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

Supporting Information

Thermoelectric properties of n-type half-Heusler NbCoSn with heavy-element Pt substitution

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Table S1. Calculated and Dulong-Petit (DP) specific heat, longitudinal and transversal sound velocities, coefficient of linear thermal expansion (CLTE) and density for $NbCo_{1-x}Pt_xSn$ with x = 0.05 and x = 0.10.

Composition	*Calc. C_p @300 K* $(Jg^{-1}K^{-1})$	*DP C_p* $(Jg^{-1}K^{-1})$	v_l (ms^{-1})	v_t (ms^{-1})	*CLTE* $(10^{-6}\ K^{-1})$	ρ (gcm^{-3})
$NbCo_{0.95}Pt_{0.05}Sn$	0.252	0.269	5563	3028	9.14	8.64 (99.2%)
$NbCo_{0.9}Pt_{0.1}Sn$	0.246	0.263	5471	2906	10.7	8.75 (98.3%)

Table S2. Structural parameters of NbCoSn and $NbCo_{0.95}Pt_{0.05}Sn$ obtained by Rietveld refinement of Synchrotron XRD patterns.

Composition	*NbCoSn*	*$NbCo_{0.95}Pt_{0.05}Sn$*
Latt.parameter a/Å	5.95386(4)	5.96556(3)
V/Å^3	211.055(2)	212.3020(17)
U_{iso}, Nb/Å^2	0.0018(16)	0.0041(13)
U_{iso}, Co/Pt/Å^2	0.0054(7)	0.0065(6)
U_{iso}, Sn /Å^2	0.0098(18)	0.0106(14)
R_I	3.15	2.06
R_p	6.18	9.42
R_{wp}	7.72	12.3
R_{exp}	4.97	7.27
χ^2	2.41	2.87

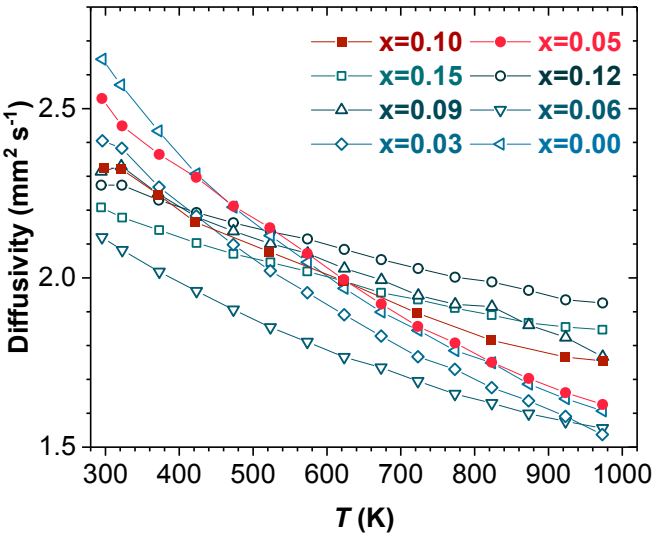

Figure S1. Temperature dependence of diffusivity for $NbCo_{1-x}Pt_xSn$.

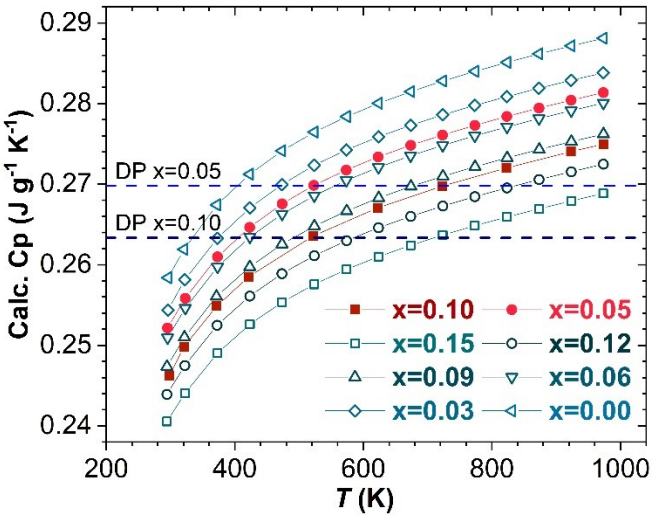

Figure S2. Calculated heat capacity from CLTE for $NbCo_{1-x}Pt_xSn$, with a comparison to the Dulong Petit (DP) values for $x = 0.05$ and $x = 0.1$.

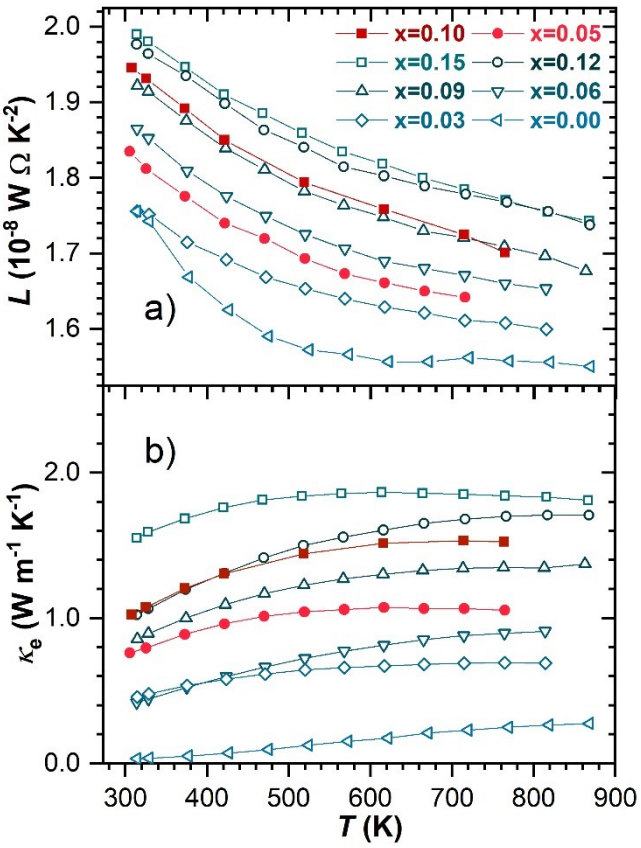

Figure S3. a) Calculated Lorentz number using the SPB model and b) Electronic thermal conductivity for $NbCo_{1-x}Pt_xSn$.

The experimental phonon scattering parameter were calculated using the following equations[1]:

$$\frac{\kappa_L}{\kappa_L^p} = \frac{tan^{-1}(u)}{u}; u^2 = \frac{\pi^2 \theta_D \Omega}{hv^2} \kappa_L^p \Gamma_{exp}$$

where $\Gamma_{expt,}$ u, v, h, Ω, and $^{\theta_D}$ are the experimental disorder scattering parameter, the disorder scaling parameter, the average lattice sound velocity, the Planck constant, the average volume/atom, and the Debye temperature, respectively.

Mass fluctuation scattering parameter was calculated by:

$$\Gamma_M = \frac{1}{3}\left(\frac{\bar{M}}{\bar{\bar{M}}}\right)^2 x(1-x)\left(\frac{M_1 - M_2}{\bar{M}}\right)^2$$

$$\bar{M} = xM_{Pt} + (1-x)M_{Co}$$

$$\bar{\bar{M}} = \frac{1}{3}(\bar{M} + M_{Nb} + M_{Sn})$$

where Γ_M and $M_{y,}$ are the experimental mass fluctuation scattering parameter and the atomic weight of the y element.

Table S3. Room temperature lattice thermal conductivity κ_L, calculated disorder parameter u, experimental (Γ_{exp}), mass (Γ_M) and strain field (Γ_S) fluctuations scattering parameters.

Composition	κ_L (W/ m K)	u	Γ_{exp}	Γ_M
NbCoSn	5.86	--	--	--
$NbCo_{0.97}Pt_{0.03}Sn$	4.79	0.89	0.0262	0.0214
$NbCo_{0.95}Pt_{0.05}Sn$	4.61	0.99	0.0329	0.0343
$NbCo_{0.94}Pt_{0.06}Sn$	4.34	1.16	0.0449	0.0404
$NbCo_{0.91}Pt_{0.09}Sn$	4.28	1.20	0.0452	0.0569
$NbCo_{0.90}Pt_{0.10}Sn$	4.00	1.39	0.0607	0.0620
$NbCo_{0.88}Pt_{0.12}Sn$	4.05	1.35	0.0579	0.0713
$NbCo_{0.85}Pt_{0.15}Sn$	3.22	2.02	0.1293	0.0837

References

1 J. Yang, G. P. Meisner and L. Chen, *Appl. Phys. Lett.*, 2004, **85**, 1140–1142.