

Supporting Information for

Photoluminescence Detection of Symmetry Transformations in Low-dimensional Ferroelectric ABO₃ Perovskites

Tochukwu Ofoegbuna,^a Khashayar R. Bajgiran,^a Orhan Kizilkaya,^b Stuart A. J. Thomson,^c Adam T. Melvin,^a and James A. Dorman ^{*a}

^a Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803, United States

^b Center for Advanced Microstructure Devices, Louisiana State University, Baton Rouge, Louisiana 70803, United States

^c Edinburgh Instruments Ltd., 2 Bain Square, Livingston EH54 7DQ, United Kingdom

* Corresponding Author

Email: jamesdorman@lsu.edu.

Figures

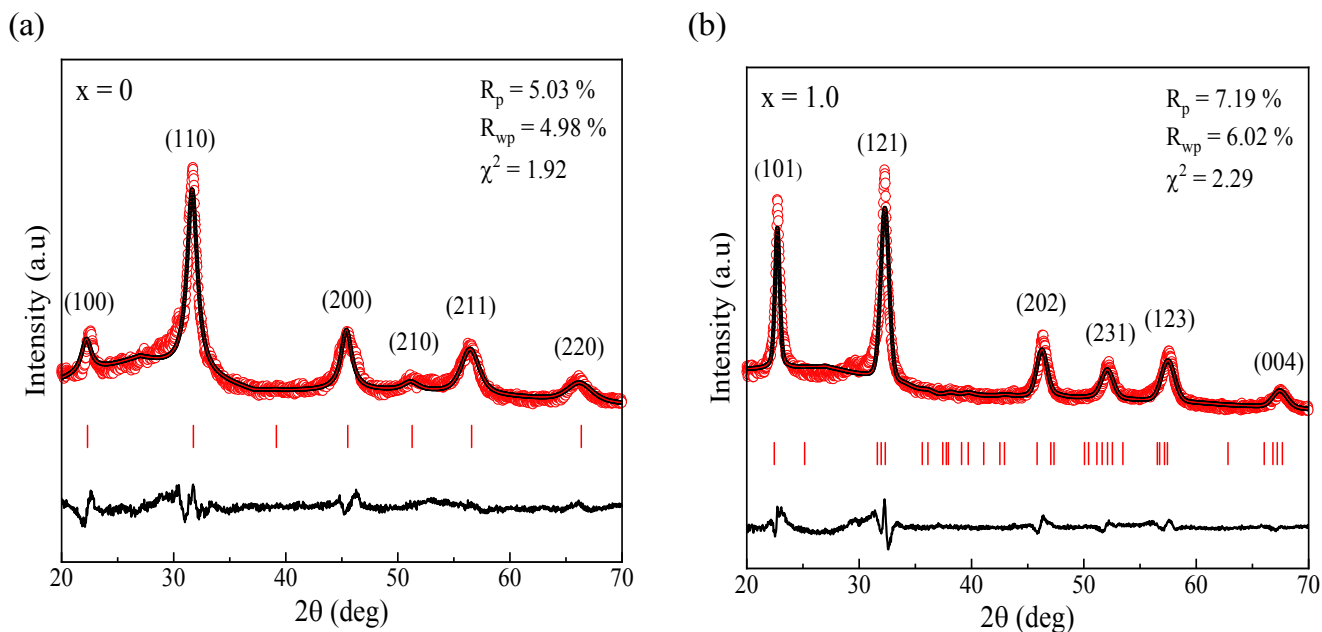


Fig. S1 (a-b) Rietveld refinement of $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3:\text{Eu}$ (2 mol%) NPs. The $x = 0$ ($\text{Sr}_{1-x}\text{NbO}_3$) and $x = 1.0$ ($\text{Ca}_{1-x}\text{NbO}_3$) compositions are references for the C and O phases. Reported spectra were collected at room temperature with $\lambda = 1.541 \text{ \AA}$. The upper symbols illustrate the observed data (circles) and the calculated pattern (solid line). The vertical markers show calculated positions of Bragg reflections and the lower curve represents the difference between observed and calculated intensities.

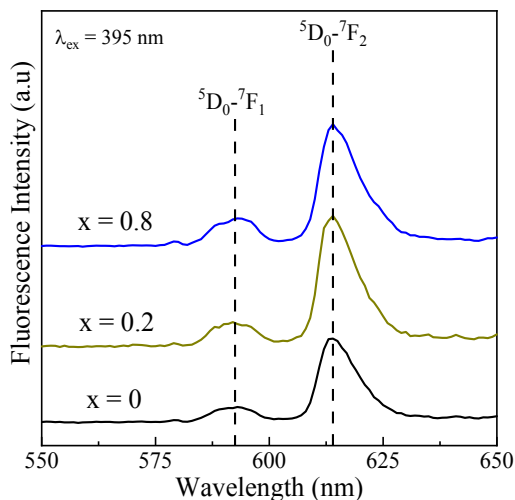


Fig. S2 PL emission spectra for $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3:\text{Eu}$ (2 mol%) nanoparticles. Spectra are offset for clarity.

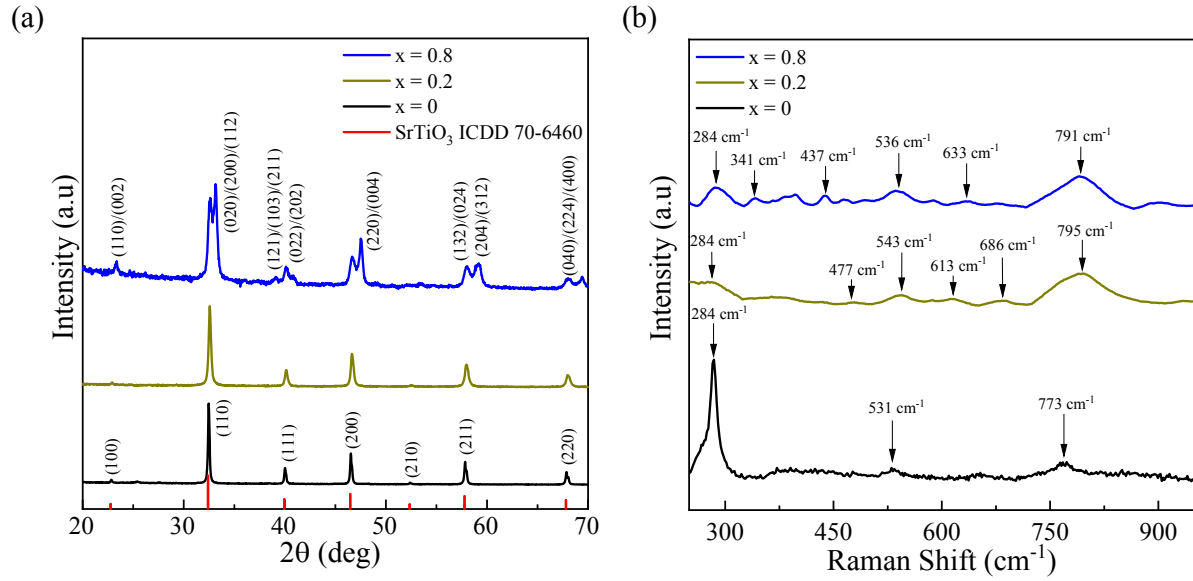


Fig. S3 (a) XRD pattern and (b) Raman spectra for CSTO:Eu (2 mol%, x = 0, 0.2 and 0.8) nanoparticles.

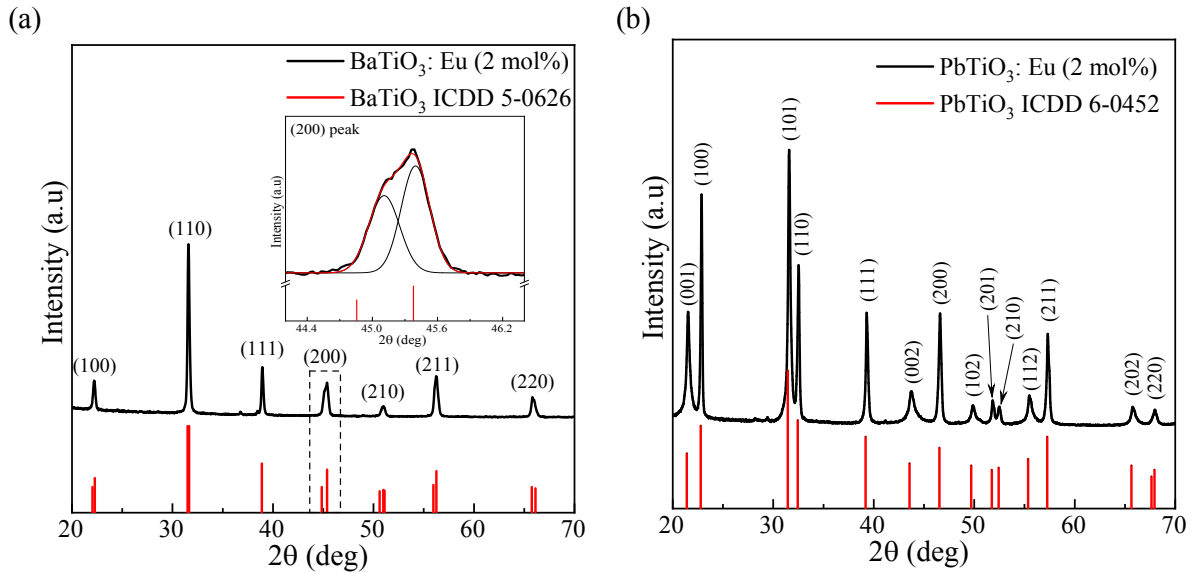


Fig. S4 Diffraction pattern for Eu-doped (a) BTO and (b) PTO NPs.

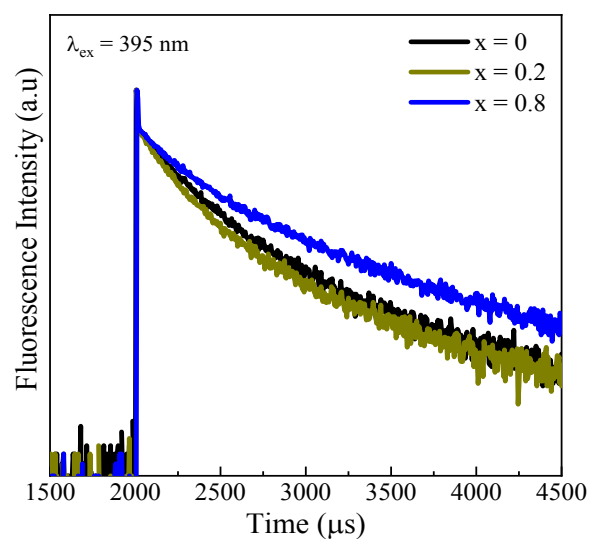


Fig. S5 Room-temperature lifetime measurements for $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3:\text{Eu}$ (2 mol%) nanoparticles.

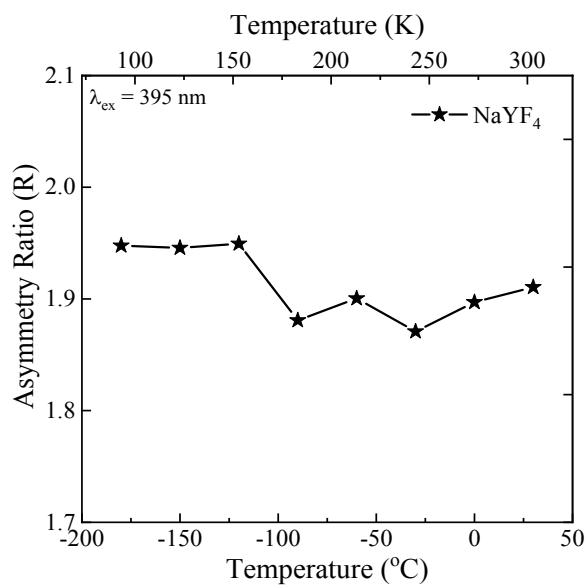


Fig. S6 Asymmetry ratio for $\text{NaYF}_4:\text{Eu}$ (2 mol%) nanoparticles in C phase. The plot highlights the absence of structural transformations in NaYF_4 at low-temperatures.

Tables

Table S1 Crystallographic Data and Refined Lattice Parameters for $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3$ Nanoparticles based on X-ray Diffraction Data

Parameters	x = 0	x = 1.0
wavelength (Å)		1.541
temperature (K)		300
2θ range (°)		20-70
space group	Pm-3m (No. 221) ^a	Pnma (No. 62) ^b
	Lattice Parameters	
a (Å)	3.988(0)	5.591(6)
b (Å)	3.988(0)	7.873(2)
c (Å)	3.988(0)	5.526(7)
α, β, γ (°)	90	90
V (Å ³)	63.411	243.306
	Atomic Coordinates	
Sr/Ca (x,y,z)	0.5, 0.5, 0.5	0.02602, 0.25, 0.02512
Nb (x,y,z)	0, 0, 0	0, 0, 0.5
O1 (x,y,z)	0.5, 0, 0	0.03976, 0.25, 0.54792
O2 (x,y,z)	-	0.19040, -0.022, 0.73890

^{a-b} space group ref.: ICSD 19-2410, ICSD 47-1668. The occupancy was fixed to 0.7 at the Sr site and 1 at Nb and O sites for the $\text{Sr}_{1-x}\text{NbO}_3$ structure and to 1 at all atom sites for the $\text{Ca}_{1-x}\text{NbO}_3$ structure. For the $\text{Sr}_{1-x}\text{NbO}_3$, the isotropic displacement parameter U_{iso} is 0.021(0), 0.017(9), and 0.044(5) Å² for Sr, Nb, and O sites, respectively. For the $\text{Ca}_{1-x}\text{NbO}_3$, the isotropic displacement parameter U_{iso} is 0.060(7), 0.003(9), 0.025(2), and 0.043(0) Å² for Ca, Nb, O1, and O2 sites, respectively.

Table S2 Lattice Parameter and Crystal Structure for $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3:\text{Eu}^{3+}$ (2 mol%) Nanoparticles

x	a (Å)	b (Å)	c (Å)	V (Å ³)	Crystal Structure
0	3.98	3.98	3.98	63.13	C
0.1	3.98	3.98	4.04	64.03	C and T
0.2	3.98	3.98	4.03	63.85	C and T
0.5	5.67	7.97	5.33	241.06	Mixture
0.8	5.75	7.91	5.29	240.81	O
1.0	5.75	7.88	5.28	239.49	O

Table S3 Lifetime for $\text{Ca}_x\text{Sr}_{1-x}\text{NbO}_3:\text{Eu}^{3+}$ (2 mol%) Nanoparticles Fit to a Double-Exponential Decay Curve

x	τ_1 (μs)	τ_2 (μs)	R ² (%)
0	179.03	571.99	99.8
0.2	174.46	629.20	99.8
0.8	211.04	798.55	99.8