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ELECTRONIC SUPPLIMENTARY INFORMATION FOR DALTON TRANSACTIONS

Effect of the Y:B ratio on phase purity and development of thermally stable nano-sized Eu⁺³-doped YBO₃ red phosphor using sodium borohydride

BY

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Figure S1 indicates the excitation spectra of YBO₃: Eu³⁺ sample at an emission wavelength of 612 nm. This gives the basis for using 230 nm as the excitation wavelength.

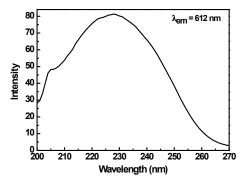


Figure S1: Excitation spectra of YBO₃: Eu³⁺ sample.

The crystallite size (nm) of YBO₃: Eu³⁺ sample, heated at different temperatures is given in Table S1. The crystallite size was calculated using Scherrer's formula [*B. D. Cullity, Elements of X-ray Diffraction, 2nd edition, Addison-Wesley Publishing Company, Inc., Page no: 102*] i.e. crystallite size (nm) = $0.9 \, \lambda \, / (\beta \times \text{Cos}\theta_B)$, where λ is the wavelength of Cu K_{\alpha} (0.154 nm), β is the Full width at half maximum (FWHM) and θ_B is the Bragg's angle. β is expressed as $(\beta_s^2 - \beta_{std}^2)^{1/2}$, where β_s is the FWHM of sample and β_{std} is the FWHM value (0.0511) for standard Siwafer sample. The Table S1 suggests that the crystallite size of un-doped and Eu³⁺-doped sample varies in between around 35 to 50 nm. The obtained lattice parameter and cell volume are also given in Table S1.

Table S1: Crystallite size, lattice parameter and cell volume of un-doped and Eu³⁺-doped YBO₃ sample heated at different temperatures.

			crystallite	Lattice parameter	Cell volume
	2θ (degree)	FWHM	size (nm)	a=b, c (Å)	$(Å^3)$
Un-doped YBO ₃					
800 °C	27.057	0.2337	35.44	3.79, 8.84	110.14
1000°C	27.225	0.2012	41.55	3.77, 8.80	108.85
1100°C	27.277	0.1922	43.65	3.77, 8.79	108.53
1200°C	27.175	0.1842	45.69	3.78, 8.81	108.90
1300°C	27.172	0.1783	47.33	3.78, 8.80	108.88
1400°C	27.225	0.1712	49.49	3.77, 8.80	108.79
Eu ³⁺ -doped YBO ₃					
800°C	27.072	0.2245	36.98	3.79, 8.83	110.45
1000°C	27.165	0.2179	38.17	3.78, 8.81	109.37
1100°C	27.185	0.1898	44.23	3.78, 8.82	109.50
1200°C	27.095	0.1837	45.81	3.79, 8.83	109.95
1300°C	27.146	0.1755	48.15	3.79, 8.83	109.83
1400°C	27.185	0.1707	49.64	3.78, 8.83	109.26

Figure S2 (a) and (b) shows FESEM micrograph of un-doped YBO₃, calcined at 800 °C and 1200 °C, respectively. The particles are agglomerated in nature for both calcined samples. However, the average agglomerated particle size was 100 to 200 nm at 800 °C, whereas 500 nm to 2 μ m at 1200 °C.

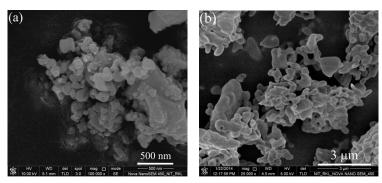


Figure S2: FESEM micrograph of un-doped YBO₃, calcined at (a) 800 °C and (b) 1200 °C.

The particle morphology of un-doped YBO₃ was also observed in TEM. Fig. S3 (a) and (b) indicates the TEM micrographs of un-doped YBO₃, calcined at 800 °C and 1200 °C, respectively. The particle size of un-doped YBO₃, calcined at 800 °C was ~8-10 nm, whereas, for the sample calcined at 1200 °C, the particles were agglomerated in nature and the average particle size was found to be 100-300 nm.

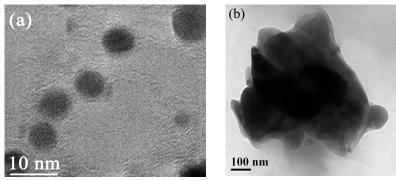


Figure S3: TEM micrograph of un-doped YBO₃, calcined at (a) 800 °C and (b) 1200 °C.

In order to confirm the purity along with the qualitative and quantitative composition of Y_{0.9}Eu_{0.1}BO₃, its EDS analysis was performed. Figure S4 shows EDS mapping of YBO₃: Eu³⁺ phosphor calcined at two different temperatures. It was confirmed that the sample contained yttrium, boron, oxygen and europium and no impurities. The typical EDS spectrum was also shown in Fig. S4 and it was used to further characterize the composition of the phosphor sample. The EDS spectrum of YBO₃: Eu³⁺ sample shows the presence of Y, B, O and Eu. Quantitative testing of the atom concentrations of the sample performed at different point

positions are listed in Table S2. The Eu concentration was calculated by the Eu atomic concentration divided by the sum of Y and Eu atomic concentration [Q. Dong, Y. Wang, Z. Wang, X. Yu, and B. Liu, *J. Phys. Chem. C*, 2010,**114**, 9245], which are also shown in Table S2. From EDS quantitative microanalysis, the amount of Eu³⁺ in YBO₃ phosphor is calculated as nearly 10 %.

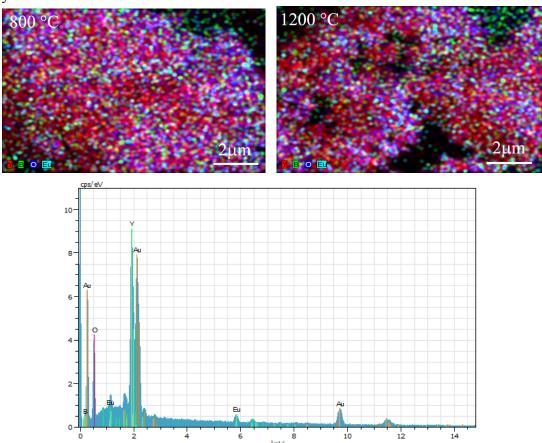


Figure S4: EDS mapping and EDS spectra of YBO₃: Eu³⁺ phosphor.

Table S2: Concentration of Eu in YBO₃ phosphor was determined based on atom concentration measured by EDS at different position.

Different position		Atomic % obt	Calculated Eu% from EDS data		
	Y	В	О	Eu	
1	35.67	14.60	45.26	4.47	11.13
2	42.29	16.12	36.93	4.66	9.92
3	30.95	16.6	48.88	3.57	10.34