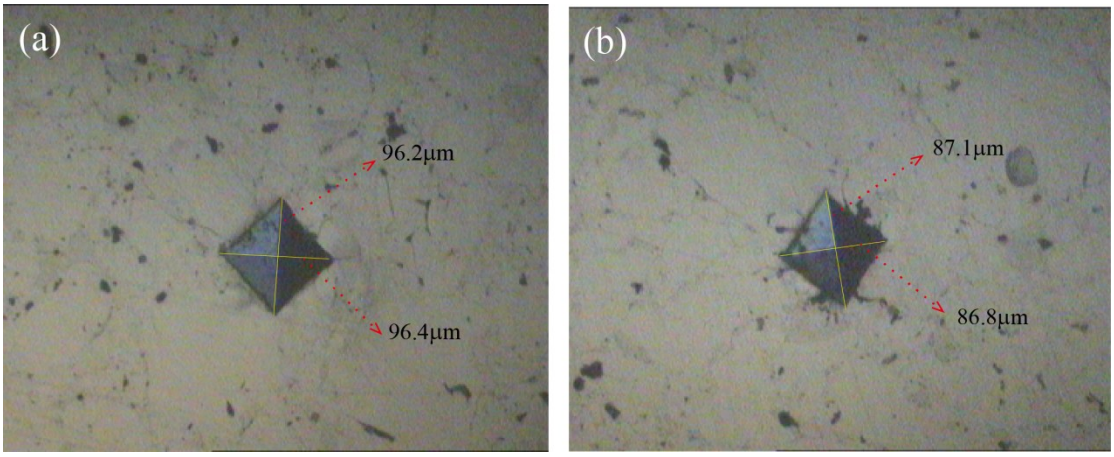

Fig. S4 Vickers micro indentation of (a) MnTe and (b) 0.5 at% Na_2S-doped MnTe, respectively.

SI5: 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 follow 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: $F_n(\varphi) = \int_0^\infty \frac{x^n}{1+e^{x-n}} dx$, r is the scattering (parameter typical r=-1/2 for acoustic phonon scattering near room temperature) and φ 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_2S-doped samples (x = 0-1).

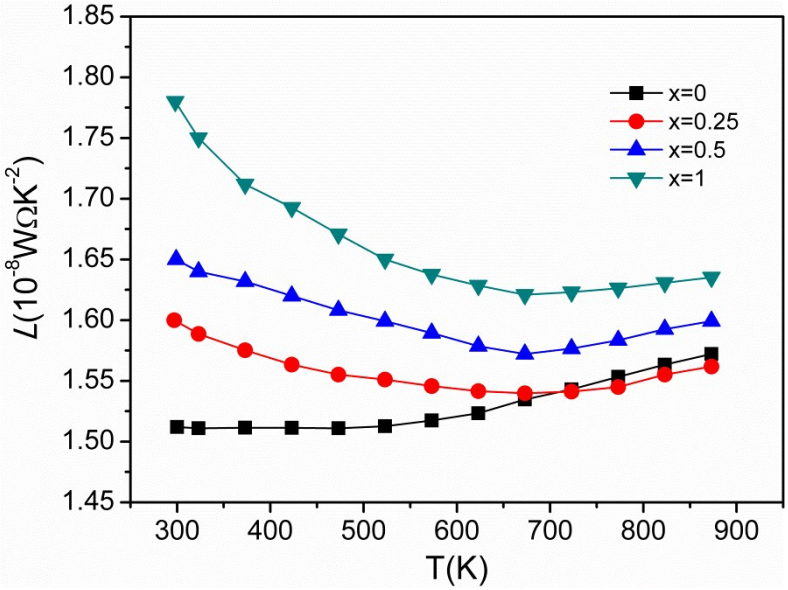

Fig. S6 Temperature dependence of the calculated Lorenz number.

Reference

[1] W. Xie, S. Populoh, K. Gałzka, X. Xiao, L. Sagarna, Y. Liu, M. Trottmann, J. He and A. Weidenkaff, J. Appl. Phys., 2014, 115, 103707.