Electronic Supplementary Information (ESI)

Realization of White Light Emission as a Manifestation of Dy^{3+} to Eu^{3+} Energy Transfer in Single Component $MgAl_2O_4$: Dy^{3+}, Eu^{3+} Nanophosphor: A Promising Candidate For Solid State Lighting & Self referencing Optical Thermometry Applications

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Method of Rietveld analysis:

The Rietveld method of powder structure refinement[1-2] is one of the best known methods to ascertain different (micro/nano) structure parameters of single/multi-phase materials. Adoption of this method becomes incumbent for quantitative phase analysis of a multiphase material where reflections from the constituent phases are severely overlapped. The experimental XRD pattern is simulated using analytical functions that depend on different structural and microstructure parameters of each individual phase.[3] The calculated intensities (y_{ic}) are determined from the following equation:[3]

$$Y_{ic} = S\sum_k L_k |F_k| 2\Phi(2\theta_i - 2\theta_k) P_k A + y_{bi} \qquad (1)$$

where S is the scale factor, k represents the Miller indices (h,k,l) for a Bragg reflection, L_k represents the Lorentz polarization and multiplicity factors, Φ is the reflection profile function, P_k is the preferred orientation function, A is absorption function, F_k is the structure factor for the k^{th} Bragg reflection and y_{bi} is the background intensity of the i^{th} step. Marquardt least-square refinement procedure is used to monitor the difference between the observed and the calculated pattern with the help of the reliability index parameters, $R_{wp} = \left[\frac{\sum_i w_i (Y_{io} - Y_{ic})^2}{\sum_i w_i {Y_{io}}^2}\right]^{\frac{1}{2}}$ (weighted residual error), and $R_{exp} = \left[\frac{(N-P)}{\sum_i w_i Y_{io}^2}\right]^{\frac{1}{2}}$ (expected error). Where w_i is the statistical weight, Y_{io} and Y_{ic} are the observed and calculated X-ray diffraction intensity, N is the weight and number of experimental observations and P is the number of fitting parameters. Goodness of Fit (GoF)[4-5], which is the ratio of R_{wp} and R_{exp} , indicates the refinement quality. The peak shape is assumed to be to be a pseudo-Voigt (pV) function with asymmetry to take into account the individual broadening caused by particle size and strain respectively.[6-7] In the present study, Rietveld software MAUD (Materials Analysis Using Diffraction)[8] version 2.79 is utilized for simultaneous

refinement of different structural and microstructure parameters of $MgAl_2O_4:Eu^{3+}$, Dy^{3+} nanostructures.

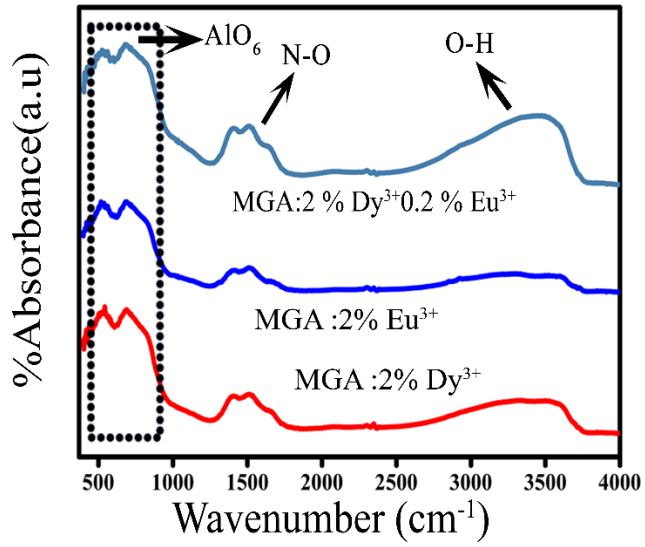

Figure S1: FTIR of synthesize samples.

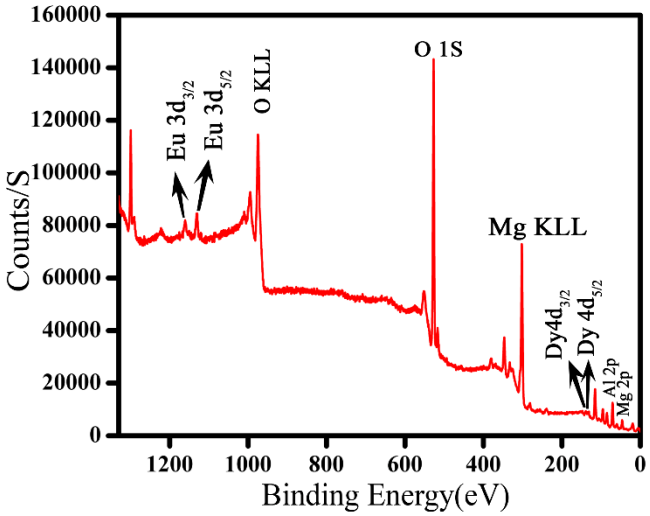

Figure S2: XPS survey scan of Eu^{3+}, Dy^{3+} co-doped $MgAl_2O_4$ nanophosphor

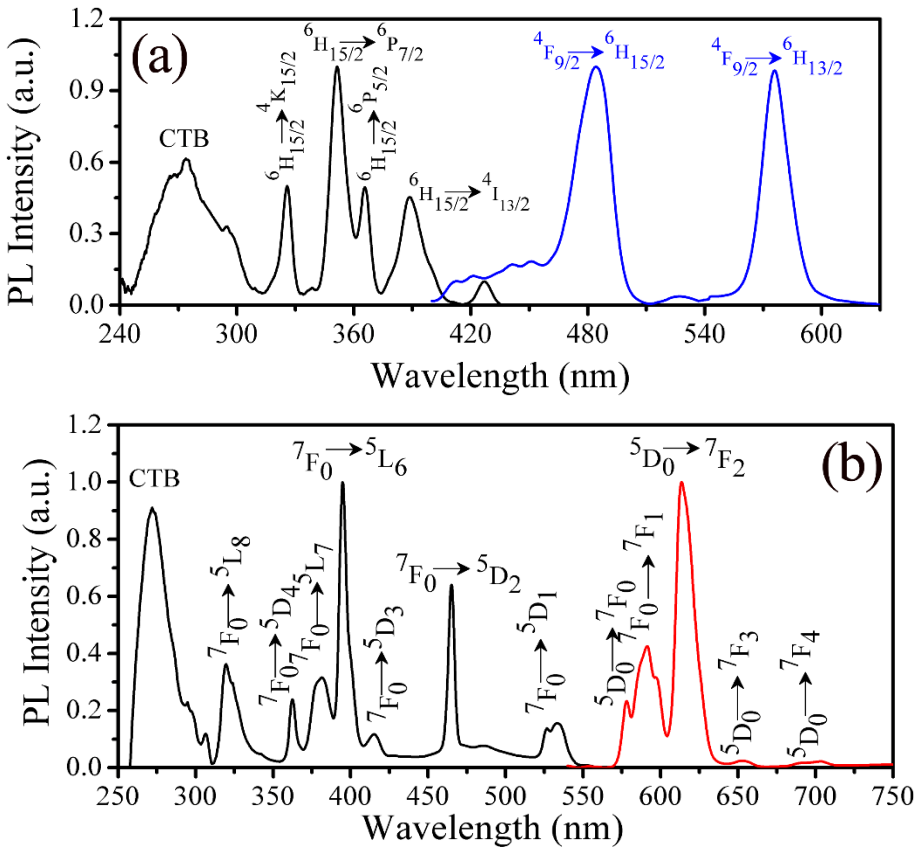

Figure S3: (a) PL excitation (left side, monitored at 575nm) and emission spectra (right side, excited by 351nm) of MGA:2% Dy^{3+} nanophosphors (b) PL excitation (left side, monitored at 616 nm) and emission spectra (right side, excited by 394 nm) of MGA: 2% Eu^{3+} nanophosphors.

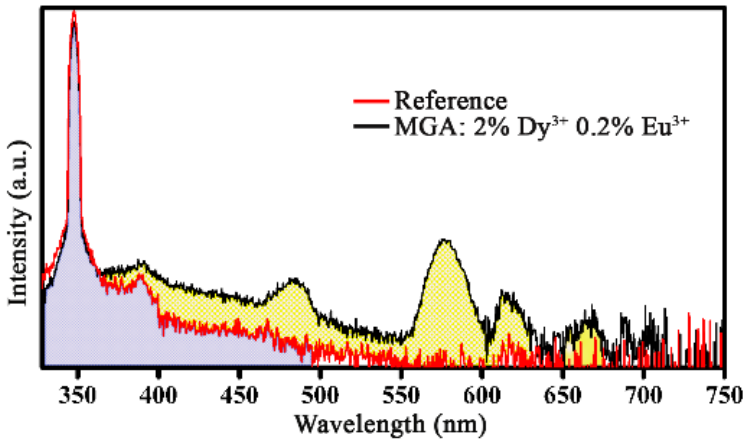

Figure S4: PL spectra of MGA: 2% Dy^{3+}, 0.2% Eu^{3+} and reference sample (Benflect recorded in an integrating sphere attached with PL spectrometer for quantum yield measurement.

References:

1. Rietveld, H.M. Line profiles of neutron powder-diffraction peaks for structure refinement. *Acta Crystallographica* 1967, 22, 151-152.

2. Rietveld, H.M. A profile refinement method for nuclear and magnetic structures. *Journal of Applied Crystallography* 1969, 2, 65-71.

3. Young, R.A. The Rietveld Method. IUCr, Oxford University Press, 1996.

4. Lutterotti, L.; Scardi, P.; Maistrelli, P. LSI - a computer program for simultaneous refinement of material structure and microstructure. *Journal of Applied Crystallography* 1992, 25, 459-462.

5. Young, R.A.; Willes, D.B. Profile shape functions in Rietveld refinements. *Journal of Applied Crystallography* 1982, 15, 430-438.