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Supplementary Information for:

Thermoelectric properties of the aliovalent half-Heusler alloy $Zn_{0.5}Ti_{0.5}NiSb$ with intrinsic low thermal conductivity

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Table S1: Half-Heusler compositions for hot-pressed $Zn_{1-x}Ti_xNiSb$ disks derived from EDX elemental maps shown in Fig. S1.

Nominal Composition	**EDX Composition**
$Zn_{0.35}Ti_{0.65}NiSb$	$Zn_{0.32}Ti_{0.65}NiSb_{1.02}$
$Zn_{0.40}Ti_{0.60}NiSb$	$Zn_{0.39}$ $Ti_{0.61}NiSb$
$Zn_{0.45}Ti_{0.55}NiSb$	$Zn_{0.42}Ti_{0.54}NiSb_{1.03}$
$Zn_{0.50}Ti_{0.50}NiSb$	$Zn_{0.47}Ti_{0.53}NiSb$
$Zn_{0.55}Ti_{0.45}NiSb$	$Zn_{0.55}Ti_{0.46}NiSb_{1.02}$
$Zn_{0.60}Ti_{0.40}NiSb$	$Zn_{0.58}Ti_{0.41}NiSb_{1.01}$

Table S2: Overview of resistivity fit parameters for the $Zn_{1-x}Ti_xNiSb$ samples,[1] see manuscript for further details.

	E_g (eV)	ρ_0 (μΩ.m)	B(×10^{-4} μΩ.m.$K^{-1.5}$)	A (μΩ.m)	ρ_0/B ($K^{1.5}$)
n-type					
$Zn_{0.35}Ti_{0.65}NiSb$	0.39 (fixed)	7(1)	2.5(3)	5.4(1)	27500
$Zn_{0.40}Ti_{0.60}NiSb$	0.39 (fixed)	14(1)	4.7(3)	4.0(1)	29978
$Zn_{0.45}Ti_{0.55}NiSb$	0.39(2)	33(3)	-	2.0(1)	-
p-type					
$Zn_{0.50}Ti_{0.50}NiSb$	0.39(2)	53(3)	-	2.1(1)	-
$Zn_{0.55}Ti_{0.45}NiSb$	0.39 (fixed)	15(1)	-	1.8(1)	-
$Zn_{0.60}Ti_{0.40}NiSb$	0.39 (fixed)	7(1)	0.7(1)	1.9(1)	105980

Table S3: Measured, crystallographic and % density of the hot pressed $Zn_{1-x}Ti_xNiSb$ ($0.4 \leq x \leq 0.65$) disks characterised in this manuscript.

Composition	Measured Density ($g.cm^{-3}$)	Crystallographic Density ($g.cm^{-3}$)	% Density
$Zn_{0.35}Ti_{0.65}NiSb$	7.37(2)	7.58	97.2
$Zn_{0.40}Ti_{0.60}NiSb$	7.41(2)	7.58	97.7
$Zn_{0.45}Ti_{0.55}NiSb$	7.48(2)	7.59	98.5
$Zn_{0.50}Ti_{0.50}NiSb$	7.5(2)	7.60	98.7
$Zn_{0.55}Ti_{0.45}NiSb$	7.51(2)	7.60	98.8
$Zn_{0.60}Ti_{0.40}NiSb$	7.56(2)	7.61	99.3

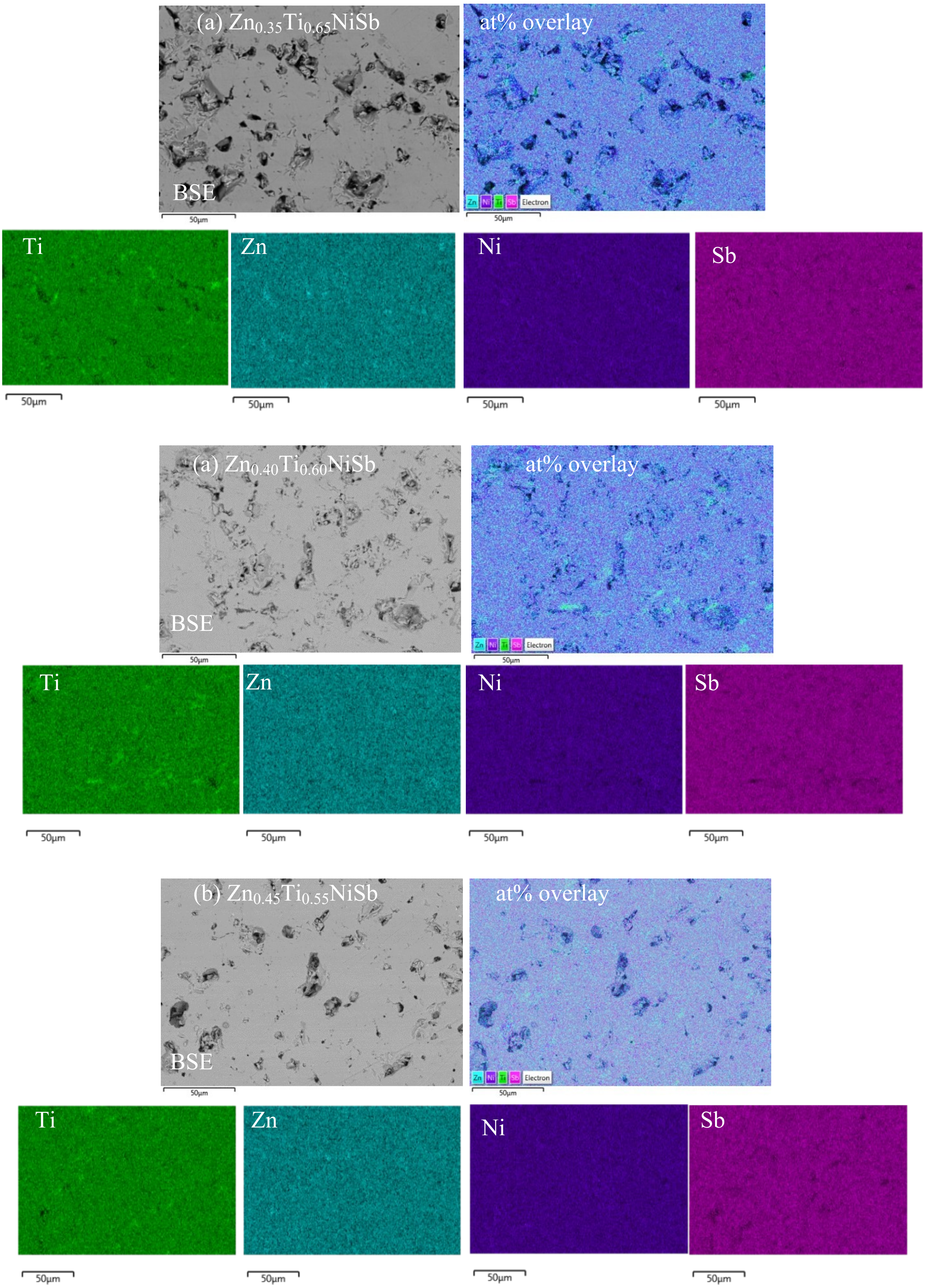

Figure S1: Backscattered Secondary Electron SEM images, at% composite and individual elemental at% maps for n-type $Zn_{1-x}Ti_xNiSb$ disks.

Figure S2: Backscattered Secondary Electron SEM images, at% composite and individual elemental at% maps for p-type $Zn_{1-x}Ti_xNiSb$ disks.

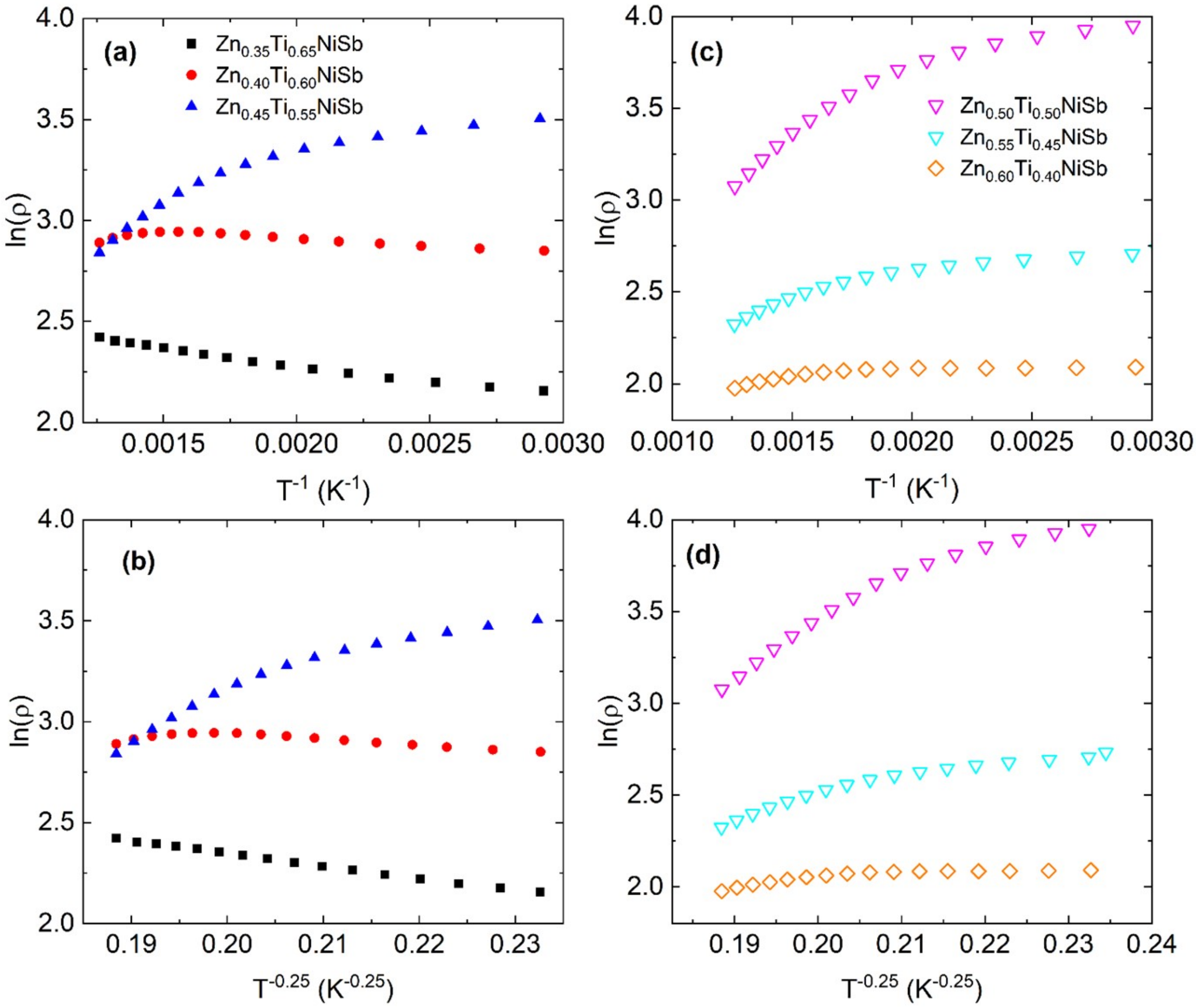

Figure S3: Temperature dependence of ln[$p(T)$] plotted against T^{-1} and $T^{-0.25}$ to check for pure thermally activated semiconducting and variable range hopping transport in **(a-b)** n-type and **(c-d)** p-type $Zn_{1-x}Ti_xNiSb$.

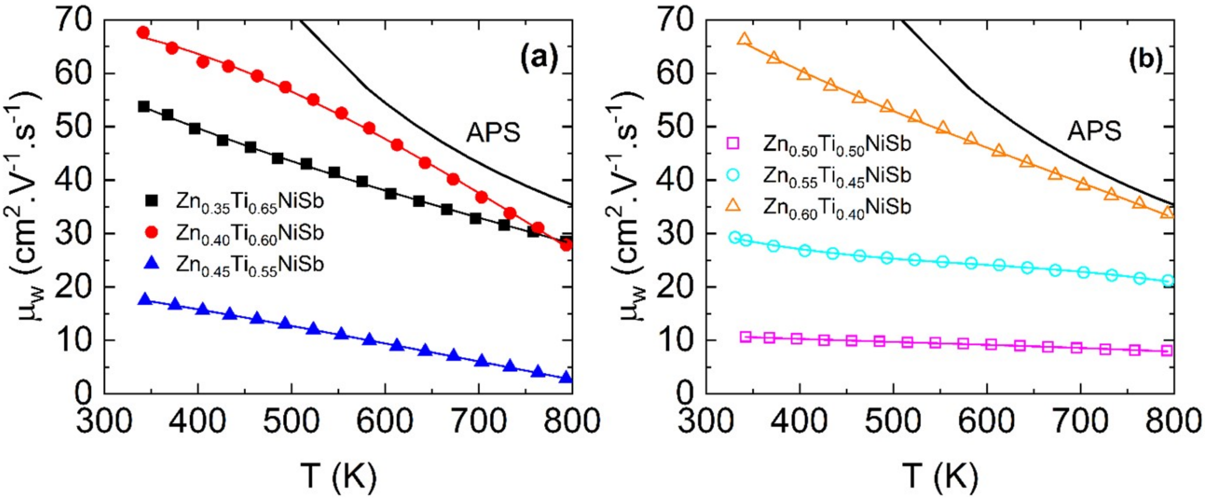

Figure S4: Temperature dependence of the weighted mobility (μ_w) calculated from *S(T)* and *ρ(T)* for **(a)** n-type and **(b)** p-type $Zn_{1-x}Ti_xNiSb$.[2]

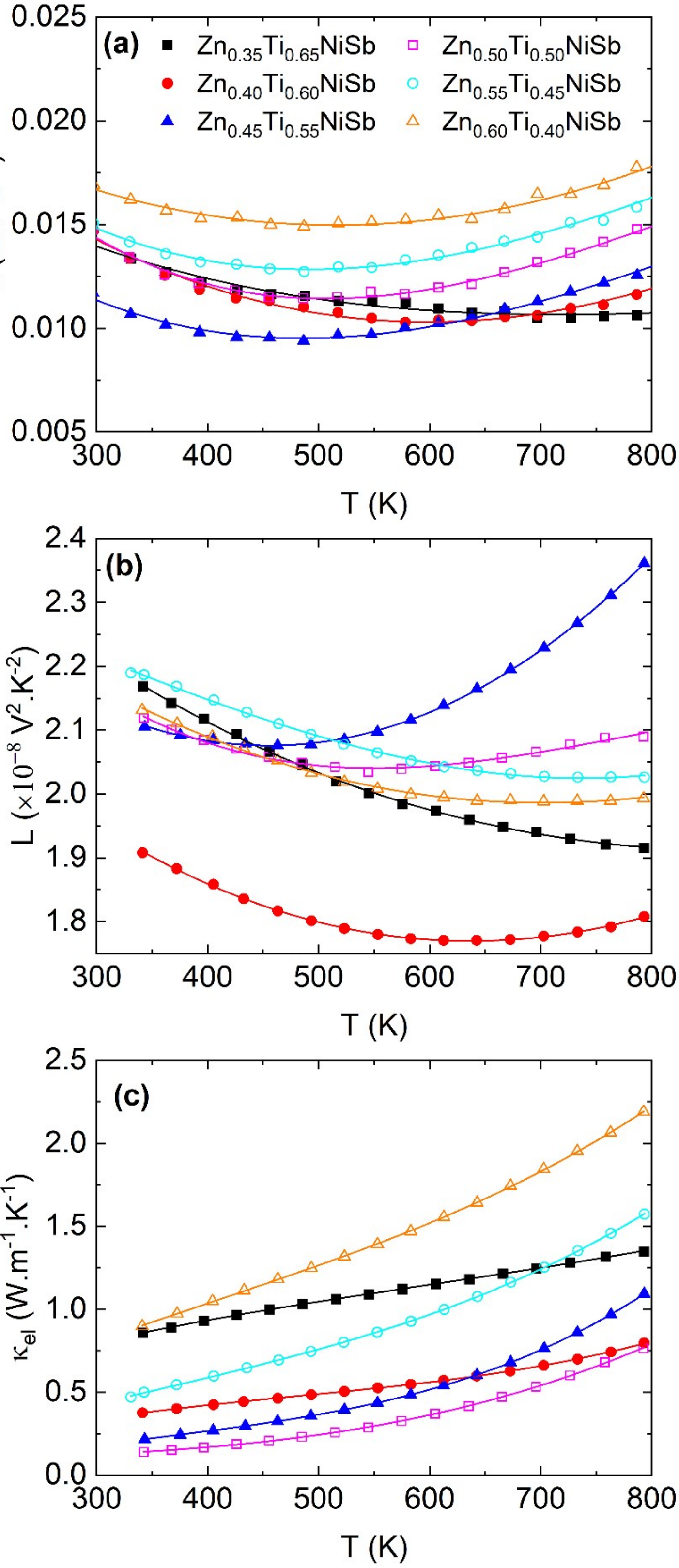

Figure S5: Temperature dependence of the **(a)** thermal diffusivity, **(b)** calculated Lorenz number,[3] and **(c)** electronic thermal conductivity ($\kappa_{el} = LT/\rho$) for the $Zn_{1-x}Ti_xNiSb$ samples.

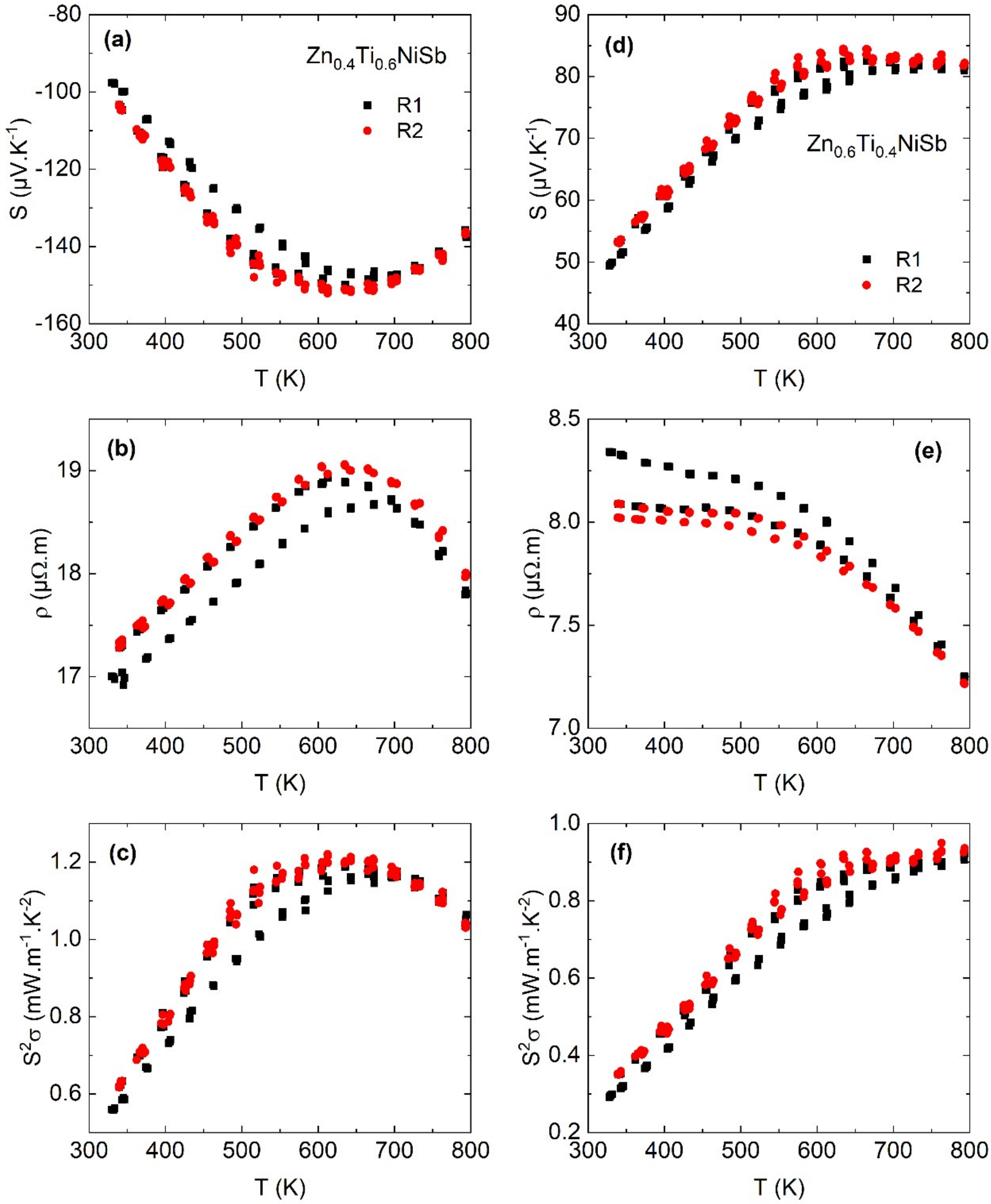

Figure S6: Thermal cycling for the best performing n-type $Zn_{0.4}Ti_{0.6}NiSb$ **(a-c)** and p-type $Zn_{0.6}Ti_{0.4}NiSb$ **(d-f)** samples. The first measurement on heating is slightly offset, but subsequent cooling-heating measurements fall on top of each other.

References

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3. H.-S. Kim, Z. M. Gibbs, Y. Tang, H. Wang and G. J. Snyder, *APL Materials*, 2015, **3**, 041506.