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

Supporting Information

Lead-free antiferroelectric borate crystal $K_3Nb_3B_2O_{12}$ with polar structure

Pai Shan, Junjie Xiong, Zujian Wang, Chao He, Xiaoming Yang, Rongbing Su, Xifa Long**

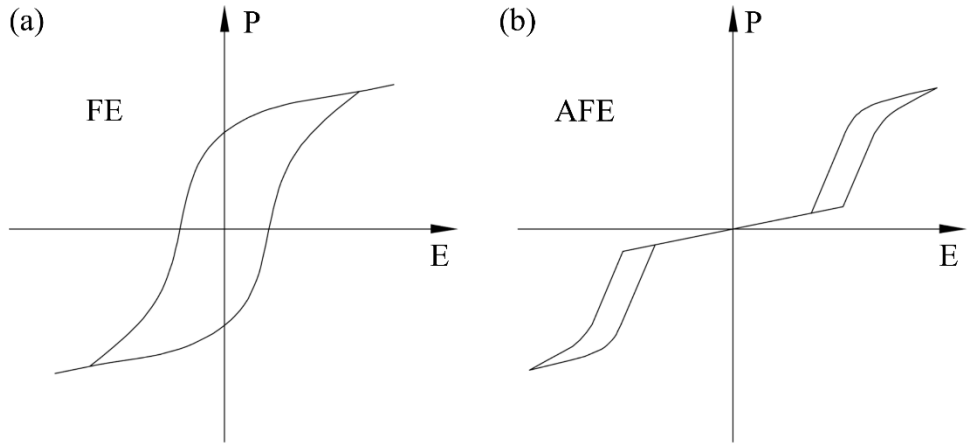

Figure S1. Schematic illustrations of (a) single *P*–*E* hysteresis loop for FEs and (b) double *P*–*E* hysteresis loop for AFEs.

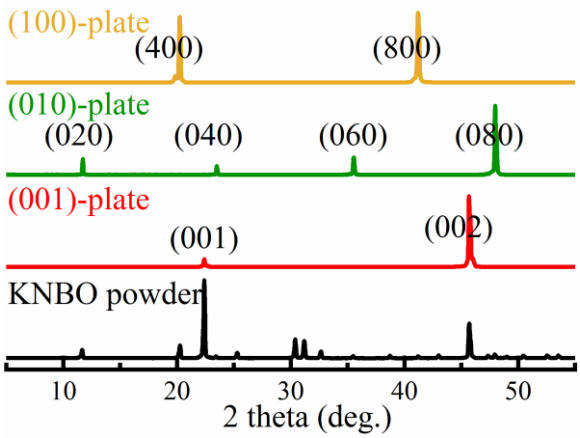

Figure S2. XRD patterns of KNBO powder, (001), (010) and (100) crystal plates.

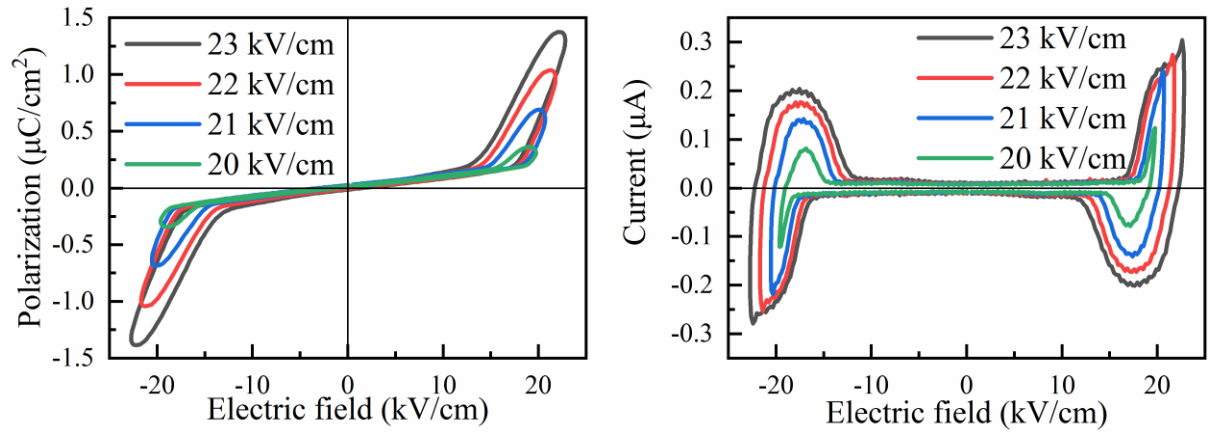

Figure S3. (a) Double *P*–*E* hysteresis loops and (b) corresponding *I*–*E* curves of KNBO crystal measured at different electric fields, by 50 Hz, at room temperature.

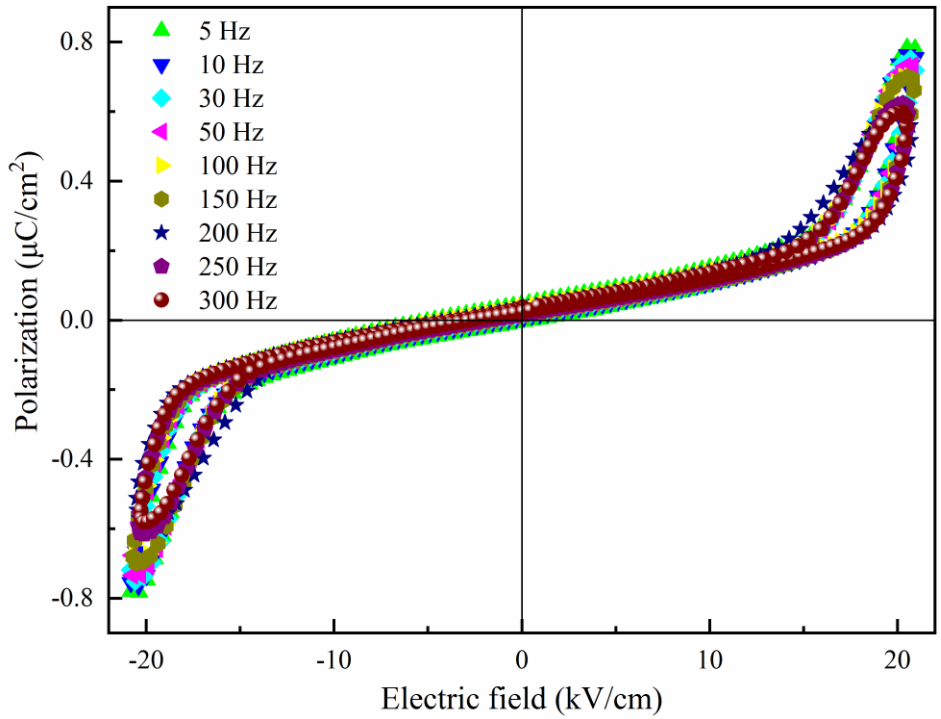

Figure S4. Double *P–E* hysteresis loops of KNBO crystal measured with different frequencies, by 21 kV/cm, at room temperature.

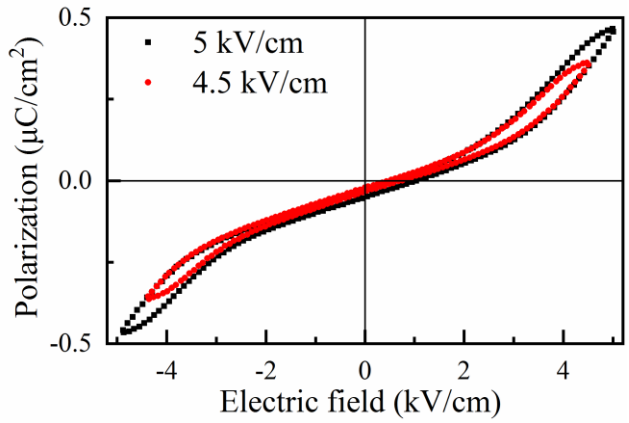

Figure S5. Double *P–E* hysteresis loops of KNBO crystal measured at 374 K, by 50 Hz.

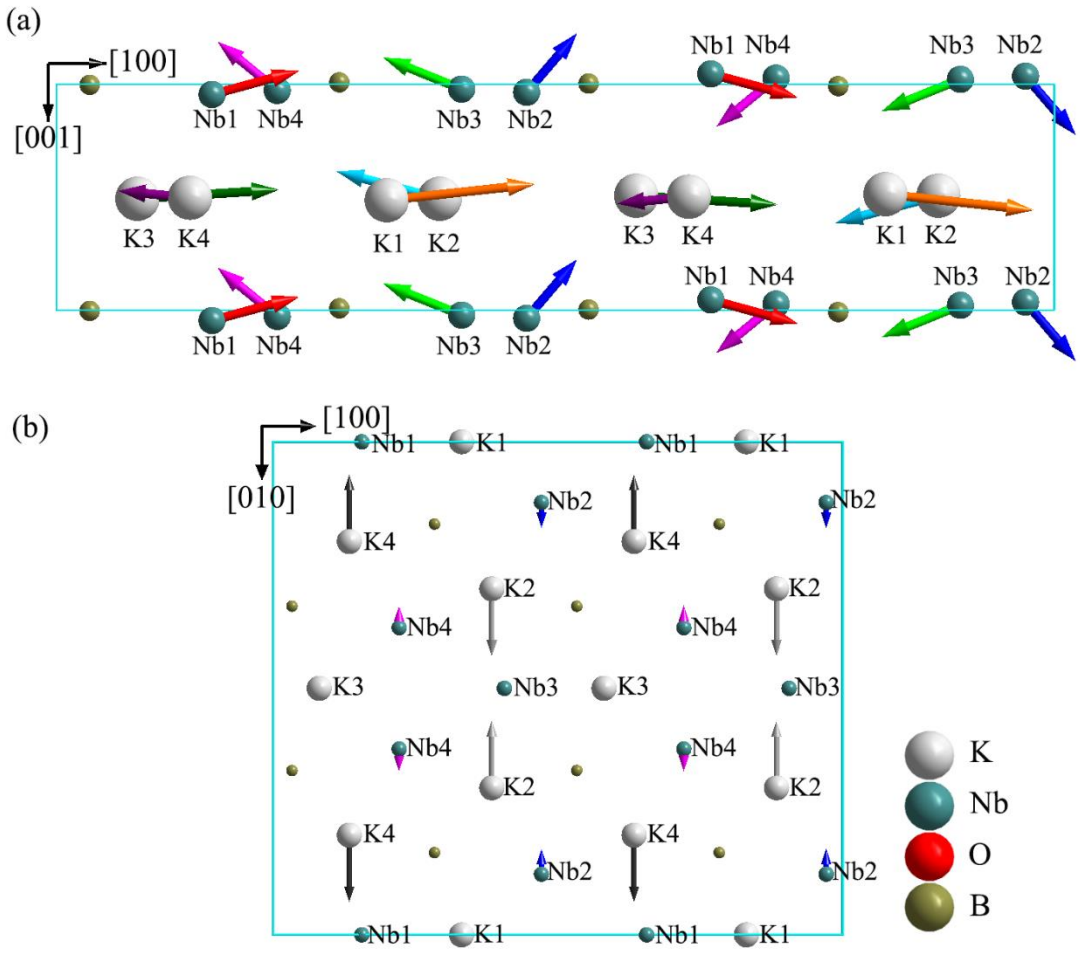

Figure S6. Orientation of the dipole moment vectors for NbO_6, KO_{13} and BO_3 polyhedra in a unit cell of KNBO crystal, (a) in (010) plane and (b) along [010] direction. All O atoms are omitted for clarity. The numbers represent cations possessing different crystallographically independent sites.

Table S1. Crystal data and structure refinement for KNBO crystal at room temperature.

Formula sum	$K_3Nb_3B_2O_{12}$
Formula weight (g/mol)	609.65
Crystal color	colorless
Crystal system	orthorhombic
Space group	$P2_1ma$
a/Å	17.5219(7)
b/Å	15.1708(6)
c/Å	3.96882(11)
V/Å^3	1055.00(7)
Z	4
Crystal size	0.18 × 0.13 × 0.09 mm^3
F(000)	1144
Limiting indices	-4 ≤ h ≤ 4, -21 ≤ k ≤ 19, -18 ≤ l ≤ 18
GOF(F^2)	1.096
Final *R* indices [$F_o^2 > 2\sigma(F_c^2)$.] [a]	R_1 = 0.0232, wR_2 = 0.0557
Final R indices (all data) [a]	R_1 = 0.0316, wR_2 = 0.0616

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$ and $wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$ for $F_o^2 > 2\sigma(F_c^2)$

Table S2. Calculation of dipole moments for NbO_6, KO_{13} and BO_3 polyhedra within a unit cell of KNBO crystal.

Cation of polar polyhedra	Dipole Moment [Debye]			
	[100]-component	[010]-component	[001]-component	total magnitude
Nb(1 [a]-1 [b])O_6	1.016	0.000	-1.218	1.586
Nb(1-2)O_6	1.015	0.000	1.218	1.586
Nb(2-1)O_6	-0.259	0.788	-1.337	1.574
Nb(2-2)O_6	-0.259	-0.788	-1.337	1.574
Nb(2-3)O_6	-0.254	0.786	1.337	1.571
Nb(2-4)O_6	-0.254	-0.786	1.337	1.571
Nb(3-1)O_6	0.740	0.000	-1.300	1.496
Nb(3-2)O_6	0.730	0.000	1.299	1.490
Nb(4-1)O_6	-0.362	-0.683	-1.305	1.516
Nb(4-2)O_6	-0.362	0.683	-1.305	1.516
Nb(4-3)O_6	-0.362	-0.677	1.307	1.516
Nb(4-4)O_6	-0.362	0.677	1.307	1.516
K(1-1)O_{13}	2.362	0.000	1.129	2.618
K(1-2)O_{13}	2.362	0.000	-1.129	2.618
K(2-1)O_{13}	-1.216	2.064	1.424	2.787
K(2-2)O_{13}	-1.216	-2.064	1.424	2.787
K(2-3)O_{13}	-1.216	2.063	-1.425	2.787
K(2-4)O_{13}	-1.216	-2.063	-1.425	2.787
K(3-1)O_{13}	2.397	0.000	0.675	2.491
K(3-2)O_{13}	2.397	0.000	-0.675	2.491
K(4-1)O_{13}	-1.164	-2.060	0.498	2.418
K(4-2)O_{13}	-1.164	2.060	0.498	2.418
K(4-3)O_{13}	-1.164	-2.061	-0.498	2.419
K(4-4)O_{13}	-1.164	2.061	-0.498	2.419
B(1-1)O_3	-0.072	-0.048	-0.151	0.174
B(1-2)O_3	-0.072	0.048	-0.151	0.174
B(1-3)O_3	-0.071	-0.048	0.151	0.174
B(1-4)O_3	-0.071	0.048	0.151	0.174
B(2-1)O_3	-0.085	0.025	0.054	0.104
B(2-2)O_3	-0.085	-0.025	0.054	0.104
B(2-3)O_3	-0.085	0.023	-0.054	0.104
B(2-4)O_3	-0.085	-0.023	-0.054	0.104

[a] The first number represents cations possessing different crystallographically independent sites, these numbers obtain identical implication with Figure 3; [b] The second number represents serial number of cations occupying in the same crystallographically independent sites.