Low thermal conductivity in a new mixed metal telluride $Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$

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Electronic Supplementary Information (ESI)

Table S1: Important structural and refinement details of the $Mn_{1.78(5)}In_{0.84(2)}Si_2Te_6$ structure obtained from the Rietveld refinement of the PXRD data of the sample with the loaded composition of $Mn_{1.8}In_{0.8}Si_2Te_6$[a].

Refined composition	$Mn_{1.78(5)}In_{0.84(2)}Si_2Te_6$
Space group	$P\bar{3}1m$
a (Å)	7.0370(2)
c (Å)	7.1131(2)
V (Å^3)	305.04(3)
Z	2
ρ (g cm^{-3})	5.51
GOF on F^2	1.98
[b]R_p	5.54
[c]R_{wp}	8.34

[a]λ = 1.5406 Å, T = 298(2) K.

[b]$R_p = \Sigma\,|Y_{o,m} - Y_{c,m}| \,/\, \Sigma\, Y_{o,m}$

[c]$R_{wp} = \{\Sigma\,[w_m(Y_{o,m} - Y_{c,m})^2] \,/\, \Sigma w_m\, Y_{o,m}^2\}^{1/2}$ For $w_m = 1/\sigma\,(Y_{o,m})^2$

Table S2: Fractional atomic coordinates and site occupancy factors (SOF) obtained from the Rietveld refinement of the $Mn_{1.78(5)}In_{0.84(2)}Si_2Te_6$ structure using the PXRD data.

Atoms	Wyckoff Position	Site Symmetry	*x*	*y*	*z*	SOF
In1	2*d*	3·2	1/3	2/3	0	0.42(2)
Mn1	2*d*	3·2	1/3	2/3	0	0.58(2)
Mn2	2*c*	3·2	1/3	2/3	1/2	0.31(5)
Si1	2*e*	3·*m*	0	0	0.1630(5)	1
Te1	6*k*	··*m*	0.3422(5)	0	0.2602(5)	1

Table S3 Atomic displacement parameters (Å^2) for the $Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$ structure obtained from the SCXRD study.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
$Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$						
In1	0.0238(7)	0.0238(7)	0.0512(15)	0.0119(4)	0.000	0.000
Mn1	0.0238(7)	0.0238(7)	0.0512(15)	0.0119(4)	0.000	0.000
Mn2	0.032(5)	0.032(5)	0.018(6)	0.016(2)	0.000	0.000
Si1	0.0130(14)	0.0130(14)	0.030(3)	0.0065(7)	0.000	0.000
Te1	0.0143(3)	0.0187(4)	0.0272(4)	0.00934(19)	-0.0017(3)	0.000

Table S4 All the bond angles (in degrees) in the $Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$ structure obtained from the SCXRD study.

Te1i—In1—Te1ii	96.17 (3)	Te1viii—Mn2—Te1ix	88.382 (18)
Te1i—In1—Te1iii	85.181 (17)	Te1ii—Mn2—Te1ix	177.97 (2)

Te1ii—In1—Te1iii	93.502 (19)	Te1iv—Mn2—Te1vi	88.382 (18)
Te1i—In1—Te1iv	93.502 (19)	Te1vii—Mn2—Te1vi	93.05 (3)
Te1ii—In1—Te1iv	85.181 (17)	Te1viii—Mn2—Te1vi	177.97 (2)
Te1iii—In1—Te1iv	178.03 (2)	Te1ii—Mn2—Te1vi	88.382 (18)
Te1i—In1—Te1v	85.181 (17)	Te1ix—Mn2—Te1vi	90.22 (2)
Te1ii—In1—Te1v	178.03 (2)	Si1x—Si1—Te1	106.10 (14)
Te1iii—In1—Te1v	85.181 (17)	Si1x—Si1—Te1xi	106.10 (14)
Te1iv—In1—Te1v	96.17 (3)	Te1—Si1—Te1xi	112.62 (12)
Te1i—In1—Te1vi	178.03 (2)	Si1x—Si1—Te1iv	106.10 (14)
Te1ii—In1—Te1vi	85.181 (17)	Te1—Si1—Te1iv	112.62 (12)
Te1iii—In1—Te1vi	96.17 (3)	Te1xi—Si1—Te1iv	112.62 (12)
Te1iv—In1—Te1vi	85.181 (17)	Si1—Te1—Mn2vii	122.44 (8)
Te1v—In1—Te1vi	93.502 (19)	Si1—Te1—Mn2xii	122.44 (8)
Te1iv—Mn2—Te1vii	177.97 (2)	Mn2vii—Te1—Mn2xii	89.78 (2)
Te1iv—Mn2—Te1viii	90.22 (2)	Si1—Te1—In1iii	100.84 (10)
Te1vii—Mn2—Te1viii	88.382 (18)	Mn2vii—Te1—In1iii	75.007 (12)
Te1iv—Mn2—Te1ii	88.382 (18)	Mn2xii—Te1—In1iii	135.10 (3)
Te1vii—Mn2—Te1ii	90.22 (2)	Si1—Te1—In1xii	100.84 (10)
Te1viii—Mn2—Te1ii	93.05 (3)	Mn2vii—Te1—In1xii	135.10 (3)
Te1iv—Mn2—Te1ix	93.05 (3)	Mn2xii—Te1—In1xii	75.007 (12)
Te1vii—Mn2—Te1ix	88.382 (18)	In1iii—Te1—In1xii	86.50 (2)

Symmetry codes: (i) *y*, -*x*+*y*+1, -*z*; (ii) *x*, *y*+1, *z*; (iii) -*x*+1, -*y*+1, -*z*; (iv) -*y*, *x*-*y*, *z*; (v) *x*-*y*, *x*, -*z*; (vi) -*x*+*y*+1, -*x*+1, *z*; (vii) -*x*+1, -*y*+1, -*z*+1; (viii) *y*, -*x*+*y*+1, -*z*+1; (ix) *x*-*y*, *x*, -*z*+1; (x) -*x*, -*y*, -*z*; (xi) -*x*+*y*, -*x*, *z*; (xii) *x*, *y*-1, *z*.

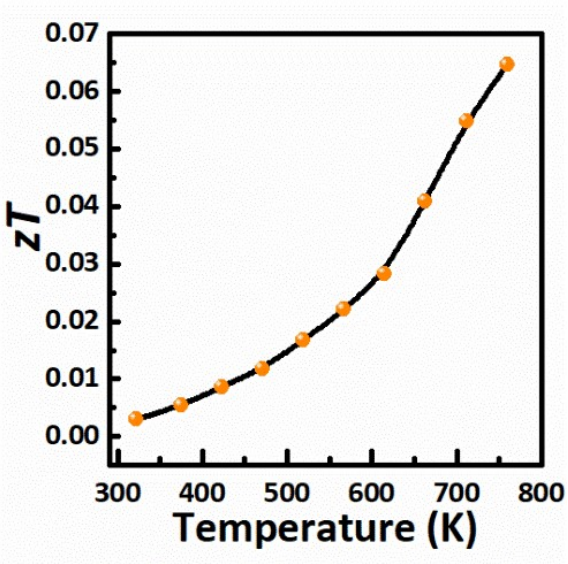

Fig. S1: The thermoelectric figure of merit (zT) of the polycrystalline sample $Mn_{1.8}In_{0.8}Si_2Te_6$. Each data point has an estimated error of 20%.