Supplementary information for:

Impact of Nb vacancies and p-type doping of the NbCoSn-NbCoSb half-Heusler thermoelectrics

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Table S1: Lattice parameters (Å) from x-ray powder diffraction for all NbCoSn based compositions synthesised using Ta foil.

Composition	*a* (Å)
NbCoSn	5.9500(5)
$NbCo_{1.05}Sn$	5.9506(4)
$Nb_{0.8}Ti_{0.2}Co_{1.05}Sn$	5.9660(5)
$Nb_{0.8}Zr_{0.2}Co_{1.05}Sn$	HH 1 5.9970(2) HH 2 5.9605(3) HH 3 5.9822(3)
$NbCo_{1.05}Sn_{0.75}Sb_{0.25}$	5.9438(1)
$NbCo_{1.05}Sn_{0.5}Sb_{0.5}$	5.9429(1)
NbCoSb	5.9004(1)
$NbCo_{1.05}Sb$	5.9028(1)

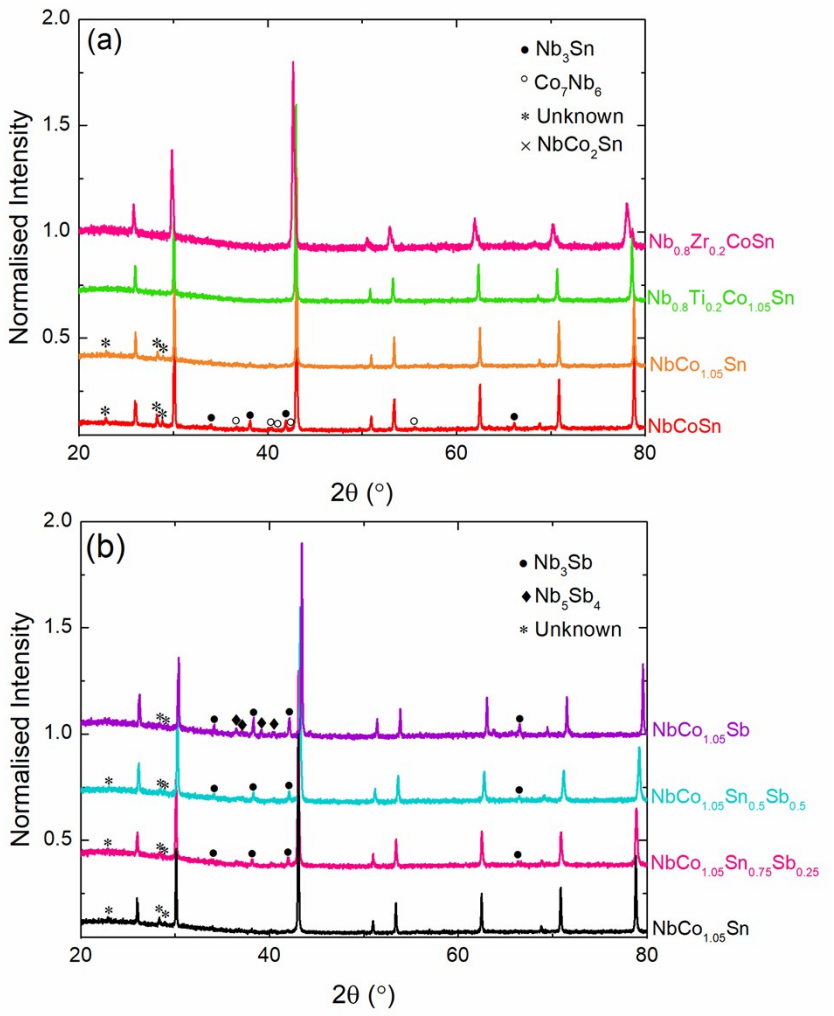

Figure S1: X-ray powder diffraction data for compositions annealed using Ta foil **(a)** $NbCo_{1+y}Sn$ (y = 0, 0.05), $Nb_{0.8}Ti_{0.2}Co_{1.05}Sn$, $Nb_{0.8}Zr_{0.2}CoSn$ and **(b)** $NbCo_{1.05}Sn_{1-z}Sb_z$ ($0 \leq z \leq 1$), after hot pressing.

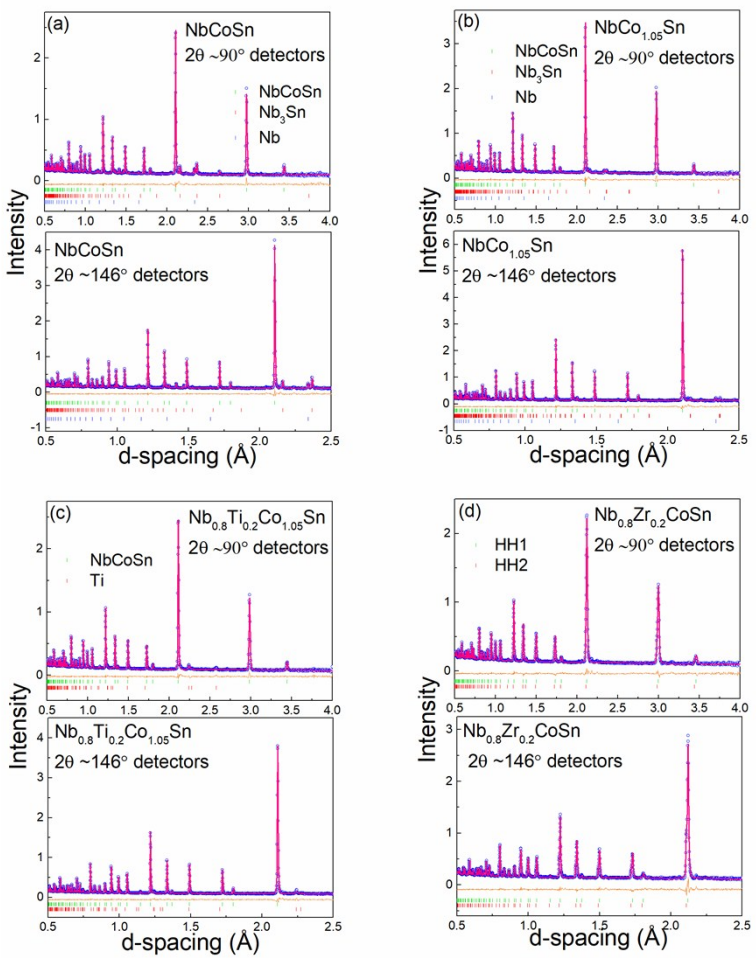

Figure S2: Fitted powder neutron diffraction profiles for **(a-b)** $NbCo_{1+y}Sn$ (y = 0, 0.05), **(c)** $Nb_{0.8}Ti_{0.2}CoSn$ and **(d)** $Nb_{0.8}Zr_{0.2}CoSn$. Blue circles are observed data, red lines are calculated profile, orange lines are difference profiles (obs-calc). Vertical lines indicate Bragg reflection positions (phases indicated in figures).

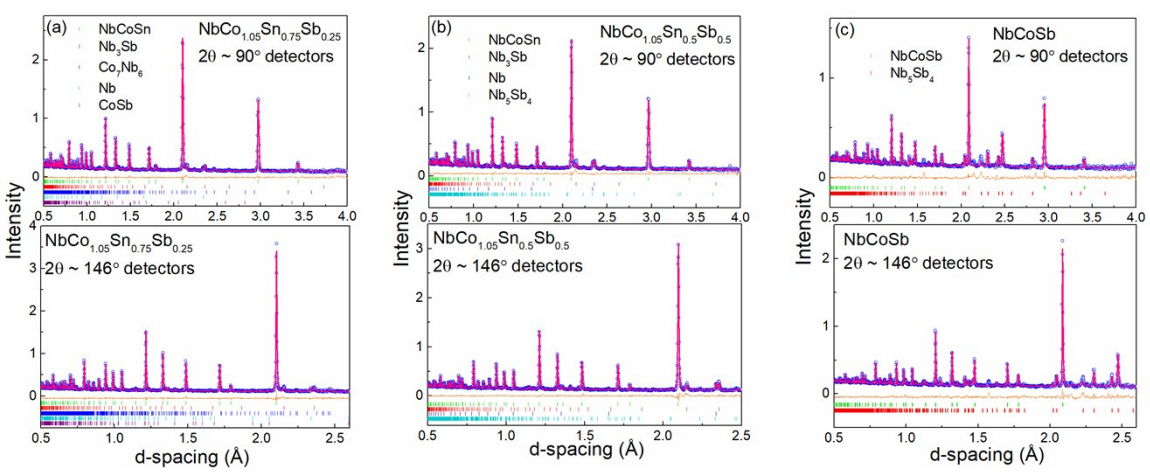

Figure S3 Fitted powder neutron diffraction profiles for **(a-c)** $NbCo_{1.05}Sn_{1-z}Sb_z$ (z = 0.25, 0.5, 1). Blue circles are observed data, red lines are calculated profile, orange lines are difference profiles (obs-calc). Vertical lines indicate Bragg reflection positions (phases indicated in figures).