Electronic Supplementary Material (ESI) for RSC Advances.

Size induced modification of boron structural unit in YBO_3: Systematic investigation by experimental and theoretical methods

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Supporting Information

Table-S1: The calculated coordination parameters (using PAW–PBE) for monoclinic YBO_3 as compared with experiment.

Atom	Position	DFT results in present work			Rietveld refinement of XRD pattern of 800°C heated sample in the present work			Values reported in *Chem. Mater.* 2004, *16*, 2418-2424		
		x	y	z	x	y	z	x	y	z
Y1	4c	0.2500	0.2500	0.0000	0.2500	0.2500	0.0000	0.2500	0.2500	0.0000
Y2	8f	0.0854	0.2557	0.4993	0.0843	0.2561	0.5007	0.0825	0.2487	0.4985
B1	8f	0.1201	0.0377	0.2469	0.1220	0.0382	0.2476	0.1257	0.0815	0.2371
B2	4e	0.0000	0.6759	0.2500	0.0000	0.6780	0.2500	0.0000	0.6393	0.2500
O1	8f	0.1261	0.0919	0.1030	0.1258	0.0830	0.1057	0.1182	0.1152	0.1005
O2	8f	0.2227	0.0929	0.3883	0.2209	0.0900	0.3894	0.2233	0.1035	0.3847
O3	8f	0.0480	0.5659	0.3917	0.0478	0.5650	0.3938	0.0605	0.5911	0.3758
O4	8f	0.3914	0.3082	0.2517	0.3932	0.3090	0.2543	0.3814	0.3398	0.2639
O5	4e	0.0000	0.1354	0.2500	0.0000	0.1399	0.2500	0.0000	0.1583	0.2500

Table-S2: Relative concentration of BO_3 and BO_4 structural units determined by ^{11}B MAS NMR Studies

sample	Duration of heating	BO_3	BO_4
As prepared	5h	Could not be determined accurately, as the phase formed is some sort of a complex/different from YBO_3	
500°C heated	5h	56%	44%
600°C heated	5h	53%	47%
800°C heated	5h	~0%, could not be determined	Almost 100%

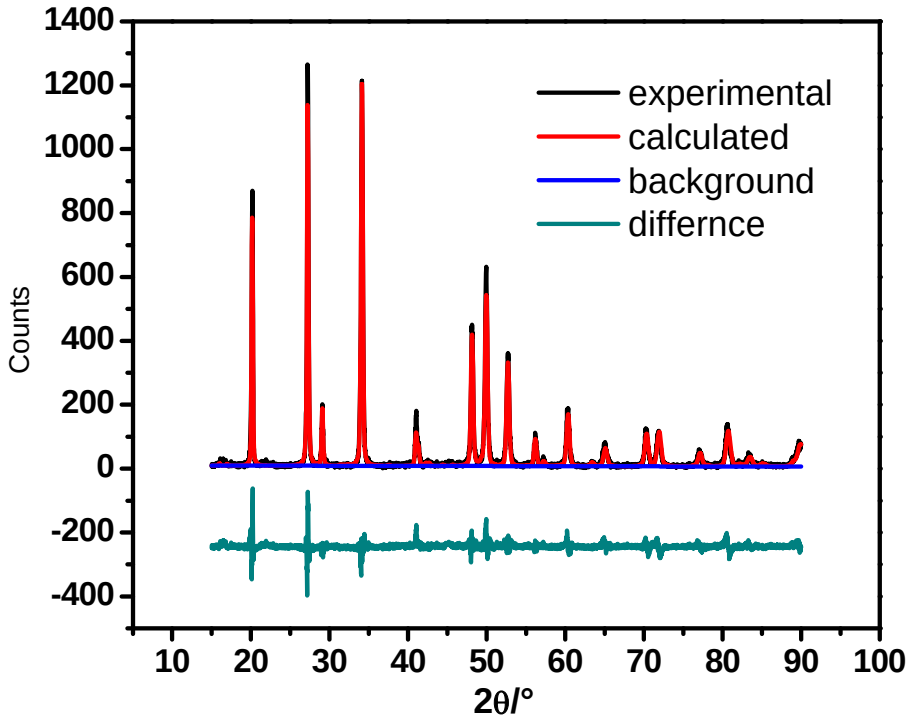

Figure-S1: Rietveld refined XRD pattern for YBO_3 sample annealed at 800°C

Formula : YBO_3

space group : C2/c

Lattice constants : a = 11.328(1)Å, b = 6.5274(7)Å and c = 9.5461(7)Å

with $\alpha = \gamma = 90^{o}$ and $\beta = 113.05^{o}$.

Goodness of fit ($\chi 2$) = 1.872

Rp, Rwp = 0.1559, 0.2194

Rf^2 = 0.1163

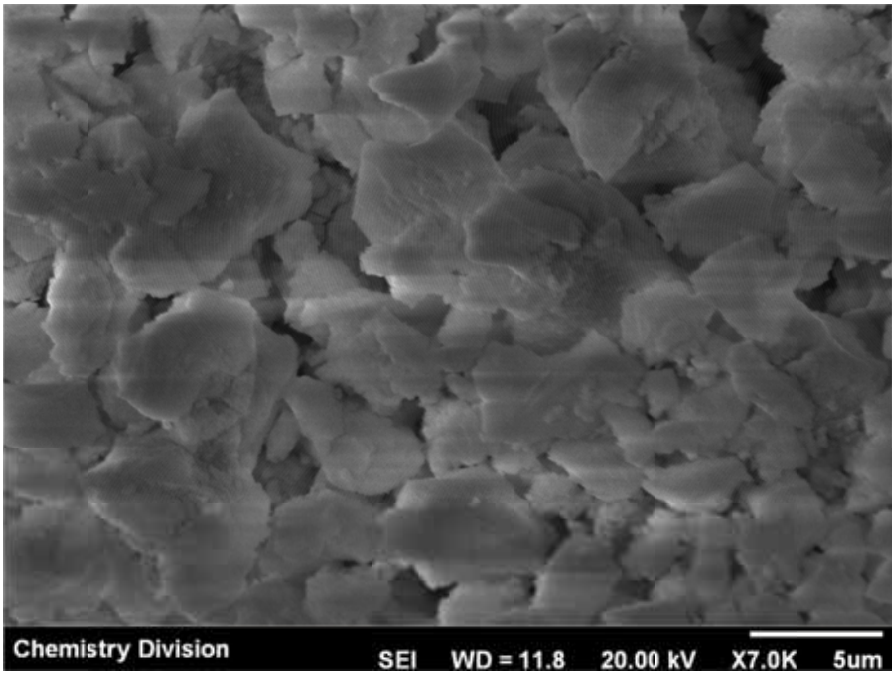

Figure-S2: SEM micrograph of 800^{o}C heated YBO_3 samples.

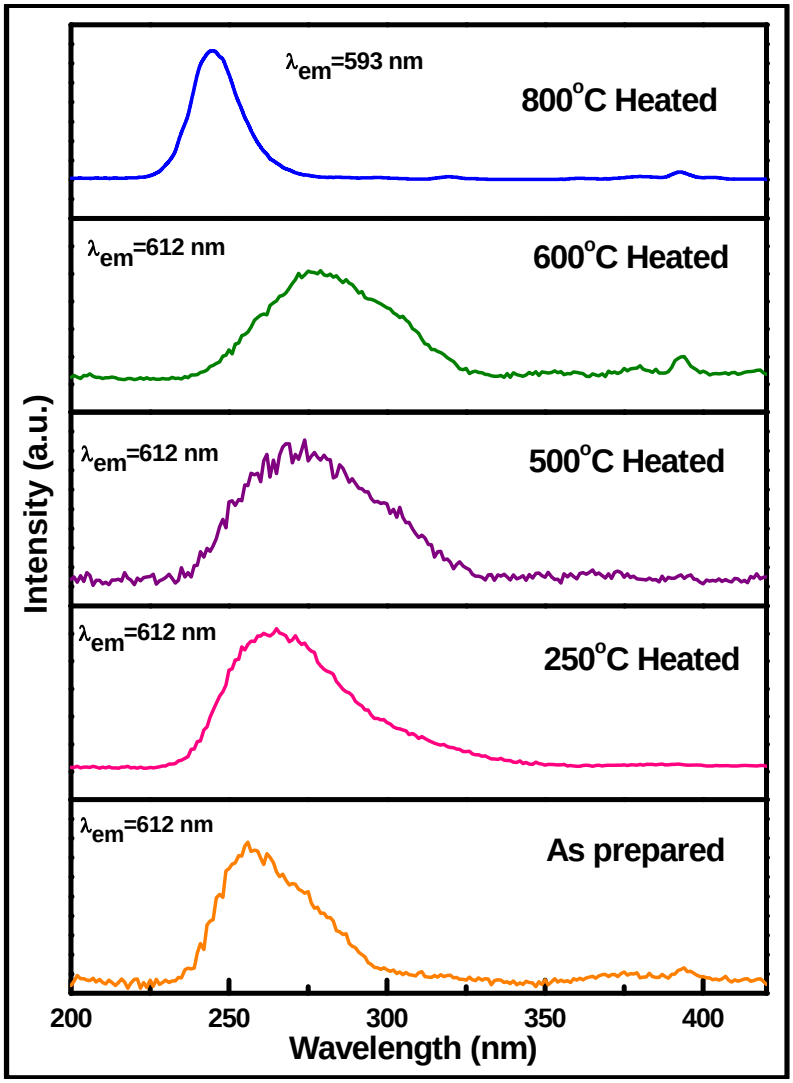

Figure-S3: Excitation spectra from Eu-doped precursor sample obtained by the reaction of Y^{3+} ions with boric acid followed by heating at different temperatures. The spectrum was recorded by monitoring the strongest emission peak of Eu^{3+} ions in corresponding emission spectra.

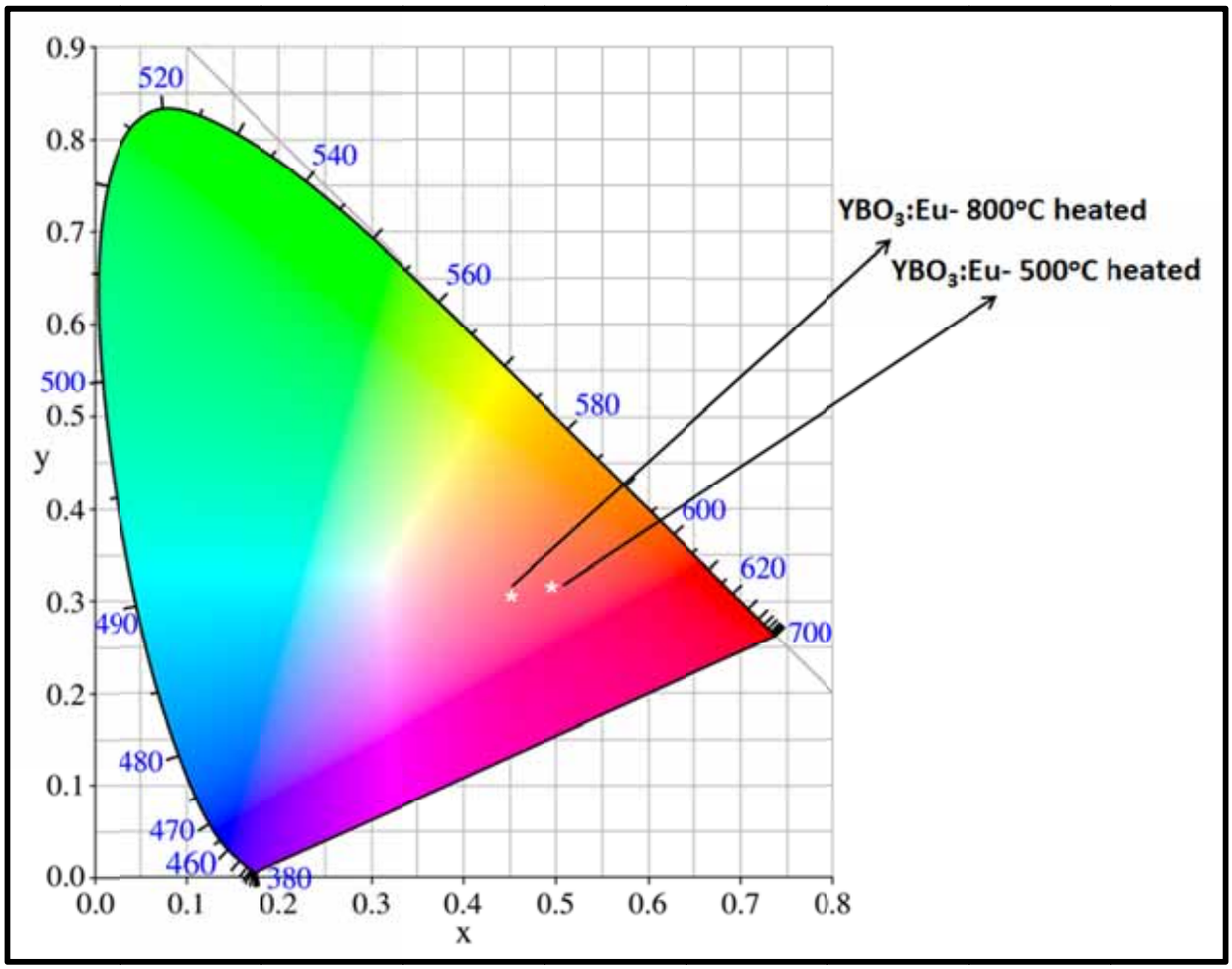

Figure-S4: CIE color coordinates of YBO_3 samples.

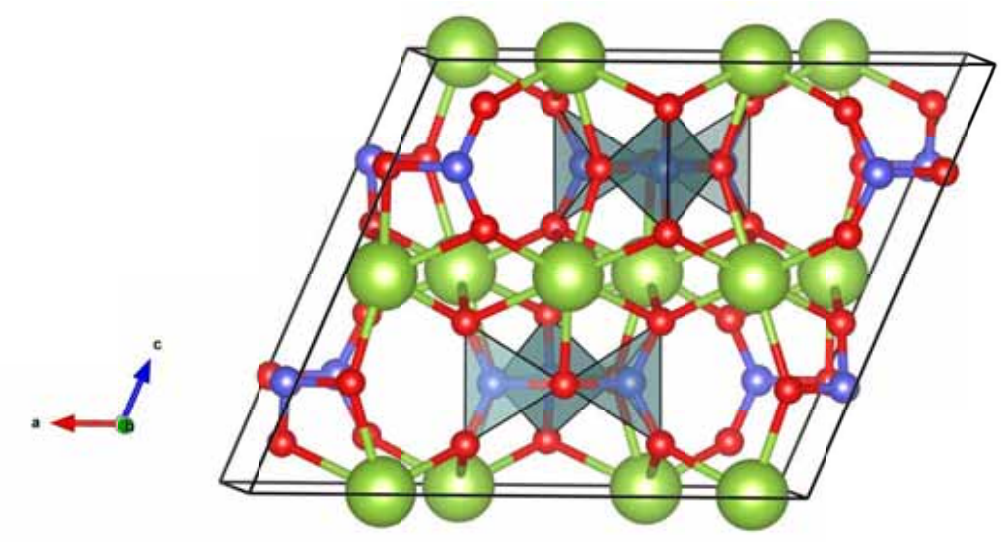

Figure S5: Representative crystal unit cell of YBO_3.

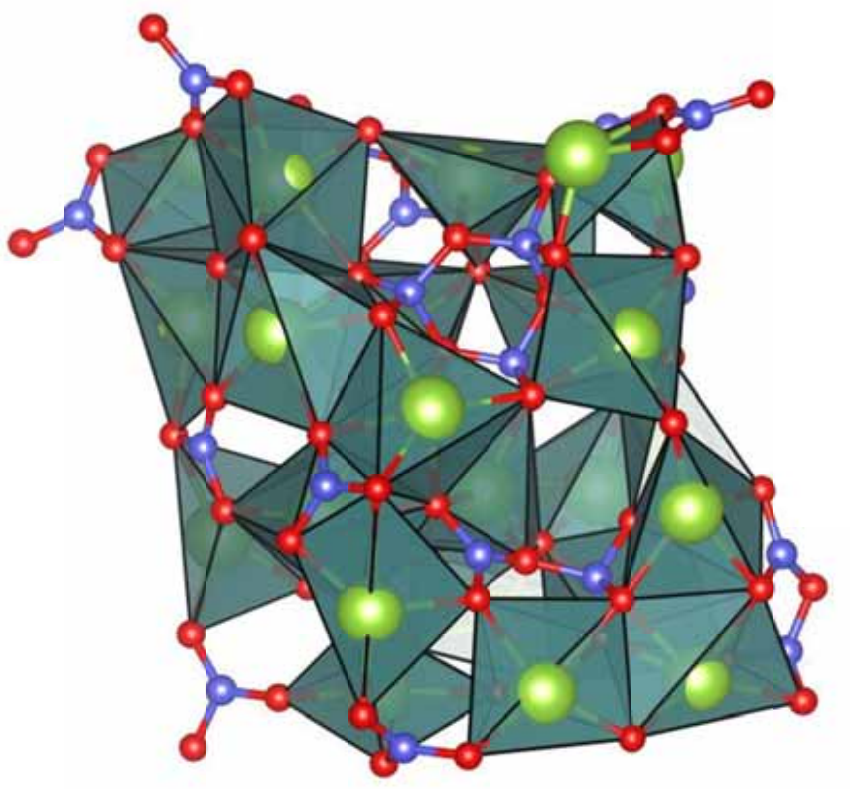

Figure-S6: YBO_3 nanoparticle structure obtained from DFT calculations.