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Supporting information

Evolution of different defect clusters in Eu³⁺ doped KMgF₃ and Eu³⁺, Li⁺ co-doped KMgF₃ compounds and the immediate consequences on the phosphor characteristics

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Instrumentation

X-Ray diffraction (XRD)

A rotating anode based powder X-ray diffractometer (model Rigaku, Japan) has been used to characterise the prepared compounds. A CuK_{α} (λ = 1.5406 and 1.5444 Å) monochromatic radiation was used as X-ray radiation source. The diffraction patterns were collected within the 2 θ range of 10-70 with a step width of 0.02 and scan rate of 5s.

Fourier-transform infrared spectroscopy (FTIR) study

The FTIR spectrum was recorded using a Bruker Platinum ATR FTIR spectrometer in the spectral range 5000-500 cm⁻¹

Photoluminescence study (PL)

An Edinburgh CD-920 unit with M 300 monochromators was used for PL study and the data acquisition and analysis were carried with the help of F-900 software provided by Edinburgh Analytical Instruments, UK. A Xenon flash with a frequency of 100 Hz was utilized as a source to record the emission, excitation and lifetime spectra. For each of the spectrum, multiple scans (at least five) were taken to minimize the peak intensity fluctuation and to maximize S/N ratio. While for lifetime study, we have used the well established Time-correlated single-photon counting (TCSPC) technique.

Electron Paramagnetic Resonance (EPR) study:

A Bruker EMX (micro) 10/12 EPR spectrometer, operating at X-band frequency (9.4218 GHz) was used for EPR experiment. The spectrometer is equipped with 100 kHz field modulation and phase sensitive detection for obtaining the first derivative signal. For calibration of g-values we have used Diphenyl picrylhydrazyl (DPPH).

Positron Annihilation Lifetime Spectroscopy (PALS) study

We have followed the same procedure as that of earlier to record the PALS measurements at room temperature using two BaF₂ scintillation detectors connected to a fast–fast coincidence system and ²²Na as positron source (~ 10 μ Ci). The source was deposited in a thin Kapton foil and then kept inside the powder sample in an aluminum vial, which was kept between two BaF₂ detectors. A resolving time of 250 ps for the positron window settings was measured with ⁶⁰Co source was and the time calibration was 12.5 ps/channel. In each the measurement,

the spectrum with approximately 2 x 10^6 counts was acquired. PALSFIT analysis program was used to analyze the data.



Figure S1: Decay profile of KMgF₃ at 250 nm excitation and at emission wavelength a) 440 nm, 480 nm, 530 nm, 605 nm



Figure S2: Excitation spectra of 0.5 mol% Eu³⁺-doped KMgF₃



Figure S3: Emission spectra of 5.0 mol % $\rm Li^{+}$ and 0.5 mol % $\rm Eu^{3+}$ doped

KMgF₃