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Scandium-doped Zinc Cadmium Oxide as New Stable n-type Oxide Thermoelectric Materials

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1. Calculated results from Rietveld refinements of XRD spectrums

Table S1 Results from Rietveld refinement for $Zn_{1-x}Cd_xSc_{0.02}O_{1.03}$ (x = 0 to 0.15) samples.

Sample	Main phase: Zincite						Secondary phase						R-Values		
	Space group	Lattice parameters (Å)			Cell Volume (Å^3)	Wt% - Rietveld (%)	Space group	Lattice parameters (Å)			Cell Volume (Å^3)	Wt% - Rietveld (%)			
		a	b	c				a	b	c			R_{exp}	R_{wp}	GOF
$ZnSc_{0.02}O_{1.03}$	P63mc	3.25	3.25	5.20	47.59	99.440	I213	9.84	9.84	9.84	954.5	0.560	2.95	10.6	3.62
$Zn_{0.95}Cd_{0.05}Sc_{0.02}O_{1.03}$	P63mc	3.27	3.27	5.23	48.38	99.276	I213	9.84	9.84	9.84	953.5	0.724	3.66	8.69	2.37
$Zn_{0.9}Cd_{0.1}Sc_{0.02}O_{1.03}$	P63mc	3.28	3.28	5.25	49.18	99.683	I213	9.85	9.85	9.85	956.5	0.317	3.54	7.41	2.09
$Zn_{0.875}Cd_{0.125}Sc_{0.02}O_{1.03}$	P63mc	3.29	3.29	5.25	49.33	97.817	Fm3m	4.69	4.69	4.69	103.33	2.183	3.81	8.99	2.36
$Zn_{0.85}Cd_{0.15}Sc_{0.02}O_{1.03}$	P63mc	3.28	3.28	5.24	48.98	93.392	Fm3m	4.69	4.69	4.69	103.18	6.608	3.61	8.80	2.44

Table S2 Results from Rietveld refinement for $Zn_{0.9}Cd_{0.1}Sc_yO_{1+1.5y}$ (y = 0 to 0.04) samples.

Sample	Main phase: Zincite						Secondary phase						R-Values		
	Space group	Lattice parameters (Å)			Cell Volume (Å^3)	Wt% - Rietveld (%)	Space group	Lattice parameters (Å)			Cell Volume (Å^3)	Wt% - Rietveld (%)			
		a	b	c				a	b	c			R_{exp}	R_{wp}	GOF
$Zn_{0.9}Cd_{0.1}O$	P63mc	3.28	3.28	5.25	49.06	100	-	-	-	-	-	-	2.89	9.69	3.35
$Zn_{0.9}Cd_{0.1}Sc_{0.01}O_{1.015}$	P63mc	3.29	3.29	5.25	49.14	100	-	-	-	-	-	-	3.53	7.70	2.18
$Zn_{0.9}Cd_{0.1}Sc_{0.02}O_{1.03}$	P63mc	3.29	3.29	5.25	49.18	99.683	I213	9.85	9.85	9.85	956.5	0.317	3.54	7.41	2.09
$Zn_{0.9}Cd_{0.1}Sc_{0.03}O_{1.045}$	P63mc	3.29	3.29	5.25	49.18	99.059	I213	9.85	9.85	9.85	955.2	0.941	3.57	8.08	2.27
$Zn_{0.9}Cd_{0.1}Sc_{0.04}O_{1.06}$	P63mc	3.29	3.29	5.25	49.10	98.618	I213	9.85	9.85	9.85	954.5	1.382	3.57	8.08	2.27

2. Parameters used for Callaway model

Table S3 An overview of the parameters used in Callaway calculations.

Sample	$ZnSc_{0.02}O_{1.03}$	$Zn_{0.95}Cd_{0.05}Sc_{0.02}O_{1.03}$	$Zn_{0.9}Cd_{0.1}Sc_{0.02}O_{1.03}$	$Zn_{0.875}Cd_{0.125}Sc_{0.02}O_{1.03}$	$Zn_{0.85}Cd_{0.15}Sc_{0.02}O_{1.03}$
θ/K	400	400	400	400	400
v/ms^{-1}	3097	3097	3097	3097	3097
α/K^{-4}s^{-1}	230	1600	3200	3900	2900
β/K^{-5}s^{-1}	0.015	0.015	0.015	0.015	0.015
L/m	1× 10^{-5}	3× 10^{-6}	4.5× 10^{-6}	4× 10^{-6}	3× 10^{-6}

Sample	$Zn_{0.9}Cd_{0.1}Sc_{0.006}O_{1.009}$	$Zn_{0.9}Cd_{0.1}Sc_{0.01}O_{1.015}$	$Zn_{0.9}Cd_{0.1}Sc_{0.02}O_{1.03}$	$Zn_{0.9}Cd_{0.1}Sc_{0.03}O_{1.045}$	$Zn_{0.9}Cd_{0.1}Sc_{0.04}O_{1.06}$
θ/K	400	400	400	400	400
v/ms^{-1}	3097	3097	3097	3097	3097
α/K^{-4}s^{-1}	3050	3100	3200	3300	3400
β/K^{-5}s^{-1}	0.015	0.015	0.015	0.015	0.015
L/m	5× 10^{-6}	5× 10^{-6}	4.5× 10^{-6}	4× 10^{-6}	3.5× 10^{-6}

3. Calculated phonon density of states for $Zn_{0.875}Cd_{0.125}O$ and ZnO by DFT calculation

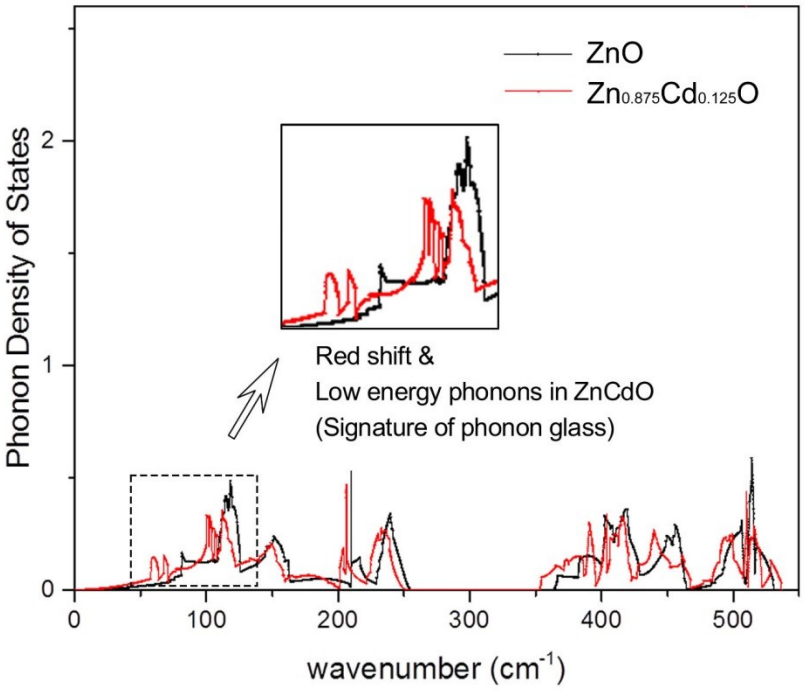

Fig. S1 Calculated phonon density of states for $Zn_{0.875}Cd_{0.125}O$ and ZnO by DFT calculation

4. Supplement TE properties

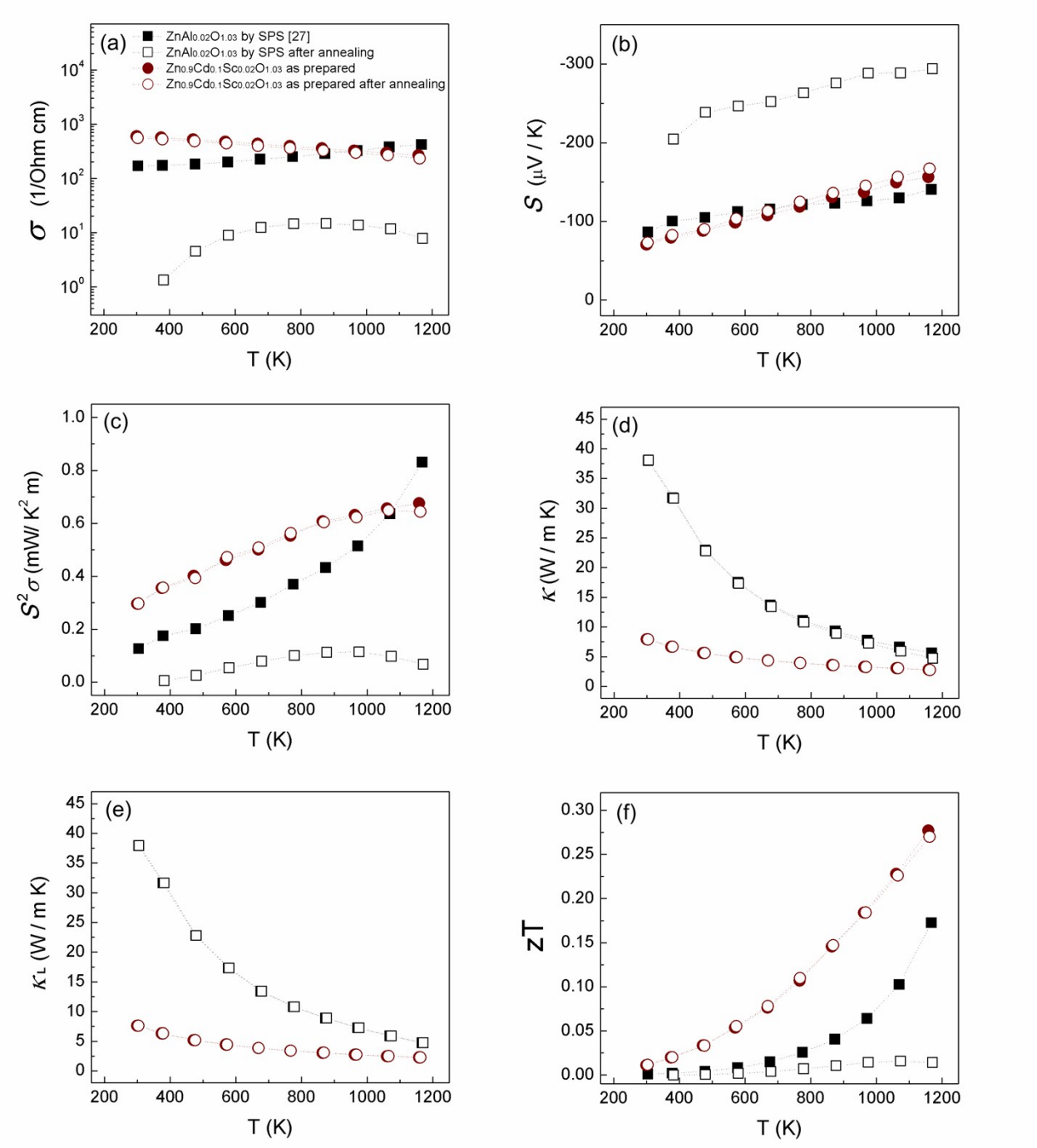

Fig. S2 TE properties of the conventional $Zn_{0.98}Al_{0.02}O_{1.03}$ samples and new $Zn_{0.9}Cd_{0.1}Sc_{0.02}O_{1.03}$ samples under the influence of annealing in air at 1073K for 72 hours.