Supporting Information

The Solid Solution $Yb_{2-x}Ca_xCdSb_2$: Structure, Thermoelectric Properties, and Quality Factor

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Table S1: EMPA Compositions for Polycrystalline Samples of $Yb_{2-x}Ca_xCdSb_2$ (x = 0, 0.2, 03, 0.5)

Sample		At %				Formula	
	x	Yb	Ca	Cd	Sb		Cation Total
Yb_2CdSb_2	0	39.6(2)		20.3(1)	40.2(2)	$Yb_{1.98(1)}Cd_{1.016(7)}Sb_{2.01(1)}$	1.98(1)
$Yb_{1.8}Ca_{0.2}CdSb_2$	0.2	35.7(4)	3.8(2)	20.6(3)	40.0(1)	$Yb_{1.78(2)}Ca_{0.189(9)}Cd_{1.03(1)}Sb_{2.000(7)}$	1.97(2)
$Yb_{1.7}Ca_{0.3}CdSb_2$	0.3	33.9(4)	5.9(4)	20.6(5)	39.7(1)	$Yb_{1.69(5)}Ca_{0.29(2)}Cd_{1.03(2)}Sb_{1.984(7)}$	1.98(3)
$Yb_{1.5}Ca_{0.5}CdSb_2$	0.5	30(1)	9.7(7)	21(2)	39.82(9)	$Yb_{1.48(5)}Ca_{0.49(4)}Cd_{1.04(8)}Sb_{1.991(4)}$	1.97(6)

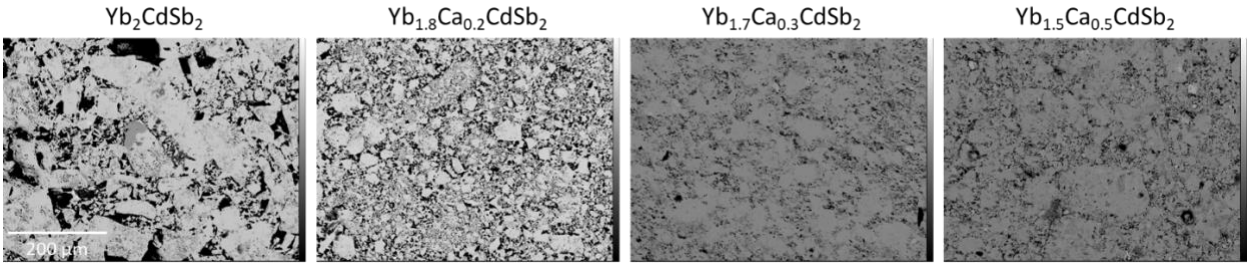


Figure S1. EMPA backscatter images for $Yb_{2-x}Ca_xCdSb_2$ (x = 0, 0.2, 03, 0.5) pressed pellets prepared via spark plasma sintering (SPS).

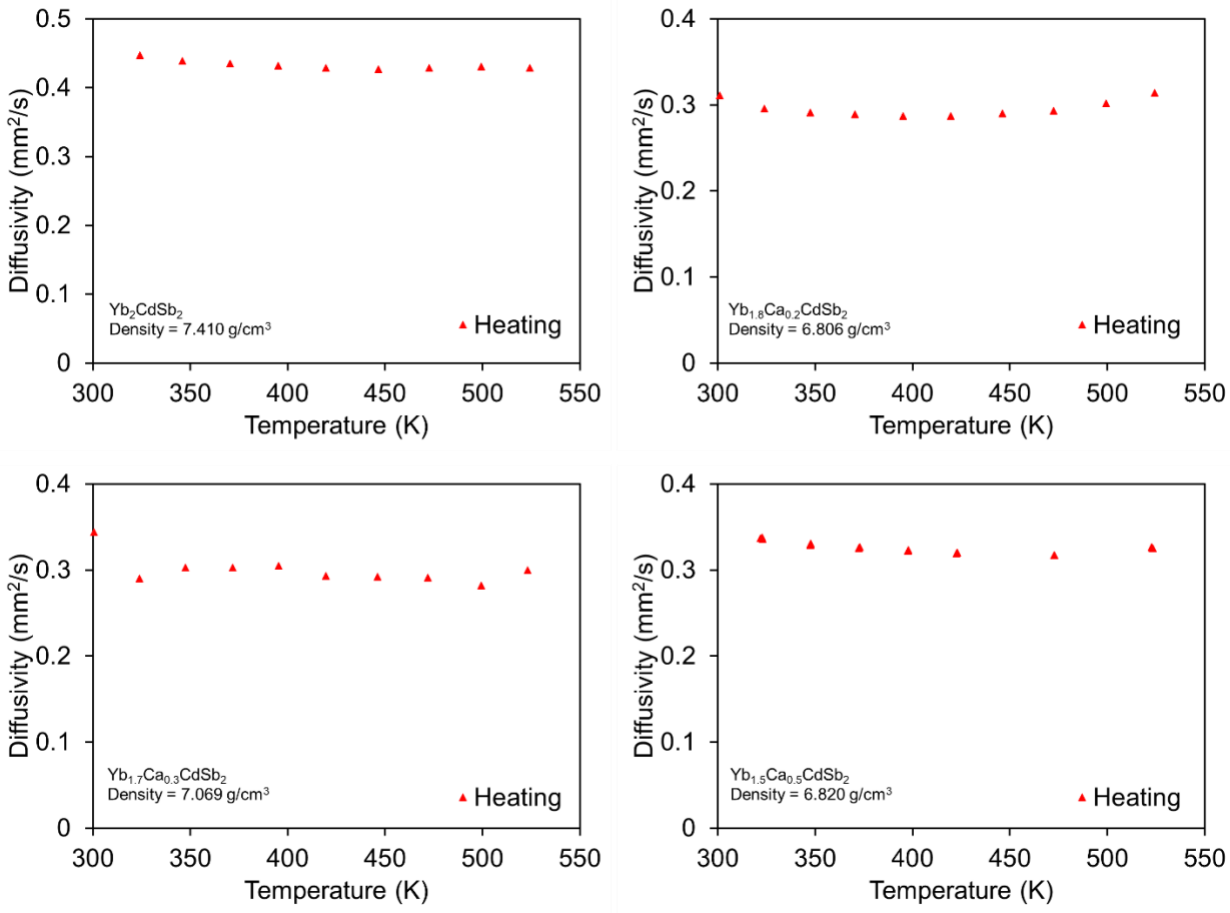


Figure S2. Caption Below

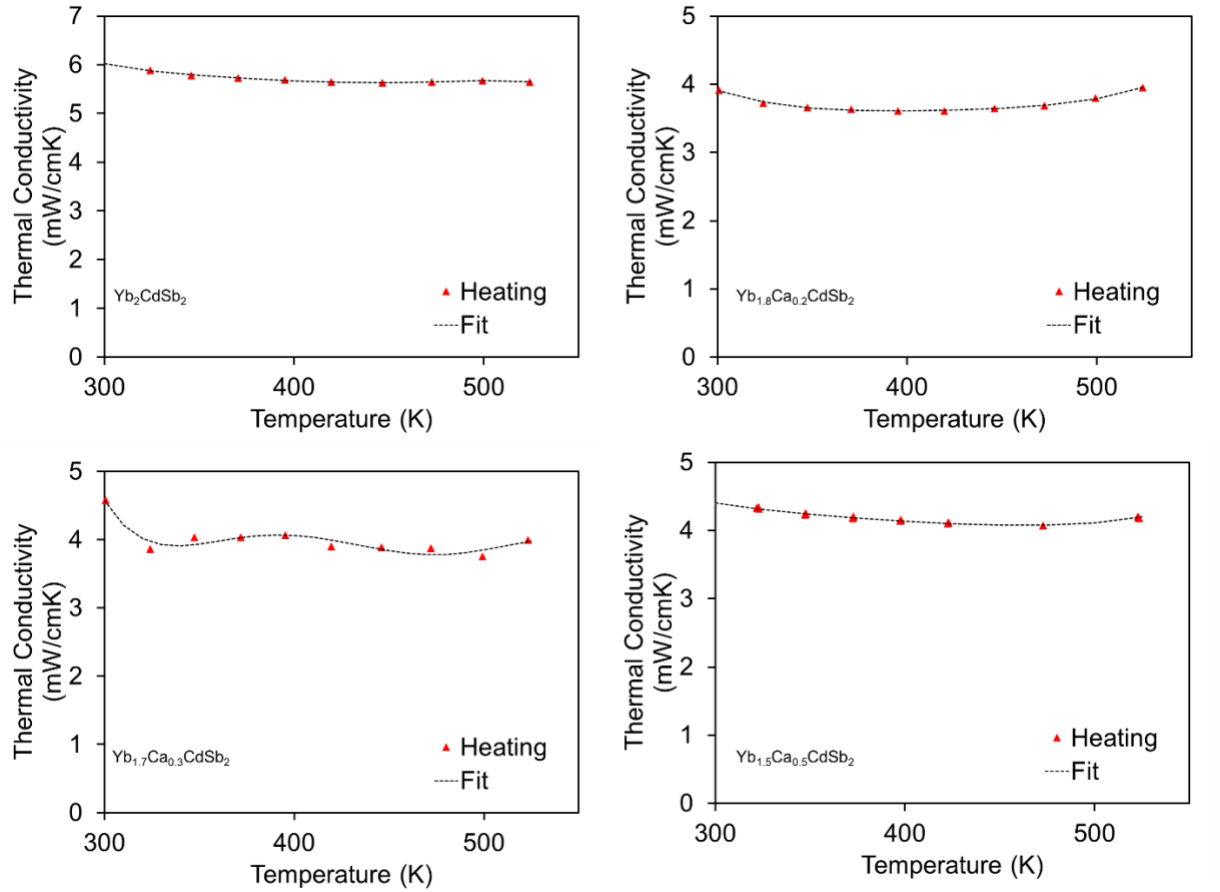
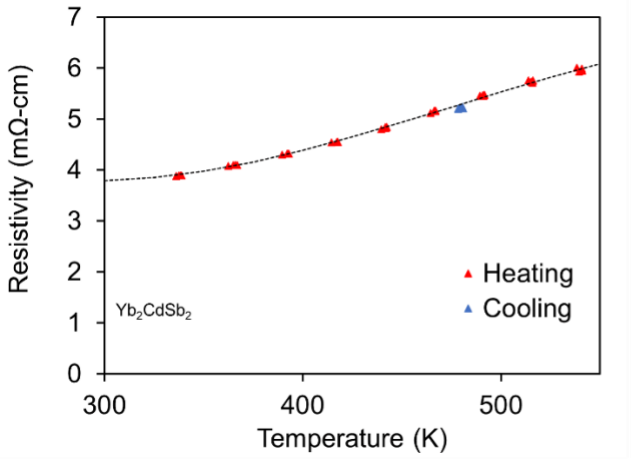
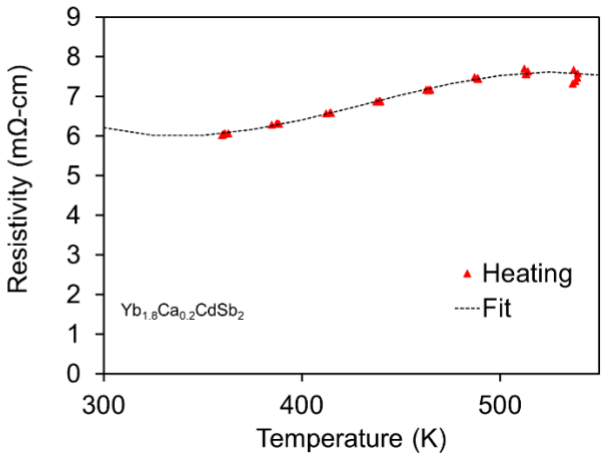
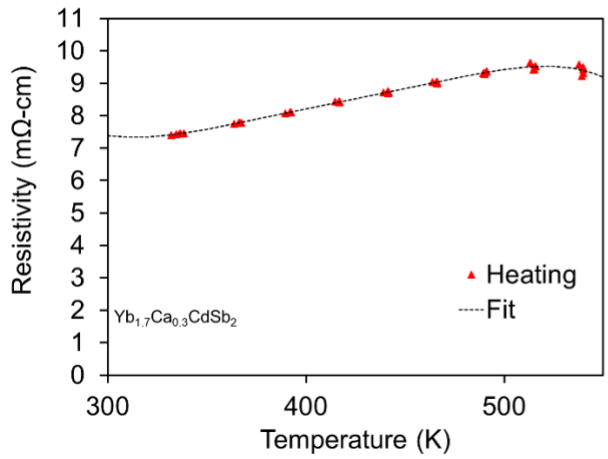


Figure S2. Caption Below


Resistivity (mΩ-cm)
Temperature (K)
Yb2CdSb2
Heating
Cooling


Resistivity (mΩ-cm)
Temperature (K)
Yb1.8Ca0.2CdSb2
Heating
Fit


Resistivity (mΩ-cm)
Temperature (K)
Yb1.7Ca0.3CdSb2
Heating
Fit

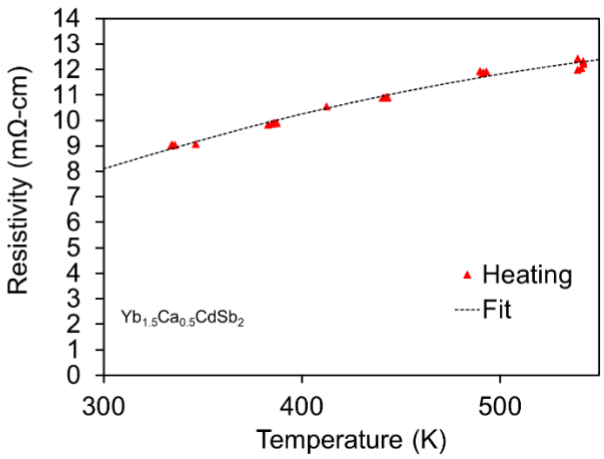

Resistivity (mΩ-cm)
Temperature (K)
Yb1.5Ca0.5CdSb2
Heating
Fit

Figure S2. Caption Below

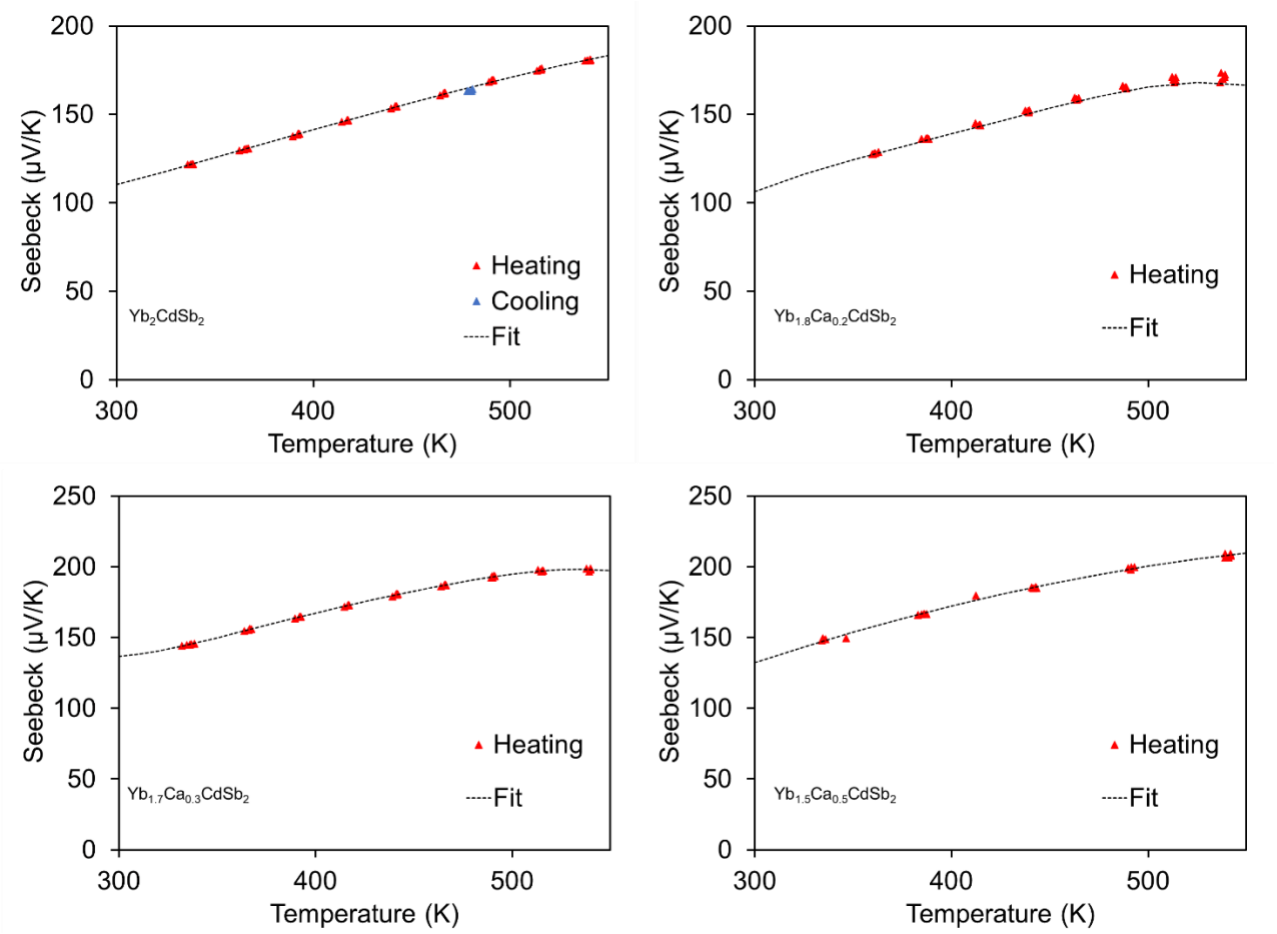


Figure S2. Experimental thermoelectric data of diffusivity, thermal conductivity, electrical resistivity, and Seebeck coefficients with polynomial fits for $Yb_{2-x}Ca_xCdSb_2$ (x = 0, 0.2, 03, 0.5) pressed pellets.

Table S2. Crystallographic Information and Structural Refinement for $Yb_{2-x}Ca_xCdSb_2$ (x = 0, 0.13, 0.27 0.39, 0.66, 0.8, 0.97, 1.25, and 1.48)

Empirical formula	Yb_2CdSb_2	$Yb_{1.87}Ca_{0.13}CdSb_2$	$Yb_{1.73}Ca_{0.27}CdSb_2$
Temperature (K)		100(2)	
Crystal system		Orthorhombic	
Space group, Z		$Cmc2_1$, 4	
Unit cell dimensions	a = 4.6091(3) Å α = 90°	a = 4.6121(2) Å α = 90°	a = 4.6225(5) Å α = 90°
	b = 17.3995(13) Å β = 90°	b = 17.4185(9) Å β = 90°	b = 17.431(2) Å β = 90°
	c = 7.1623(5) Å γ = 90°	c = 7.1702(4) Å γ = 90°	c = 7.1897(8) Å γ = 90°
Volume (Å^3)	574.39(7)	576.02(5)	579.30(11)
Density (calculated) (g/cm^3)	8.118	7.895	7.637
Absorption coefficient (mm^{-1})	45.001	42.904	40.553
F(000)	1160	1134	1106
Crystal size (mm^3)	0.151 x 0.075 x 0.063	0.118 x 0.075 x 0.041	0.060 x 0.032 x 0.022
Theta range for data collection (°)	3.685 to 30.078	3.681 to 27.287	2.337 to 30.509
Reflections collected	7575	3624	4642
Independent reflections	920 [R(int) = 0.0324]	729 [R(int) = 0.0341]	984 [R(int) = 0.0313]
Completeness to theta = 25.242° (%)	99.7	99.7	100
Max. and min. transmission	0.0867 and 0.0287	0.1290 and 0.0586	0.3468 and 0.2115
Data / restraints / parameters	920 / 1 / 33	729 / 1 / 33	984 / 13 / 44
Goodness-of-fit on F2	1.174	1.079	1.119
Final R indices [I>2sigma(I)]	R1 = 0.0170, wR2 = 0.0400	R1 = 0.0195, wR2 = 0.0480	R1 = 0.0204, wR2 = 0.0467
R indices (all data)	R1 = 0.0170, wR2 = 0.0400	R1 = 0.0195, wR2 = 0.0480	R1 = 0.0211, wR2 = 0.0470
Absolute structure parameter	0.794(12)	0.230(18)	0.538(17)
Extinction coefficient	0.00222(17)	0.0029(2)	-----
Largest diff. peak and hole (e.Å^{-3})	1.576 and -2.405	1.358 and -1.985	1.531 and -2.958

Empirical formula	$Yb_{1.61}Ca_{0.39}CdSb_2$	$Yb_{1.34}Ca_{0.66}CdSb_2$	$Yb_{1.20}Ca_{0.80}CdSb_2$
Temperature (K)		100(2)	
Crystal system		Orthorhombic	
Space group, Z		$Cmc2_1$, 4	
Unit cell dimensions	a = 4.6218(7) Å α = 90°	a = 4.6219(5) Å α = 90°	a = 4.6216(3) Å α = 90°
	b = 17.434(3) Å β = 90°	b = 17.4516(18) Å β = 90°	b = 17.4509(12) Å β = 90°
	c = 7.1930(12) Å γ = 90°	c = 7.1997(8) Å γ = 90°	c = 7.2123(5) Å γ = 90°
Volume (Å^3)	579.57(16)	580.72 (11)	581.68(7)
Density (calculated) (g/cm^3)	7.451	7.025	6.801
Absorption coefficient (mm^{-1})	38.728	34.595	32.438
F(000)	1082	1028	1000
Crystal size (mm^3)	0.111 x 0.061 x 0.033	0.029 x 0.021 x 0.017	0.061 x 0.042 x 0.030
Theta range for data collection (°)	2.336 to 27.483	2.334 to 30.470	3.665 to 28.672
Reflections collected	3692	3869	3486
Independent reflections	743 [R(int) = 0.0282]	977 [R(int) = 0.0293]	835 [R(int) = 0.0271]
Completeness to theta = 25.242° (%)	99.7	100	99.7
Max. and min. transmission	0.1830 and 0.0880	0.5745 and 0.4165	0.3704 and 0.2307
Data / restraints / parameters	743 / 1 / 32	977 / 13 / 44	835 / 13 / 45
Goodness-of-fit on F2	1.103	1.125	1.103
Final R indices [I>2sigma(I)]	R1 = 0.0174, wR2 = 0.0429	R1 = 0.0220, wR2 = 0.0487	R1 = 0.0177, wR2 = 0.0434
R indices (all data)	R1 = 0.0177, wR2 = 0.0431	R1 = 0.0238, wR2 = 0.0496	R1 = 0.0178, wR2 = 0.0434
Absolute structure parameter	0.622(18)	0.49(2)	0.79(2)
Extinction coefficient	-----	-----	0.00161(15)
Largest diff. peak and hole (e.Å^{-3})	2.045 and -1.575	1.605 and -2.465	1.816 and -1.271

Empirical formula	$Yb_{1.03}Ca_{0.97}CdSb_2$	$Yb_{0.75}Ca_{1.25}CdSb_2$	$Yb_{0.52}Ca_{1.48}CdSb_2$
Temperature (K)		100(2)	
Crystal system		Orthorhombic	
Space group, Z		$Pnma$, 4	
Unit cell dimensions	a = 7.2089(7) Å α = 90°	a = 7.2232(5) Å α = 90°	a = 7.2236(6) Å α = 90°
	b = 4.6127(5) Å β = 90°	b = 4.6120(3) Å β = 90°	b = 4.6090(4) Å β = 90°
	c = 17.5036(18) Å γ = 90°	c = 17.5201(12) Å γ = 90°	c = 17.5079(15) Å γ = 90°
Volume (Å^3)	582.04(10)	583.65(7)	582.90(9)
Density (calculated) (g/cm^3)	6.539	6.097	5.761
Absorption coefficient (mm^{-1})	29.870	25.602	22.231
F(000)	966	910	864
Crystal size (mm^3)	0.049 x 0.030 x 0.023	0.077 x 0.036 x 0.027	0.040 x 0.037 x 0.023
Theta range for data collection (°)	3.056 to 30.516	3.050 to 30.045	3.051 to 30.038
Reflections collected	7752	7217	7044
Independent reflections	993 [R(int) = 0.0452]	954 [R(int) = 0.0288]	949 [R(int) = 0.0448]
Completeness to theta = 25.242° (%)	99.7	99.8	99.8
Max. and min. transmission	0.4943 and 0.3283	0.4589 and 0.3175	0.5920 and 0.4831
Data / restraints / parameters	993 / 12 / 44	954 / 12 / 44	949 / 12 / 43
Goodness-of-fit on F2	1.112	1.061	1.139
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0559	R1 = 0.0191, wR2 = 0.0454	R1 = 0.0297, wR2 = 0.0630
R indices (all data)	R1 = 0.0407, wR2 = 0.0598	R1 = 0.0212, wR2 = 0.0465	R1 = 0.0390, wR2 = 0.0662
Absolute structure parameter	-----	-----	-----
Extinction coefficient	0.00096(8)	0.00204(14)	-----
Largest diff. peak and hole (e.Å^{-3})	2.493 and -2.321	1.169 and -1.516	1.443 and -2.029

Table S3. Atomic Coordinates (x 10^4) with Equivalent Isotropic Atomic Displacement Parameters (Ueq)[a] and Fractional Occupancy for the $Yb_{2-x}Ca_xCdSb_2$ (x = 0, 0.13, 0.27 0.39, 0.66, 0.8, 0.97, 1.25, and 1.48)

Cmc2 1

Yb_2CdSb_2

	Occ.	x	y	z	U(eq)
Yb(1)	1	0	3026(1)	5296(1)	12(1)
Yb(2)	1	0	4788(1)	2210(1)	10(1)
Cd(1)	1	0	990(1)	3960(1)	11(1)
Sb(1)	1	0	672(1)	3(1)	9(1)
Sb(2)	1	0	3215(1)	116(1)	10(1)

$Yb_{1.87}Ca_{0.13}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.910/0.090	0	3027(1)	5299(1)	10(1)
Yb/Ca(2)[b]	0.958/0.042	0	4788(1)	2210(1)	8(1)
Cd(1)	1	0	990(1)	3956(2)	9(1)
Sb(1)	1	0	671(1)	3(2)	6(1)
Sb(2)	1	0	3217(1)	109(2)	8(1)

$Yb_{1.73}Ca_{0.27}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.840/0.160	0	3025(1)	5294(1)	8(1)
Yb/Ca(2)[b]	0.892/0.076	0	4788(1)	2216(1)	4(1)
Ca(3)[c]	0.032	0	5220(60)	2840(140)	2(2)
Cd(1)[c]	0.968	0	989(1)	3956(2)	5(1)
Cd(2)[c]	0.032	0	980(20)	6100(50)	7(3)
Sb(1)	1	0	671(1)	4(2)	4(1)
Sb(2)	1	0	3215(1)	102(2)	5(1)

$Yb_{1.61}Ca_{0.39}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.756/0.244	0	3024(1)	5296(1)	11(1)
Yb/Ca(2)[b]	0.856/0.144	0	4788(1)	2215(1)	7(1)
Cd(1)	1	0	988(1)	3956(2)	9(1)
Sb(1)	1	0	671(1)	6(1)	7(1)
Sb(2)	1	0	3217(1)	96(2)	8(1)

$Yb_{1.34}Ca_{0.66}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.606/0.394	0	3026(1)	5297(1)	8(1)
Yb/Ca(2)[b]	0.738/0.212	0	4787(1)	2221(1)	4(1)
Ca(3)[c]	0.050	0	5220(30)	2940(90)	3(2)
Cd(1)[c]	0.950	0	989(1)	3957(2)	5(1)
Cd(2)[c]	0.050	0	984(13)	6030(30)	7(3)
Sb(1)	1	0	671(1)	19(1)	4(1)
Sb(2)	1	0	3217(1)	107(2)	5(1)

$Yb_{1.20}Ca_{0.80}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.526/0.474	0	3025(1)	5295(1)	9(1)
Yb/Ca(2)[b]	0.674/0.304	0	4786(1)	2210(1)	5(1)
Ca(3)[c]	0.022	0	5170(80)	2940(190)	3(3)
Cd(1)[c]	0.978	0	988(1)	3948(2)	6(1)
Cd(2)[c]	0.022	0	980(30)	6220(80)	7(4)
Sb(1)	1	0	670(1)	7(1)	4(1)
Sb(2)	1	0	3217(1)	97(1)	6(1)

Pnma

$Yb_{1.03}Ca_{0.97}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.426/0.574	2312(1)	2500	4467(1)	9(1)
Yb/Ca(2)[b]	0.584/0.360	352(1)	2500	2287(1)	6(1)
Ca/Yb(3)[c]	0.038/0.018	9640(20)	2500	2722(9)	4(2)
Cd(1)[c]	0.944	1389(1)	2500	6509(1)	5(1)
Cd(2)[c]	0.056	3580(20)	2500	6528(7)	9(1)
Sb(1)	1	2453(1)	2500	8166(1)	5(1)
Sb(2)	1	2429(1)	2500	715(1)	6(1)

$Yb_{0.75}Ca_{1.25}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.298/0.702	2307(1)	2500	4466(1)	8(1)
Yb/Ca(2)[b]	0.446/0.518	351(1)	2500	2284(1)	5(1)
Ca/Yb(3)[c]	0.028/0.008	9660(20)	2500	2728(9)	4(1)
Cd(1)[c]	0.96	1387(1)	2500	6509(1)	5(1)
Cd(2)[c]	0.036	3599(16)	2500	6515(7)	11(1)
Sb(1)	1	2454(1)	2500	8165(1)	4(1)
Sb(2)	1	2432(1)	2500	715(1)	5(1)

$Yb_{0.52}Ca_{1.48}CdSb_2$

	Occ.	x	y	z	U(eq)
Yb/Ca(1)[b]	0.196/0.804	2310(2)	2500	4468(1)	9(1)
Yb/Ca(2)[b]	0.318/0.630	350(1)	2500	2284(1)	5(1)
Ca/Yb(3)[c]	0.042/0.010	9620(30)	2500	2736(11)	5(1)
Cd(1)[c]	0.948	1384(1)	2500	6508(1)	5(1)
Cd(2)[c]	0.052	3566(18)	2500	6512(7)	7(1)
Sb(1)	1	2458(1)	2500	8165(1)	4(1)
Sb(2)	1	2438(1)	2500	715(1)	6(1)

[a] U_{eq} ($Å^2$ x 10^3) is defined as one-third of the trace of the orthogonalized Uij tensor.
[b] Ca/Yb mixed site.
[c] Partially occupied site.

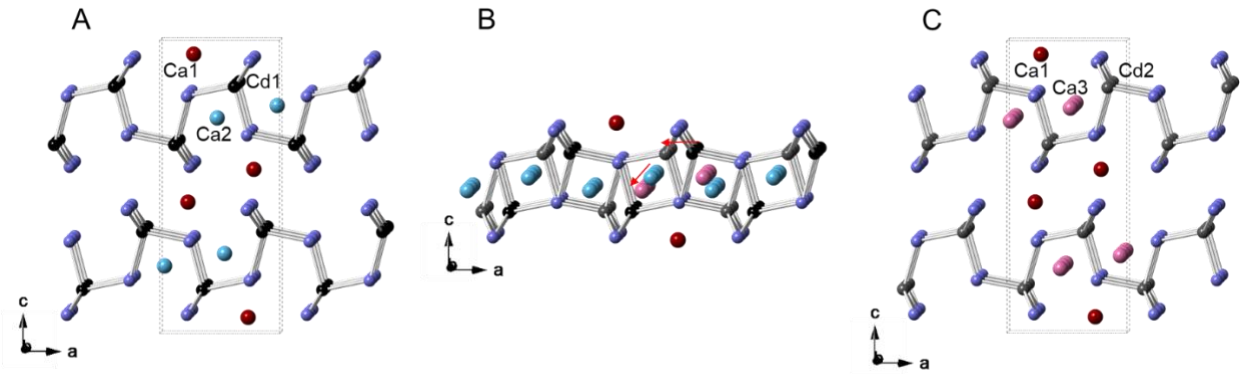


Figure S3. Shifting of the Cd1 and Yb2 sites results in a flipping of the CdSb4 chain in ~2% of the overall structure above $x = 0.6$ for $Yb_{2-x}Ca_xCdSb_2$.

A. The majority of the structure with Yb2 and Cd1 atomic positions.

B. The shifting of Cd1 atomic position to the Cd2 atomic position and the Yb2 atomic position shifting to the Ca3 atomic position.

C. The minority of the structure with Ca3 and Cd2 atomic positions.

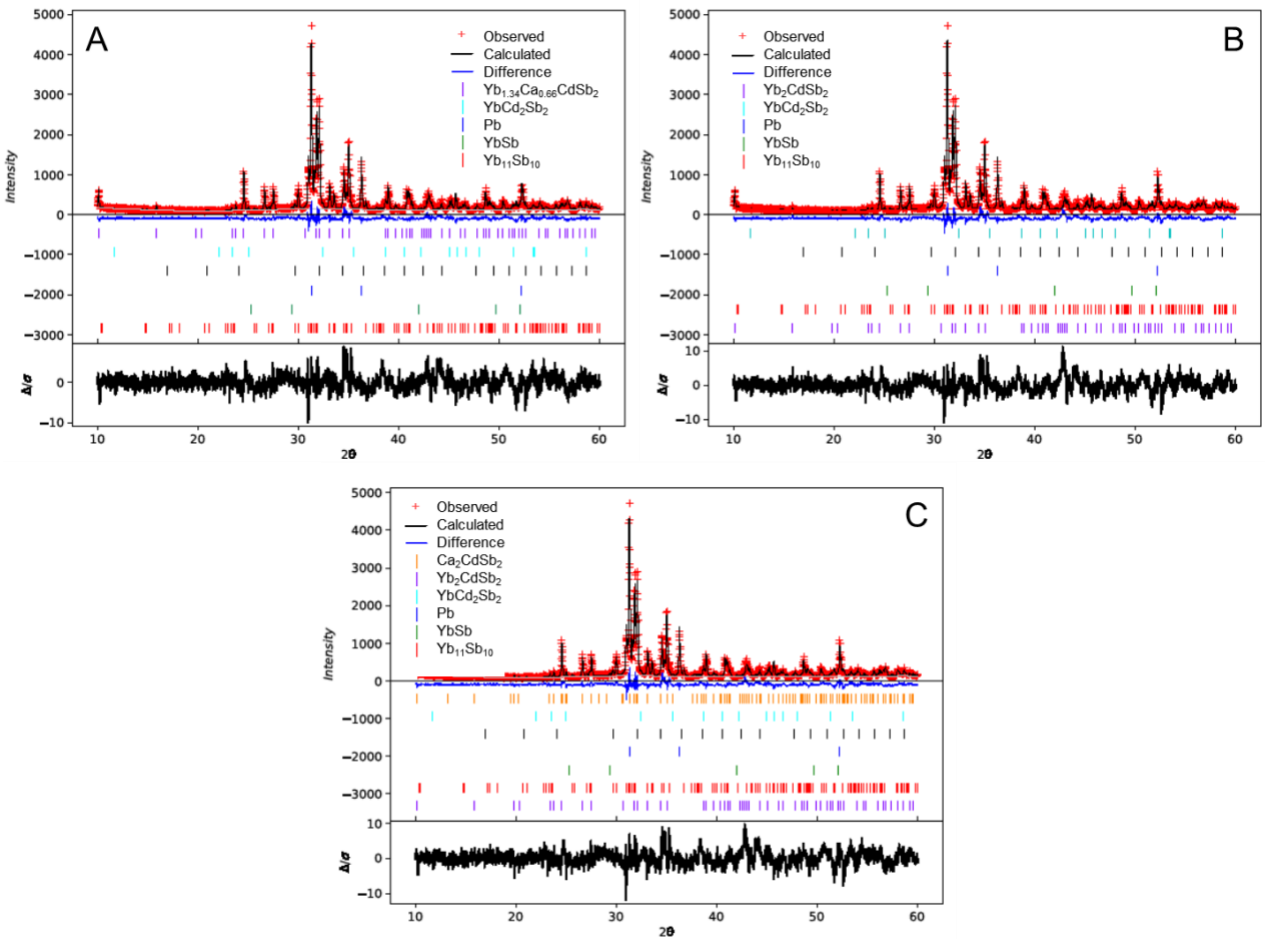


Figure S4. Rietveld refinements of $Yb_{1.03}Ca_{0.97}CdSb_2$. The data are indicated in red, calculated in black, difference in blue and the various phases as shown on the legend. Tick marks are the expected peak positions. An expanded view of the difference map is show at the bottom in black. A. with the cif file from the resulting single crystal characterization. B. Using only the cif file from the Yb_2CdSb_2 space group. C. Using both the Yb_2CdSb_2 cif and the Ca_2CdSb_2 cif.

Table S4. Refinement Statistics from the $Yb_{1.34}Ca_{0.66}CdSb_2$ Rietveld Refinements.

	A $Yb_{1.34}Ca_{0.66}CdSb_2$		B Yb_2CdSb_2		C Yb_2CdSb_2		 Ca_2CdSb_2	
Unit Cell Parameters	a =	4.6227(2)	a =	4.6225(2)	a =	4.6224(2)	a =	7.236(3)
	b =	17.4820(6)	b =	17.4809(7)	b =	17.4787(7)	b =	4.624(1)
	c =	7.2434(3)	c =	7.2429(3)	c =	7.2434(3)	c =	17.511(6)
	V =	585.37(3)	V =	585.26(3)	V =	585.2(3)	V =	585.9(3)
Rp (%), Rwp (%)		9.39, 12.35		10.25, 13.47				9.90, 12.99
Ca_2CdSb_2 (%)		---		---				6.1(4)
Yb_2CdSb_2 (%)		45.2(4)		41.6(4)				36.9(5)
$YbCd_2Sb_2$ (%)		1.2(1)		1.3(1)				1.1(1)
$Yb_{11}Sb_{10}$ (%)		41.2(5)		43.7(6)				42.9(5)
YbSb (%)		0.42(6)		0.45(7)				0.48(6)
Pb (%)		10.9(1)		11.8(1)				11.5(1)

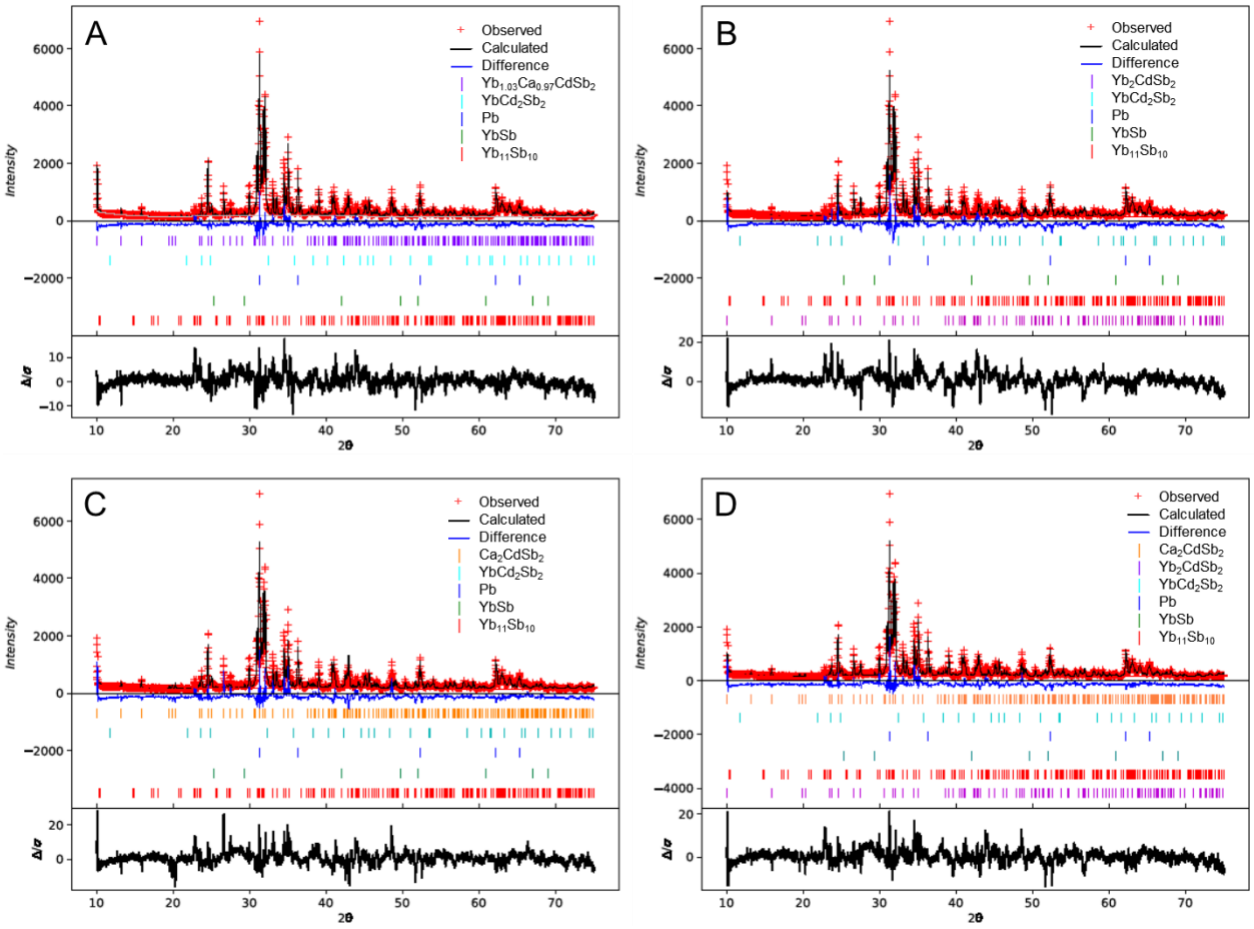


Figure S5. Rietveld refinements of $Yb_{1.34}Ca_{0.66}CdSb_2$. The data are indicated in red, calculated in black, difference in blue and the various phases as shown on the legend. Tick marks are the expected peak positions. An expanded view of the difference map is show at the bottom in black. A. Refined with the cif file from the resulting single crystal characterization. B. Using only the cif file from the Yb_2CdSb_2 space group. C. Using only the cif file from the Ca_2CdSb_2 space group. D. Using both the Yb_2CdSb_2 cif and the Ca_2CdSb_2 cif.

Table S5. Refinement Statistics from the $Yb_{1.03}Ca_{0.97}CdSb_2$ Rietveld Refinements.

	A		B		C		D			
	$Yb_{1.03}Ca_{0.97}CdSb_2$		Yb_2CdSb_2		Ca_2CdSb_2		Yb_2CdSb_2		Ca_2CdSb_2	
Unit Cell Parameters	a =	7.2523(3)	a =	4.6160(4)	a =	7.2521(5)	a =	4.6162(3)	a =	7.2530(9)
	b =	4.6160(2)	b =	17.526(1)	b =	4.6162(5)	b =	17.527(2)	b =	4.6151(9)
	c =	17.5253(8)	c =	7.2521(4)	c =	17.525(1)	c =	7.2522(8)	c =	17.527(2)
	V =	586.69(3)	V =	586.71(5)	V =	586.70(5)	V =	586.75(8)	V =	586.7(1)
Rp (%), Rwp (%)		11.70, 15.53		15.28, 19.97		15.25, 10.17				12.66, 16.70
Ca_2CdSb_2 (%)		48.9(4)		---		43.2(5)				23.9(7)
Yb_2CdSb_2 (%)		---		41.0(6)		---				23.0(8)
$YbCd_2Sb_2$ (%)		1.4(1)		2.0(2)		1.4(2)				1.43(8)
$Yb_{11}Sb_{10}$ (%)		40.9(6)		46.5(9)		45.9(8)				42.4(7)
YbSb (%)		0.54(7)		0.6(2)		0.6(1)				0.54(8)
Pb (%)		8.5(1)		9.9(2)		8.8(2)				8.7(1)

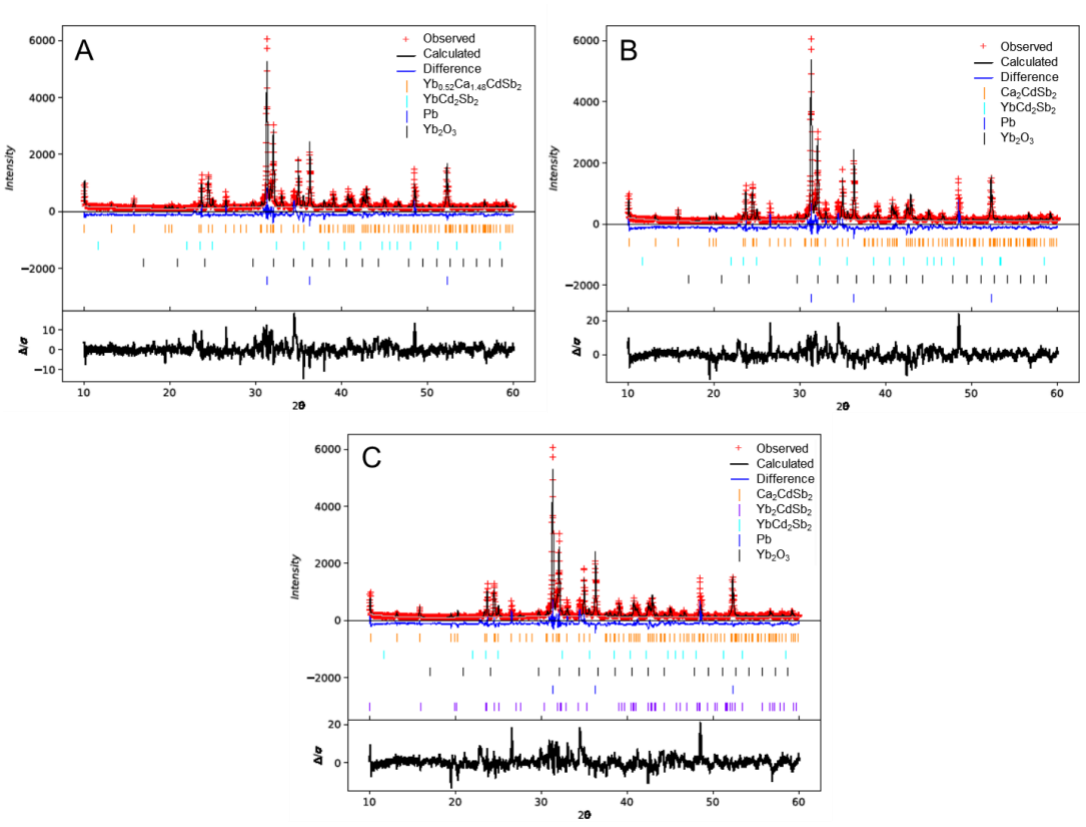


Figure S6. Rietveld refinements of $Yb_{0.52}Ca_{1.48}CdSb_2$. The data are indicated in red, calculated in black, difference in blue and the various phases as shown on the legend. Tick marks are the expected peak positions. An expanded view of the difference map is show at the bottom in black. A with the cif file from the resulting single crystal characterization. B. Using only the cif file from the Ca_2CdSb_2 space group. C. Using both the Yb_2CdSb_2 cif and the Ca_2CdSb_2 cif.

Table S6. Refinement Statistics from the $Yb_{0.52}Ca_{1.48}CdSb_2$ Rietveld Refinements.

	A		B		C			
	$Yb_{0.52}Ca_{1.48}CdSb_2$		Ca_2CdSb_2		Yb_2CdSb_2		Ca_2CdSb_2	
Unit Cell Parameters	a =	7.2704(3)	a =	7.2702(4)	a =	4.6132(4)	a =	7.2712(4)
	b =	4.6131(3)	b =	4.6134(4)	b =	17.684(4)	b =	4.6132(5)
	c =	17.5364(7)	c =	17.5371(9)	c =	7.108(3)	c =	17.535(1)
	V =	588.16(4)	V =	588.20(4)	V =	579.9(2)	V =	588.19(5)
Rp (%), Rwp (%)		12.87, 17.30		15.55, 20.88				14.69, 19.79
Ca_2CdSb_2 (%)		75.6(6)		71.9(7)				65.1(7)
Yb_2CdSb_2 (%)		---		---				8.1(7)
$YbCd_2Sb_2$ (%)		0.9(2)		0.8(2)				0.6(2)
Yb_2O_3 (%)		1.6(1)		1.9(2)				1.8(2)
Pb (%)		21.8(2)		25.3(3)				24.4(3)

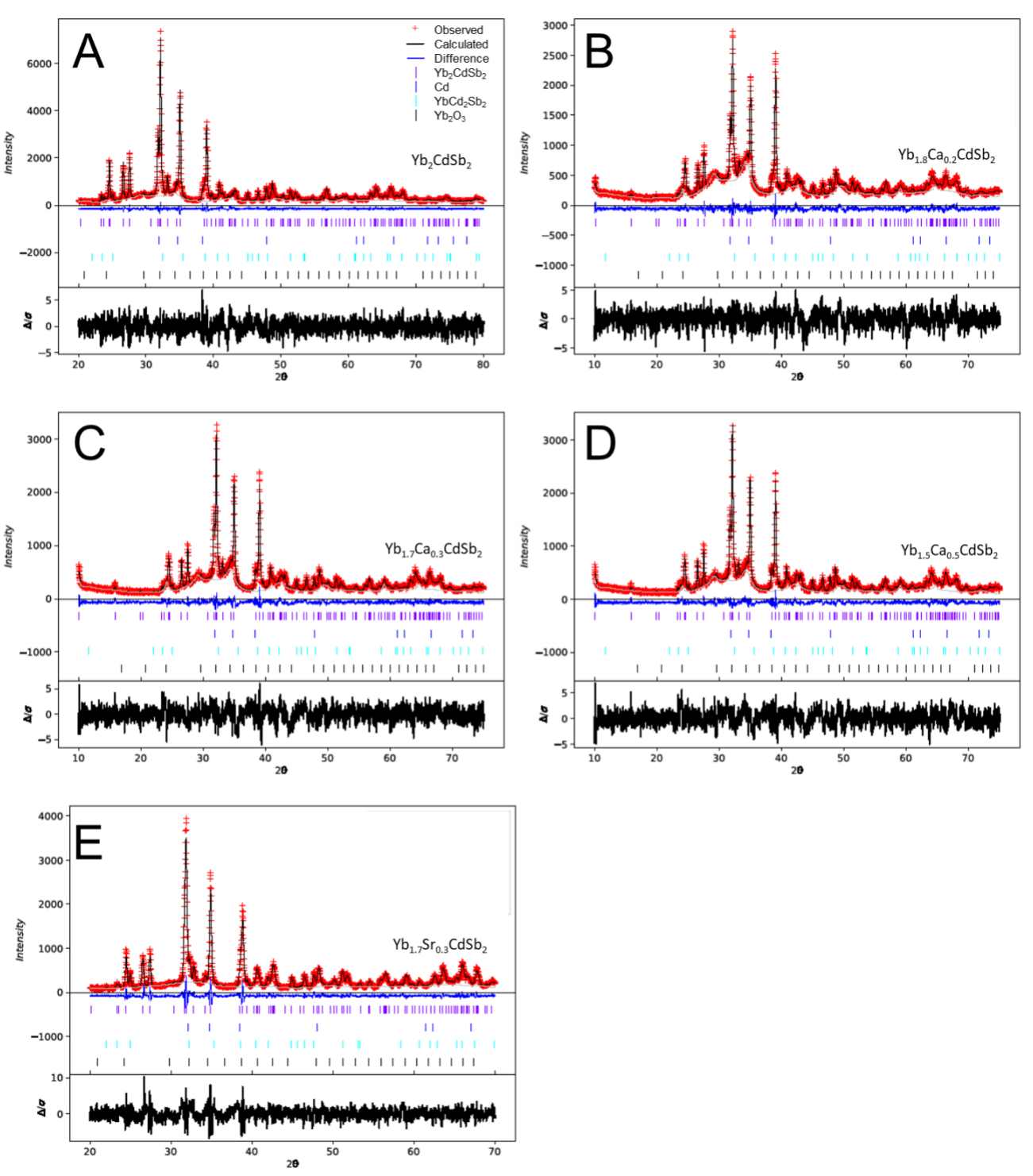


Figure S7. Rietveld refinement of polycrystalline A. Yb_2CdSb_2. B. $Yb_{1.8}Ca_{0.2}CdSb_2$. C. $Yb_{1.7}Ca_{0.3}CdSb_2$. D. $Yb_{1.5}Ca_{0.5}CdSb_2$. E. $Yb_{1.7}Sr_{0.3}CdSb_2$. The data are indicated in red, calculated in black, difference in blue and the various phases as shown on the legend in (A). Tick marks are the expected peak positions. An expanded view of the difference map is show at the bottom in black.

Table S7. Refinement Statistics from the $Yb_{2-x}A_xCdSb_2$ (A = Ca, Sr) Polycrystalline Sample Refinements.

	Yb_2CdSb_2	$Yb_{1.8}Ca_{0.2}CdSb_2$	$Yb_{1.7}Ca_{0.3}CdSb_2$	$Yb_{1.5}Ca_{0.5}CdSb_2$	$Yb_{1.7}Sr_{0.3}CdSb_2$
Unit Cell Parameters	a = 4.60806(8)	a = 4.6125(1)	a = 4.6195(1)	a = 4.6217(3)	a = 4.6267(2)
	b = 17.3936(4)	b = 17.4178(9)	b = 17.4161(9)	b = 17.461(1)	b = 17.6185(9)
	c = 7.1588(2)	c = 7.1718(4)	c = 7.1884(3)	c = 7.2003(5)	c = 7.2642(3)
	V = 573.79(2)	V = 576.18(4)	V = 578.33(3)	V = 581.1(1)	V = 592.15(3)
Rp (%), Rwp (%)	4.73, 6.10	5.65, 7.30	6.21, 7.93	6.41, 8.17	7.46, 9.26
Yb_2O_3 (%)	0.69(6)	1.2(1)	0.9(1)	1.1(1)	0.32(8)
Cd (%)	3.61(8)	3.6(2)	4.6(2)	3.9(1)	0.7(2)
$YbCd_2Sb_2$ (%)	3.60(9)	4.9(2)	3.6(2)	3.4(1)	10.6(2)

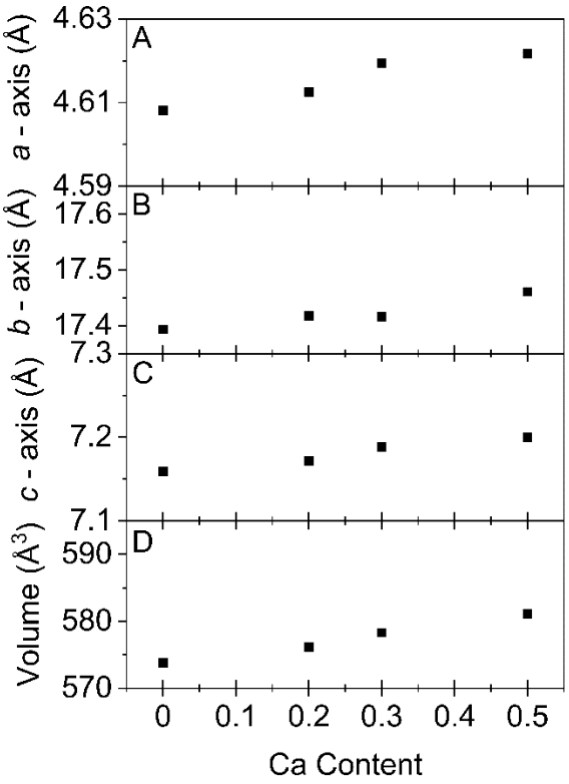


Figure S8. Lattice parameter refinement values as a function of Ca content from Rietveld refinement of PXRD. A. *a* lattice parameter B. *b* lattice parameter C. *c* lattice parameter and D. Volume of $Yb_{2-x}Ca_xCdSb_2$ compositions prepared as powders.

Table S8. EMPA Composition for $Yb_{1.7}Sr_{0.3}CdSb_2$.

Sample		At %				Formula	
	x	Yb	Sr	Cd	Sb		Cation Total
$Yb_{1.7}Sr_{0.3}CdSb_2$	0.3	34.0(6)	5.7(2)	20.8(5)	39.5(2)	$Yb_{1.70(3)}Sr_{0.286(8)}Cd_{1.04(3)}Sb_{1.97(1)}$	1.99(3)

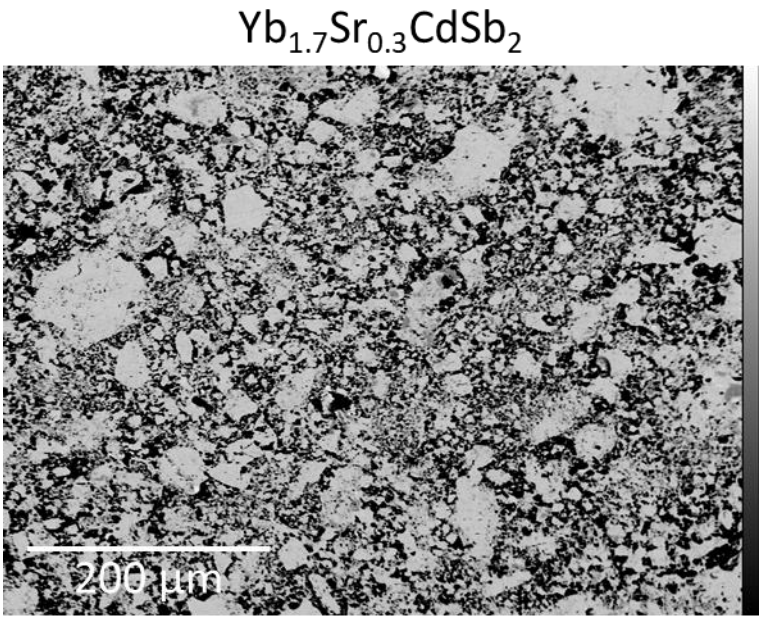


Figure S9. EMPA backscatter image for $Yb_{1.7}Sr_{0.3}CdSb_2$ pressed pellet.

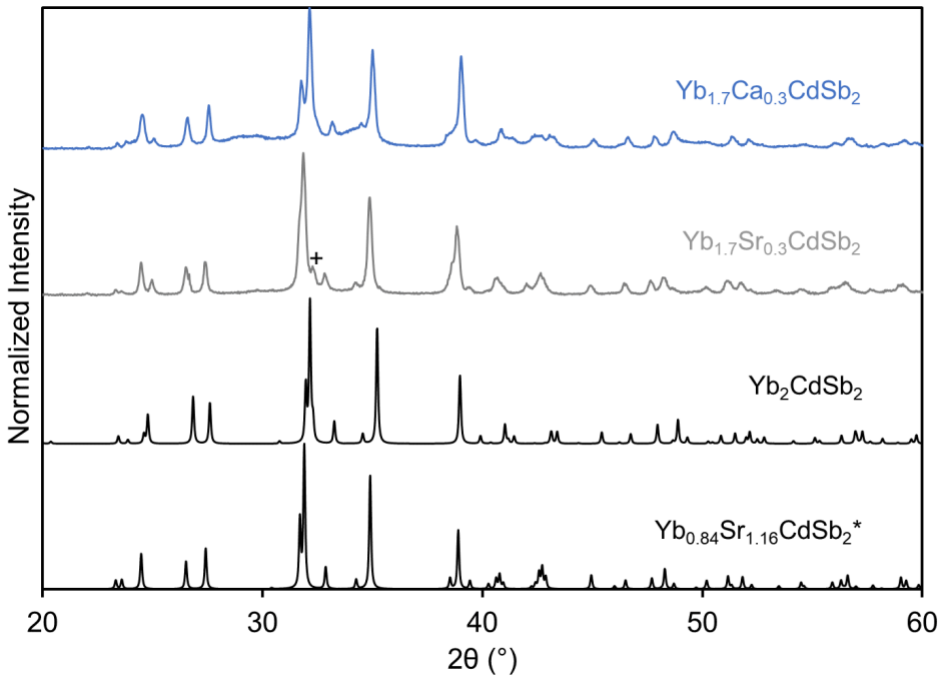


Figure S10 PXRD patterns for $Yb_{1.7}Sr_{0.3}CdSb_2$ compared to $Yb_{1.7}Ca_{0.3}CdSb_2$, the calculated Yb_2CdSb_2 pattern, and the calculated $Yb_{0.84}Sr_{1.16}CdSb_2$ pattern with the lattice parameters from the Rietveld refinement. $YbCd_2Sb_2$ is marked with "+".

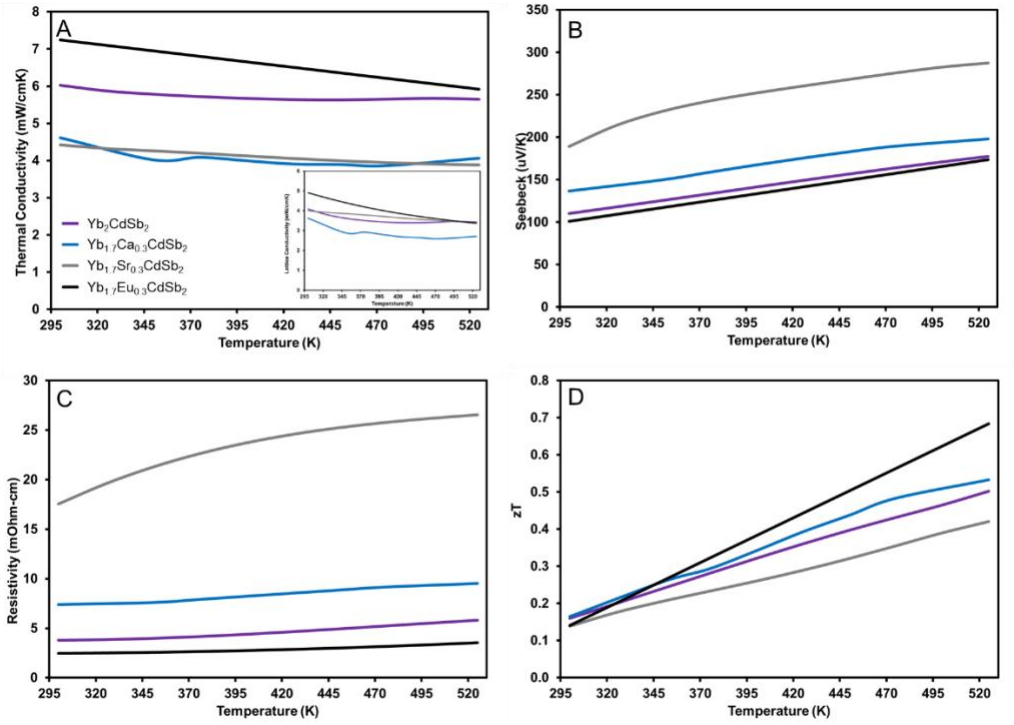


Figure S11. Thermoelectric properties versus temperature for $Yb_{1.7}A_{0.3}CdSb_2$ (A = Ca, Sr, Eu). A. Thermal conductivity B. Seebeck coefficient C. Electrical resistivity D. *zT*. The $Yb_{1.7}Eu_{0.3}CdSb_2$ data are from Cooley et. al.[13]