Supplementary Information

Single crystal growth and piezoelectric feature of $Ca_2Nb_2O_7$ crystal with an orthorhombic symmetry

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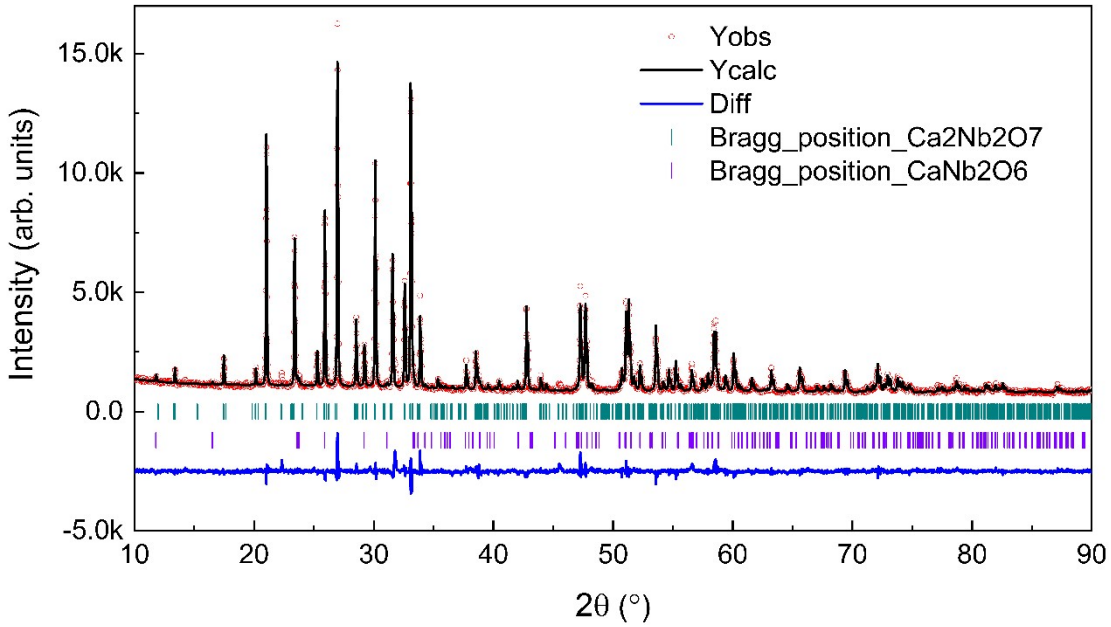

Figure S1 Rietveld refined profile example of $Ca_2Nb_2O_7$ powder.

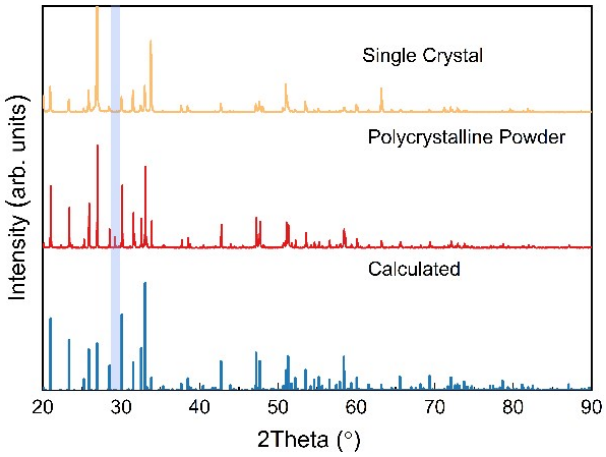

Figure S2 Experimental single crystal(yellow), polycrystalline powder(red), and calculated X-ray diffraction patterns(blue) of the $Ca_2Nb_2O_7$.

Table S1 Bond distances and bond valence for $Ca_2Nb_2O_7$ crystal

□	Bond Distances(Å)	Bond Valence		Bond Distances(Å)	Bond Valence
Nb1		4.96185255	Nb2		4.932043928
O1	2.003813364	-0.778141474	O1	2.012107109	-0.76089306
O2	1.841052841	-1.208096977	O3	1.986006729	-0.816506106
O3	1.981496328	-0.826520453	O4	1.98925785	-0.809363047
O4	2.222152782	-0.431299099	O5	1.84144884	-1.206804684
O6	1.970791432	-0.850782756	O6	2.235884024	-0.415586322
O13	1.9638	-0.867011791	O7	1.94069045	-0.922890709
Nb3	□	4.993377972	Nb4	□	□5.005184161
O7	2.129184363	-0.554500557	O2	2.27391233	-0.374994419
O8	1.784517743	-1.407540616	O9	1.99703069	-0.792537561
O9	1.993248469	-0.800680602	O11	1.843722824	-1.199410524
O5	2.304681922	-0.345070962	O12	2.001614253	-0.782780163
O10	1.867242592	-1.125540389	O13	2.089261272	-0.617678477

O12	2.012519801	-0.760044845	O14	1.832070901	-1.237783018
Ca1	□	□2.092316908	Ca2	□	2.150098347
O1	2.389134931	-0.319529647	O2	2.601635129	-0.17992232
O4	2.730707819	-0.126935628	O5	2.614040691	-0.173989796
O4	2.631789254	-0.165840679	O1	2.324153172	-0.38087698
O3	3.111551469	-0.045348311	O4	2.395725667	-0.313888322
O7	2.410780839	-0.30137267	O6	2.401341289	-0.309160297
O6	2.327686856	-0.37725673	O7	2.482119166	-0.248524471
O6	2.716895084	-0.131763916	O12	2.465144974	-0.260191399
O1	2.643825039	-0.160532822	O13	2.508760817	-0.231258667
□O7	2.330146845	-0.374756814	O3	3.058879193	-0.052286093
□O9	2.862158434	-0.088979692			
Ca3	□	□1.69186088	Ca4	□	2.030149484
O10	2.43793167	-0.28004967	O11	2.441632911	-0.2772622
O10	2.459232604	-0.264382492	O8	2.311256676	-0.394386672
O8	2.422047191	-0.292334298	O10	2.464933047	-0.260340473
O5	2.845196905	-0.093153636	O14	2.473170836	-0.254608225
O12	2.679706988	-0.145695697	O9	2.512774943	-0.228763305
O2	2.918832168	-0.076342967	O11	2.439336831	-0.278988134
O14	2.517428371	-0.225904204	O14	2.370758105	-0.335800475
O11	2.395596505	-0.313997916			

Table S2 The dipole moments of Nb-O polyhedra and Ca-O polyhedra of $Ca_2Nb_2O_7$ crystal.

Specimens	Dipole moments				
	X	Y	Z	Debye	10^{-4} esu.cm/Å^3
$Nb1O_6$	-3.419	1.441	-1.012	3.85	274.70
$Nb2O_6$	-4.057	-1.383	-1.34	4.49	320.79
$Nb3O_6$	-2.988	-1.386	-0.642	3.36	239.73
$Nb4O_6$	-1.144	1.944	-2.943	3.81	272.18
$Ca1O_{10}$	4.647	0.181	-6.866	8.29	592.40
$Ca2O_9$	8.888	-0.241	-2.761	9.31	665.02
$Ca3O_8$	-5.452	-0.060	-1.932	5.78	413.22
$Ca4O_7$	2.815	0.289	2.971	4.10	293.08
Unit Cell	-4.003	3.144	-58.104	58.33	4167

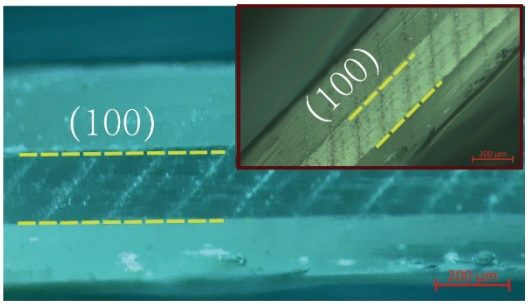

Figure S3 Polarized light microscopy images of the polished Z plate (in large visual field).

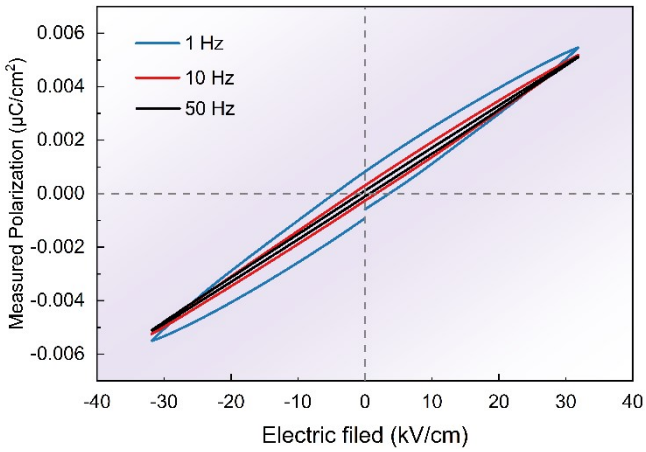

Figure S4 Polarization–Electric filed loops at 1, 10, and 50 Hz, respectively, for the Z plate with amplitudes of 32 kV/cm.