

Supplementary Information

Environmentally-benign NaNbO₃ based perovskite antiferroelectric alternative to traditional lead-based counterpart

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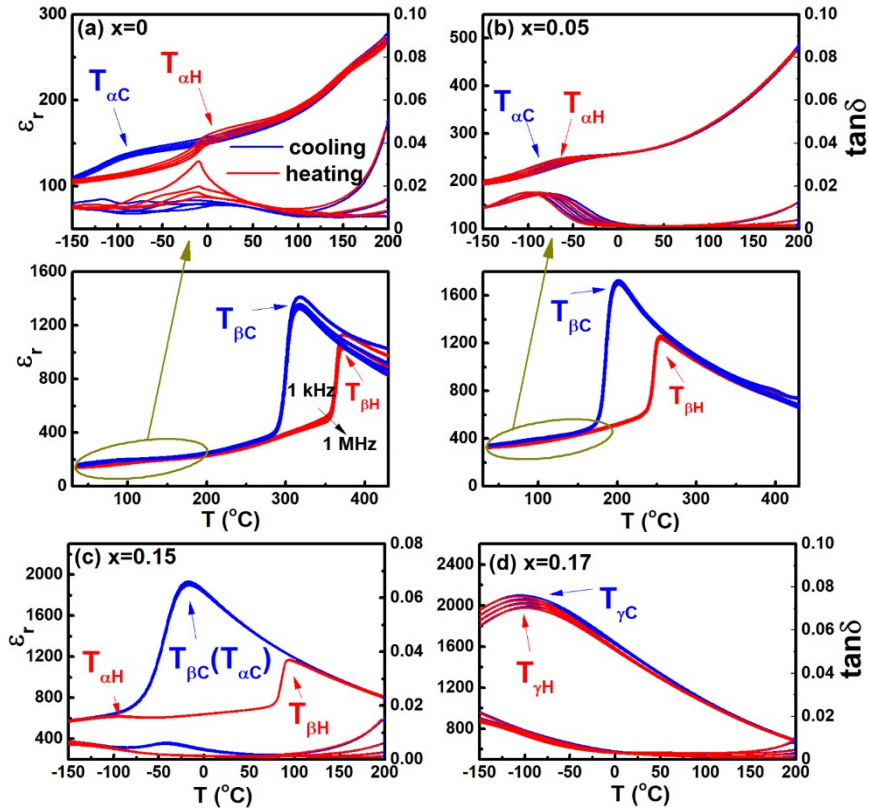


Fig. S1. The dielectric permittivity (ϵ_r) and dielectric loss ($\tan\delta$) as a function of temperature measured on heating and cooling cycles for $(1-x)\text{NN}-x\text{ST}$ ceramics: (a) $x=0$, (b) $x=0.05$, (c) $x=0.15$ and (d) $x=0.17$.

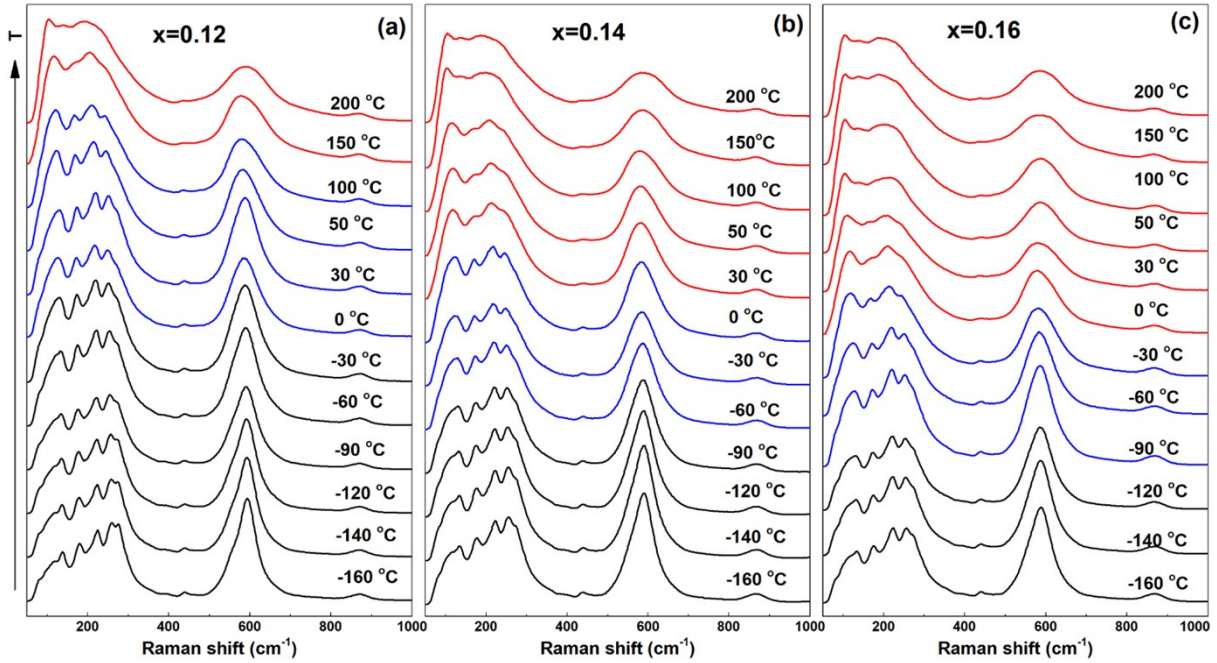


Fig. S2. Raman spectra for $(1-x)\text{NN}-x\text{ST}$ ceramics at various temperatures: (a) $x=0.12$, (b) $x=0.14$ and (c) $x=0.16$.

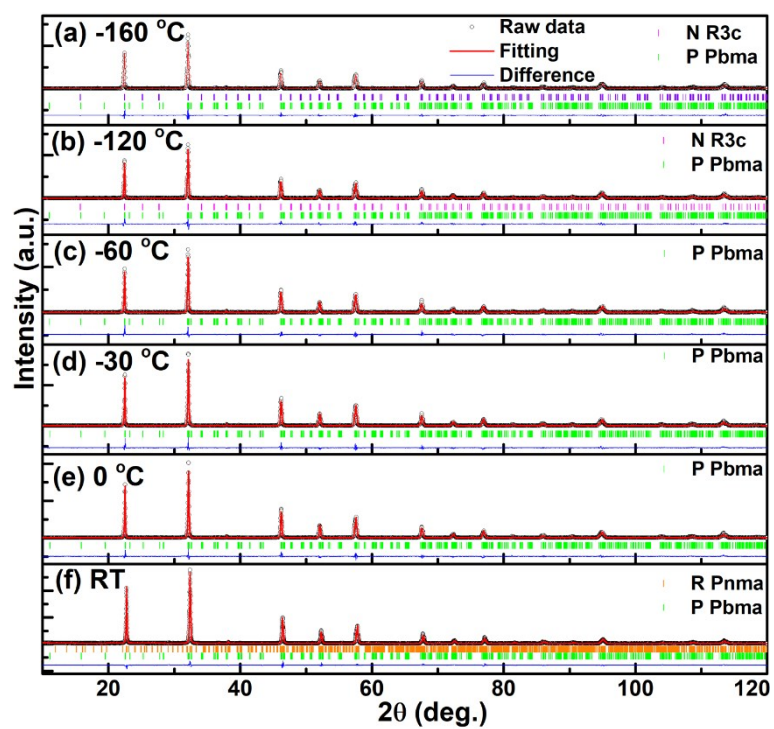


Fig. S3. Rietveld refinement plots of the $x=0.14$ ceramic measured at different temperatures.

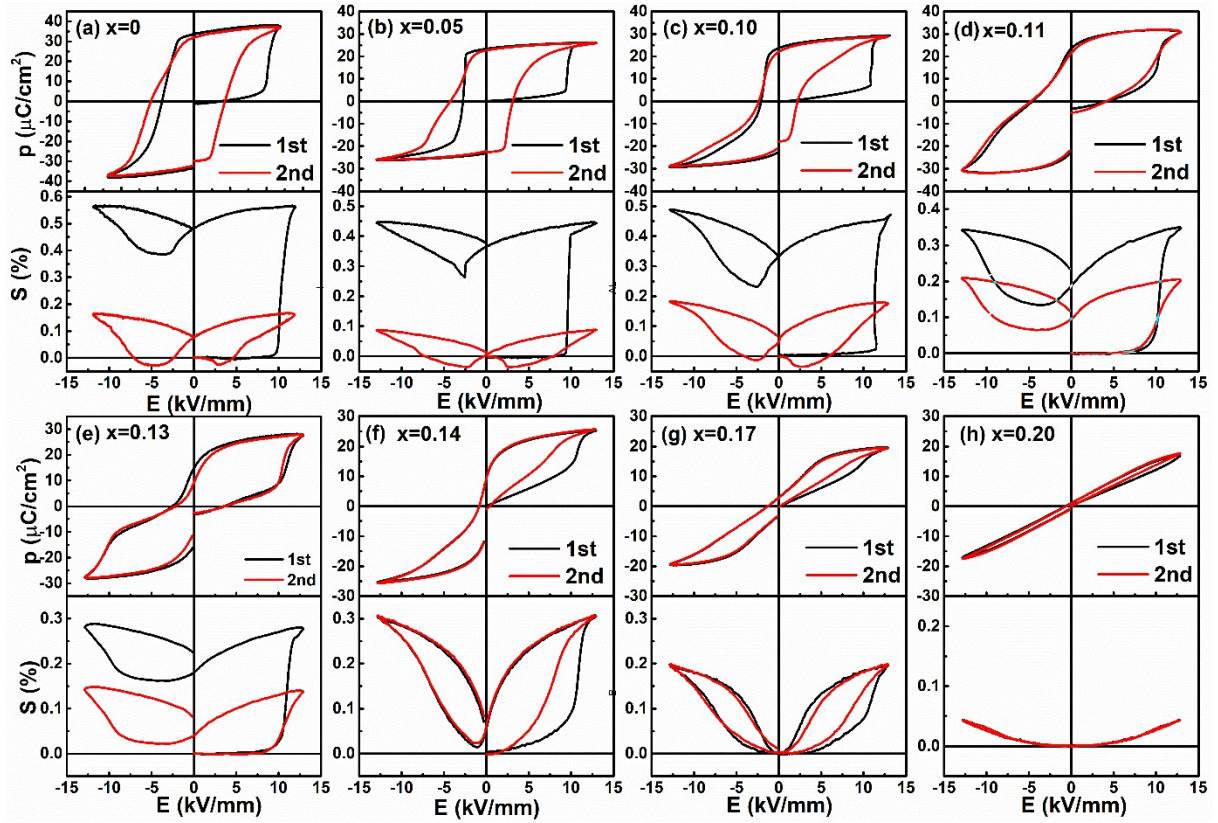


Fig. S4. Room-temperature P-E loops and bipolar S-E curves of the (1-x)NN-xST ceramic during different electric field cycles at 10 Hz: (a) $x=0$, (b) $x=0.05$, (c) $x=0.1$, (d) $x=0.11$, (e) $x=0.13$, (f) $x=0.14$, (g) $x=0.17$ and (h) $x=0.2$.

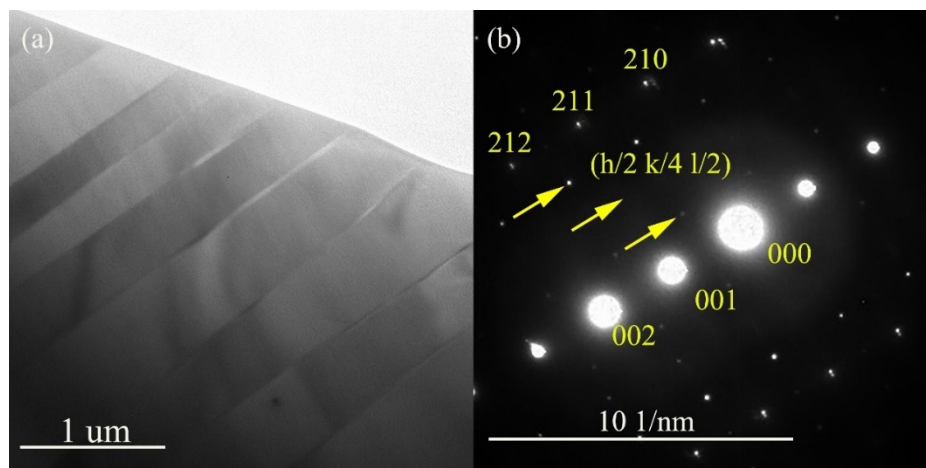


Fig. S5. (a) Bright-field TEM image and (b) the SAED patterns of the $x=0.12$ ceramic.

Table S1. Refined structure parameters by the Rietveld method for x=0.14 ceramic as function of temperature.

T (°C)	Space group	Fraction (%)	Lattice parameters	V (Å ³)	R _{wp} (%)	R _p (%)	χ ²
-160	<i>R3c</i>	54.2	a=b=c=7.8117(1) Å, α=β=γ=90.102(5)°	476.698(11)	9.41	7.55	1.78
	<i>Pbma</i>	45.8	a=5.5432(2) Å, b=15.5951(7) Å, c=5.5094(2) Å, α=β=γ=90°	476.284(35)			
-120	<i>R3c</i>	21.2	a=b=c=7.8129(5) Å, α=β=γ=90.057(8)°	476.914(21)	9.33	6.95	1.86
	<i>Pbma</i>	78.8	a=5.5438(2) Å, b=15.5963(7) Å, c=5.5091(2) Å, α=β=γ=90°	476.340(36)			
-60	<i>Pbma</i>	100	a=5.5430(2) Å, b=15.6023(7) Å, c=5.5123(2) Å, α=β=γ=90°	476.726(36)	8.88	6.72	1.70
-30	<i>Pbma</i>	100	a=5.5441(2) Å, b=15.6147(6) Å, c=5.5160(2) Å, α=β=γ=90°	477.521(33)	8.29	7.09	1.68
0	<i>Pbma</i>	100	a=5.5446(1) Å, b=15.6233(7) Å, c=5.5180(1) Å, α=β=γ=90°	478.010(34)	8.73	6.90	1.74
RT	<i>Pbma</i>	11.5	a=5.5524(1) Å, b=15.6263(2) Å, c=5.5189(1) Å, α=β=γ=90°	478.840(21)	8.92	6.91	1.61
	<i>Pnma</i>	88.5	a=7.8354(2) Å, b=7.8193(3) Å, c=23.444(9) Å, α=β=γ=90°	1436.398(44)			

RT : room temperature

Table S2. Refined structural parameters of the (1-x)NN-xST ceramic powders at room temperature.

x	State	Space group	Fraction (%)	Lattice parameters	V (Å ³)	R _{wp} (%)	R _p (%)	χ ²
0	<i>Virgin</i>	<i>Pbma</i>	86.7	a=5.5653(3) Å, b=15.5550(4) Å, c=5.5024(3) Å, α=β=γ=90°	475.315(9)	8.87	6.43	2.09
		<i>P2₁ma</i>	13.3	a=5.5712(2) Å, b=7.7802(3) Å, c=5.5016(3) Å, α=β=γ=90°	238.472(7)			
0.05	<i>Virgin</i>	<i>Pbma</i>	91.1	a=5.5608(1) Å, b=15.5802(2) Å, c=5.5101(1) Å, α=β=γ=90°	477.383(12)	9.33	7.28	2.22
		<i>P2₁ma</i>	9.9	a=5.5780(2) Å, b=7.7815(3) Å, c=5.5049(4) Å, α=β=γ=90°	238.945(9)			
0.10	<i>Virgin</i>	<i>Pbma</i>	96.2	a=5.5547(1) Å, b=15.6121(2) Å, c=5.5144(1) Å, α=β=γ=90°	478.210(13)	9.22	7.66	2.11
		<i>P2₁ma</i>	3.8	a=5.5808(1) Å, b=7.8021(5) Å, c=5.5118(4) Å, α=β=γ=90°	239.997(8)			
0.11	<i>Virgin</i>	<i>Pbma</i>	100	a=5.5513(1) Å, b=15.6255(2) Å, c=5.5164(1) Å, α=β=γ=90°	478.498(12)	9.12	7.87	2.09
0.12	<i>Virgin</i>	<i>Pbma</i>	100	a=5.5521(1) Å, b=15.6261(1) Å, c=5.5170(1) Å, α=β=γ=90°	478.645(9)	8.30	6.46	1.76
0.13	<i>Virgin</i>	<i>Pbma</i>	100	a=5.5526(1) Å, b=15.6265(2) Å, c=5.5185(1) Å, α=β=γ=90°	478.826(11)	9.07	6.95	2.03
0.14	<i>Virgin</i>	<i>Pbma</i>	11.5	a=5.5524(1) Å, b=15.6263(2) Å, c=5.5189(1) Å, α=β=γ=90°	478.840(21)	8.92	6.91	1.61
		<i>Pnma</i>	88.5	a=7.8354(2) Å, b=7.8193(3) Å, c=23.444(9) Å, α=β=γ=90°	1436.398(44)			
0.15	<i>Virgin</i>	<i>Pbma</i>	4.0	a=5.5534(3) Å, b=15.6282(4) Å, c=5.5190(4) Å, α=β=γ=90°	478.998(34)	9.63	7.35	2.41
		<i>Pnma</i>	96.0	a=7.8183(1) Å, b=7.8265(1) Å, c=23.4923(8) Å, α=β=γ=90°	1437.486(53)			
0.16	<i>Virgin</i>	<i>Pnma</i>	100	a=7.8179(3) Å, b=7.8252(1) Å, c=23.5123(9) Å, α=β=γ=90°	1438.397(42)	9.52	7.34	2.30
0.17	<i>Virgin</i>	<i>Pnma</i>	100	a=7.8290(2) Å, b=7.8289(3) Å, c=23.4790(5) Å, α=β=γ=90°	1439.082(52)	9.60	7.41	2.21
0.20	<i>Virgin</i>	<i>Pnma</i>	100	a=7.8422(1) Å, b=7.8327(1) Å, c=23.4814(3) Å, α=β=γ=90°	1442.354(27)	9.04	7.02	1.43
0.12	<i>Poled</i>	<i>P2₁</i>	100	a=5.5517(1) Å, b=15.6266(1) Å, c=5.5178(1) Å, α=γ=90°, β=90.048(1)°	478.705(11)	9.16	6.88	1.88
0.16	<i>Poled</i>	<i>Pnma</i>	100	a=7.8171(2) Å, b=7.8259(1) Å, c=23.5120(8) Å, α=β=γ=90°	1438.383(38)	9.06	7.00	2.27