Supplementary Information (SI) for Journal of Materials Chemistry A.

Title: Massive reduction in lattice thermal conductivity and strongly enhanced thermoelectric properties in Ge- and Se-doped CoSbS

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Supplementary Information:

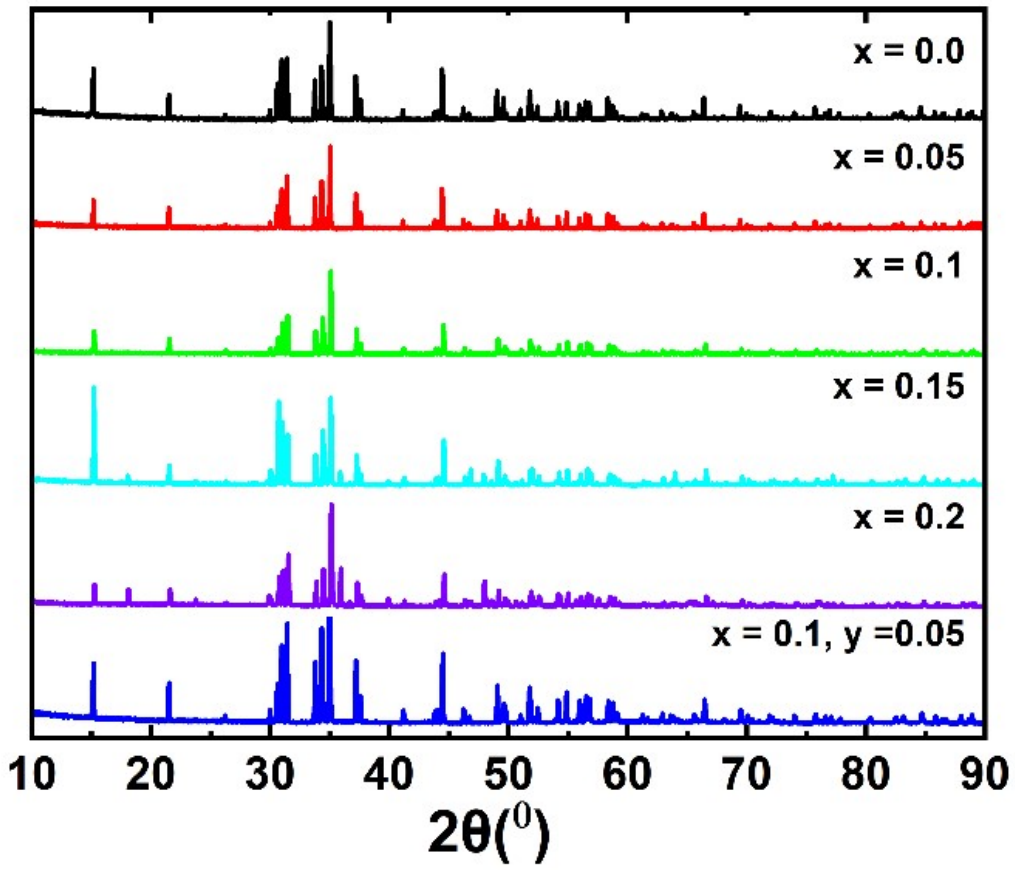

Figure S1. Powder X-ray diffraction pattern of all the polycrystalline $Co(Sb_{1+x}Ge_x)(S_{1-y}Se_y)$ samples.

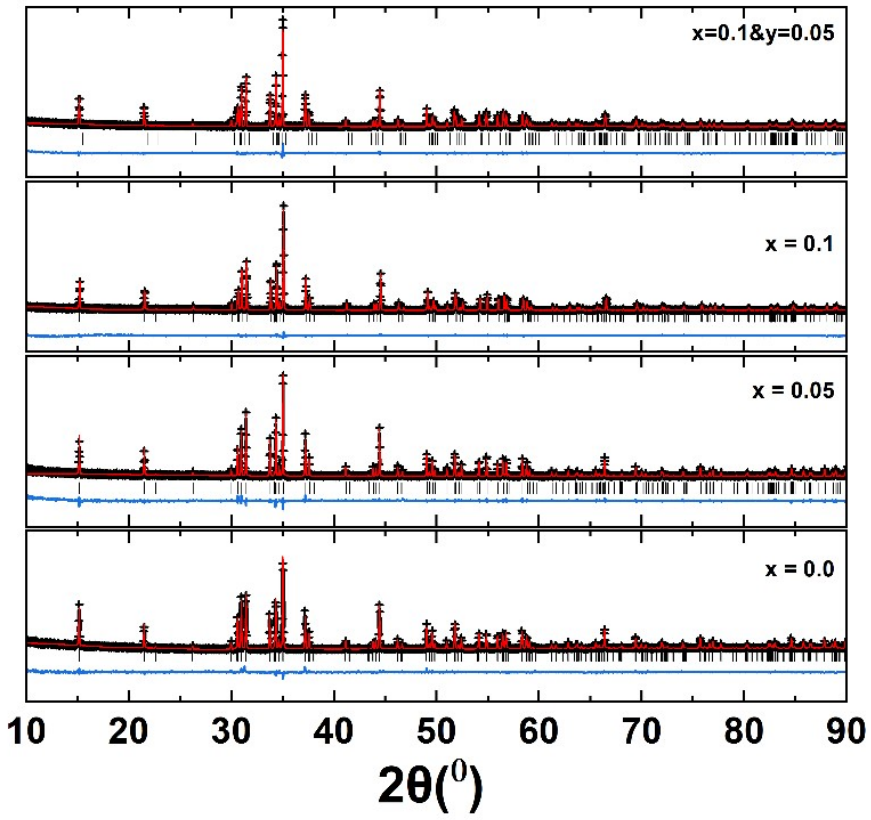

Figure S2. Rietveld refinement powder X-ray diffraction pattern of the polycrystalline $Co(Sb_{1+x}Ge_x)(S_{1-y}Se_y)$ samples. Black + are the observed pattern, Red lines represents the calculated pattern, vertical black bars are the Bragg positions, and the blue lines indicate the difference between observed and calculated patterns.

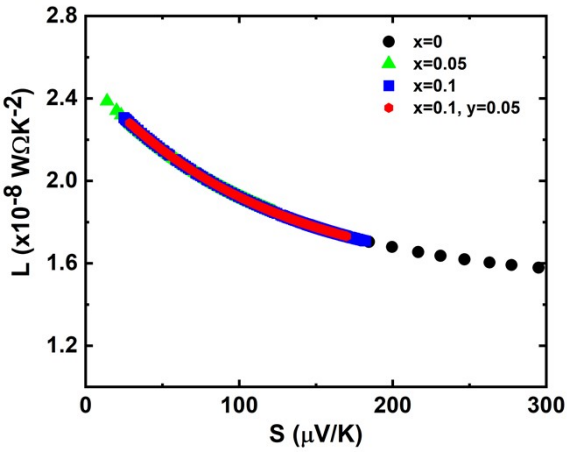

Figure S3. Lorentz number versus Seebeck coefficient for polycrystalline $Co(Sb_{1+x}Ge_x)(S_{1-y}Se_y)$ samples.

Table S1. Atomic positions and occupancies obtained from Rietveld refinement of XRD pattern for the $Co(Sb_{1+x}Ge_x)(S_{1-y}Se_y)$ samples.

Sample	Element	X	Y	Z	Biso	Occup.
x = 0.0	**Co**	0.012(4)	0.164(5)	0.384(4)	0.447	1.0000
	Sb	0.116(3)	0.050(3)	0.179(1)	0.962	0.997(3)
	S	-0.135(1)	0.306(1)	0.065(6)	1.068	0.996(2)
x = 0.05	**Co**	0.012(3)	0.166(3)	0.385(4)	1.03	1.0000
	Sb	0.117(4)	0.050(4)	0.179(4)	1.072	0.9492(3)
	Ge	0.117(4)	0.050(4)	0.179(4)	1.072	0.0503(3)
	S	-0.134(3)	0.306(3)	0.066(4)	1.048	1.0000
x = 0.10	**Co**	0.012(6)	0.165(6)	0.383(3)	1.085	1.0000
	Sb	0.118(3)	0.048(2)	0.180(3)	0.996	0.8952(3)
	Ge	0.118(3)	0.048(2)	0.180(3)	0.996	0.0997(3)
	S	-0.134(1)	0.306(8)	0.071(4)	1.114	1.0000
x = 0.15	**Co**	0.014(3)	0.153(3)	0.376(4)	1.455	1.0000
	Sb	0.115(4)	0.049(4)	0.178(4)	0.429	0.860(3)
	Ge	0.115(4)	0.049(4)	0.178(4)	0.429	0.138(3)
	S	-0.137(3)	0.304(3)	0.087(4)	2.487	1.0000
x=0.1&y=0.05	**Co**	0.013(3)	0.163(3)	0.385(4)	1.644	1.0000
	Sb	0.118(4)	0.047(4)	0.179(4)	1.323	0.9072(3)
	Ge	0.118(4)	0.047(4)	0.179(4)	1.323	0.1000(4)
	S	-0.134(3)	0.307(3)	0.066(3)	1.295	0.9778(3)
	Se	-0.134(3)	0.307(3)	0.066(3)	1.295	0.0375(3)

Table S2. Crystal lattice parameters obtained from Rietveld refinement of XRD pattern for the $Co(Sb_{1+x}Ge_x)(S_{1-y}Se_y)$ samples.

Sample	a(Å)	b(Å)	c(Å)
x = 0.0	5.8431(6)	5.9567(6)	11.6700(4)
x = 0.05	5.8386(5)	5.9513(5)	11.6593(4)
x = 0.10	5.8365(5)	5.9455(5)	11.6405(4)
x = 0.15	5.8384(4)	5.9439(4)	11.6330(4)
x = 0.2	5.8434(4)	5.9524(4)	11.6503(4)
x=0.1&y=0.05	5.8481(4)	5.9547(5)	11.6579(4)