

Supporting Information

Extrinsic nature of double broadband photoluminescence from BaTiO₃ perovskites: generation of white light emitters

J. L. Clabel H.^{a,*}, Gustavo Nicolodelli^b, G.Lozano C.^a, V. A. Garcia R.^c, S. O. Ferreira^d, Alexandre Pinto^e, M. Siu Li^a, E. Marega Jr.^a

^a Physics Institute of São Carlos, University of São Paulo, P.O. Box 369,13560-970, São Carlos, SP, Brazil.

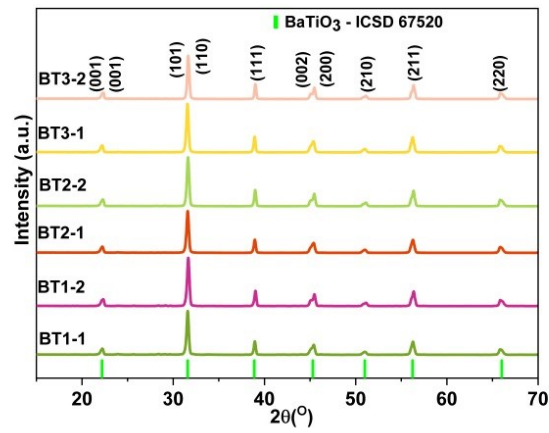
^b Department of Physics, Federal University of Santa Catarina, P.O. Box 476, 88040-900, Florianópolis, SC, Brazil.

^c Facultad de Ciencias Físicas, Universidad Nacional Mayor de San Marcos, UNMSM, Lima, Lima, Perú.

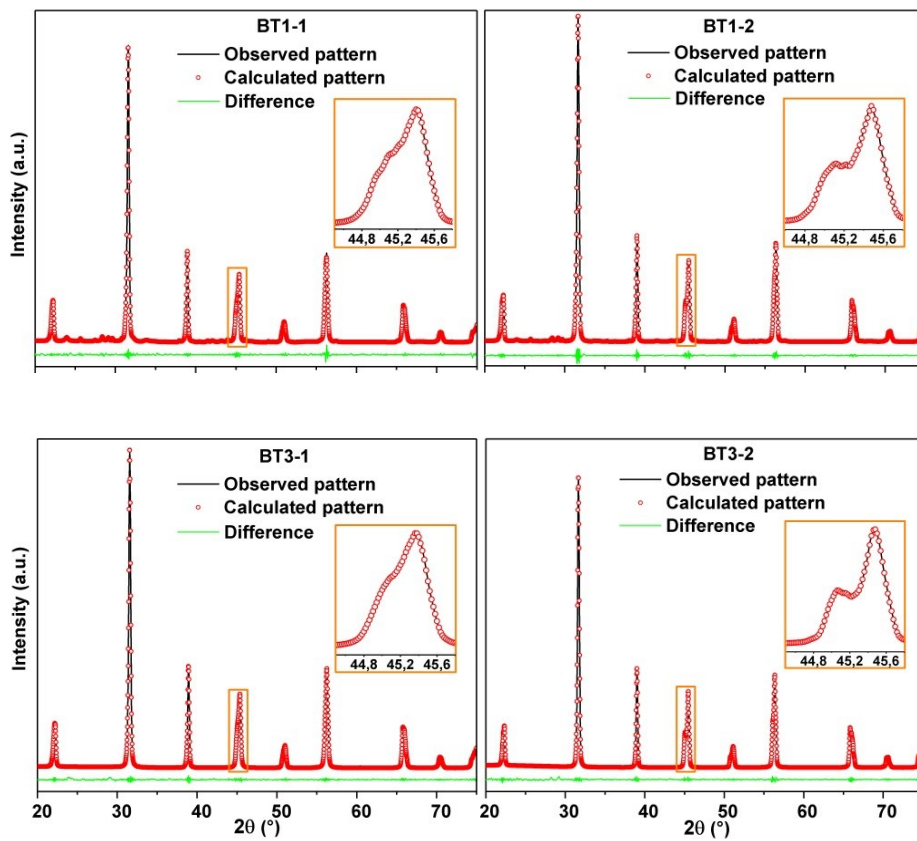
^d Department of Physics, Federal University of Viçosa, UFV, P.O. Box 36570-901, Viçosa, MG, Brazil.

^e Chemistry and Biochemistry Department, Manhattan College, Riverdale, NY 10471, USA.

*Corresponding author email addresses: jclabel@ifsc.usp.br



(a)



(b)

Figure S1. (a) X-ray diffraction patterns for different samples after thermal treatment, (b) Rietveld plots for different BaTiO₃ samples (BT1-1, BT1-2, BT3-1 and BT3-2). The amplification of X-ray diffraction profile from 44 – 46 °C in 2θ. (data extracted from the reference ¹)

Table S1. Refined structural parameters and respective agreement factors of the refinement to the BaTiO₃ samples. (data extracted from the reference ¹)

Crystallographi data	Space group	Volume (Å ³)	a, b (Å)	c (Å)	R _{Bragg} (%)	R _{wp} (%)	R _{exp} (%)	χ ²
BT1-1	P4/mm	64.390(4)	3.99899(9)	4.02642(1)	3.83	15.92	11.48	1.38
BT1-2	P4/mm	64.390(6)	3.99746(2)	4.02950(2)	3.05	15.10	11.61	1.30
BT2-1	P4/mm	64.394(5)	3.99923(1)	4.02616(2)	5.10	11.83	11.72	1.01
BT2-2	P4/mm	64.364(5)	3.99685(1)	4.02905(1)	3.53	11.88	11.22	1.06
BT3-1	P4/mm	64.391(5)	3.99898(1)	4.02544(1)	3.53	11.48	11.28	1.02
BT3-2	P4/mm	64.394(5)	3.99744(1)	4.02965(1)	5.12	13.08	12.11	1.08

Table S2. Raman mode frequency in BaTiO₃.

Raman modes	BT1-1			BT1-2			BT2-1		
	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)
A ₁ (TO)	162.03	60.46	4522.82	159.53	57.55	7391.60	158.88	59.28	5555.43
E(TO)	224.03	114.62	8469.64	208.47	100.10	9718.41	202.23	105.55	8300.67
A ₁ (TO)	279.47	57.40	3550.15	266.89	98.03	18477.8	266.07	106.33	16173.98
E(TO+LO)	307.45	9.77	2028.39	306.61	17.97	6173.7	307.03	17.04	5096.16
B ₁	321.23	163.30	6609.86	351.83	143.44	5076.88	352.98	138.36	4281.93
E(TO), A ₁ (TO)	514.04	51.31	5542.11	513.81	39.03	10997.3	514.96	40.37	9813.89
	573.53	107.26	3657.21	543.05	61.86	5452.10	544.49	65.09	4476.71
	647.32	25.09	667.83	613.38	149.58	2851.87	615.56	157.34	2516.17
E(LO), A ₁ (LO)	714.12	83.04	1486.13	715.28	59.75	2596.76	715.03	63.55	2111.20

	BT2-2			BT3-1			BT3-2		
	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)	ω (cm ⁻¹)	FWHM (cm ⁻¹)	M _I (a.u)
A ₁ (TO)	159.17	57.74	13904.54	159.89	53.71	5656.56	164.29	53.51	11692.72
E(TO)	205.24	90.85	16223.15	204.88	99.55	8161.52	211.77	78.70	14273.95
A ₁ (TO)	259.80	111.35	27508.34	265.07	96.39	15849.0	263.11	80.21	23094.66
E(TO+LO)	304.86	19.55	9191.97	307.30	17.11	5139.45	305.90	27.79	10417.84
B ₁	341.60	183.89	14647.59	340.85	159.09	4839.53	347.01	127.69	8171.07
E(TO), A ₁ (TO)	508.79	39.66	15136.09	514.77	38.45	10102.6	515.03	39.03	15474.55
	541.83	73.20	10703.58	544.33	61.50	4714.90	544.09	62.65	7232.21
	610.65	133.67	4908.79	618.70	151.09	2530.13	608.63	127.78	3219.86
E(LO), A ₁ (LO)	714.98	76.68	4312.00	715.61	58.19	2241.09	715.97	79.77	3587.99

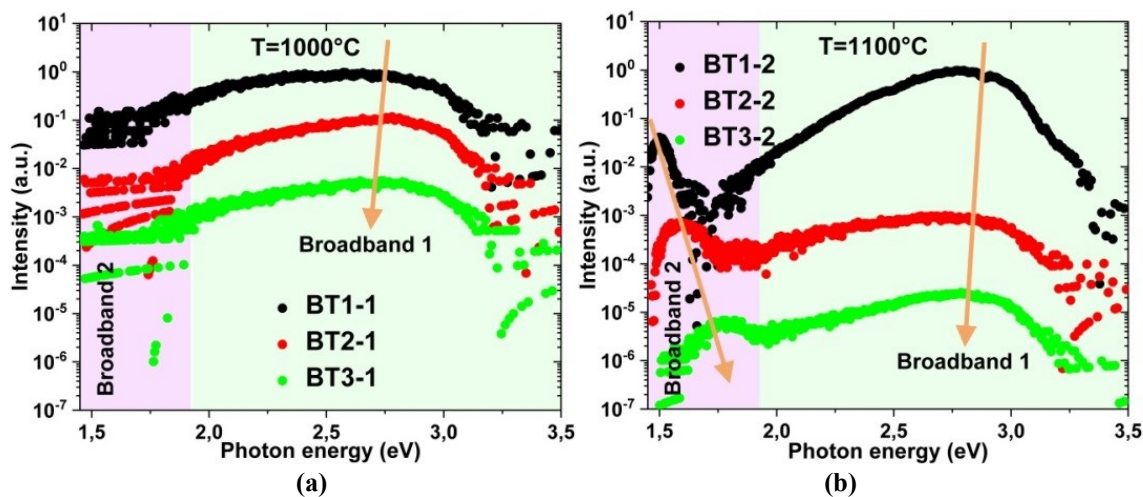


Fig. S2. Luminescence spectra of BT powder at 1000°C and 1100°C on the log scale.

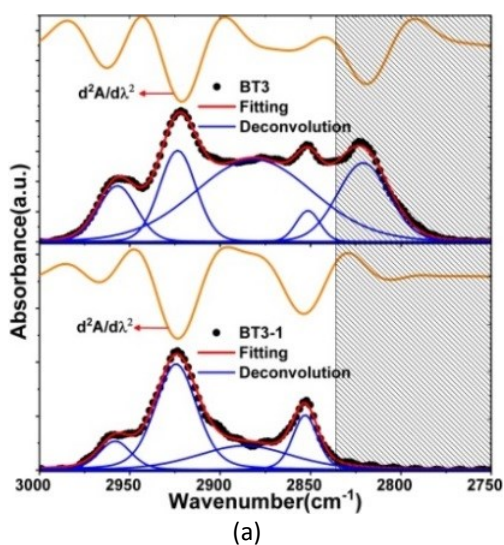


Figure S3. Fragments of FTIR spectra and deconvolution spectral bands (solid blue line) in the region between 3000 to 2750 cm^{-1} . BT3 represent the sample as mixture without thermal treatment, while BT3-1 was thermal treatment at 1000°C.

Reference

- 1 J. L. Clabel H, I. T. Awan, A. H. Pinto, I. C. Nogueira, V. D. N. Bezzon, E. R. Leite, D. T. Balogh, V. R. Mastelaro, S. O. Ferreira and E. Marega, *Ceram. Int.*, 2020, **46**, 2987–3001.