# Engineering the defect clusters in distorted $NaMgF_3$ perovskite and their important roles in tuning the emission characteristics of $Eu^{3+}$ dopant ion

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## Instrumentation:

### X-Ray diffraction (XRD):

All the XRD patterns for Undoped and doped compounds are recorded using a rotating anode based powder X-ray diffractometer (model Rigaku, Japan). As a X-ray source a $CuK_\alpha$ ($\lambda$= 1.5406 and 1.5444 Å) monochromatic radiation was used. We have collected the diffraction patterns within the 2$\theta$ range of 10-70 with a step width of 0.02 and scan rate of 5s.

### Fourier-transform infrared (FTIR) spectroscopy:

We have recorded all the FTIR spectra in the spectral range 5000-500 $cm^{-1}$ using a Bruker Platinum ATR FTIR spectrometer

### Scanning electron microscope (SEM) and Energy-dispersive X-ray spectroscopy (EDX) analysis:

A SNE4500MSEC instrument with Minisem software was used to record the SEM figures while the EDX spectrum was recorded on a Bruker Nano GmbH XFlash detector 410-M (Berlin, Germany) and the spectrum was analysed using Quantax Esprit 2.0 Bruker microanalysis software.

### Photoluminescence (PL) spectroscopy:

We have used an Edinburgh CD-920 unit with M 300 monochromators for PL measurements of all the compounds. All the data acquisition and the analysis were carried using F-900 software which was provided by Edinburgh Analytical Instruments, UK. As a source we have used a Xenon flash with a frequency of 100 Hz was utilized as a source. For each of the measurements such as excitation and emission spectra, multiple scans (at least five) were taken to maximize the S/N ratio. The widely used and well established Time-correlated single-photon counting (TCSPC) technique was used for lifetime study.

### Electron Paramagnetic Resonance (EPR) spectroscopy:

We have carried out the EPR experiments using a Bruker EMX (micro) 10/12 EPR spectrometer, which operates at X-band frequency (9.4218 GHz). The instrument is equipped with 100 kHz field modulation and phase sensitive detection for obtaining the first derivative signal. Diphenyl picrylhydrazyl (DPPH) used a standard to calibrate the g-values of the resonance signal.

**Positron Annihilation Lifetime Spectroscopy (PALS) study:**

Positron annihilation lifetime measurements were carried out using two $BaF_2$ scintillation detectors connected to fast-fast coincidence system. A $^{22}Na$ positron source (~ 10 μCi) sealed within a thin Kapton foil was put inside the powder sample in an aluminum vial. Subsequently, the vial was kept between two $BaF_2$ detectors. The time resolution measured with $^{60}Co$ in the $^{22}Na$ energy window settings was 250ps. The time calibration was kept 12.5 ps/channel. In each the measurement, the spectrum with approximately 2 x $10^6$ counts was acquired. The PAL spectra were analysed for discrete lifetime components using PALSfit analysis program.[1]

[1] P. Kirkegaard, J. V. Olsen, M. M. Eldrup and N. J. Pedersen. PALSfit. Roskilde: DanmarksTekniskeUniversitet, Risø National laboratoriet for BæredygtigEnergi. (Denmark. ForskningscenterRisoe. Risoe-R; No. 1652(EN)), 2009.

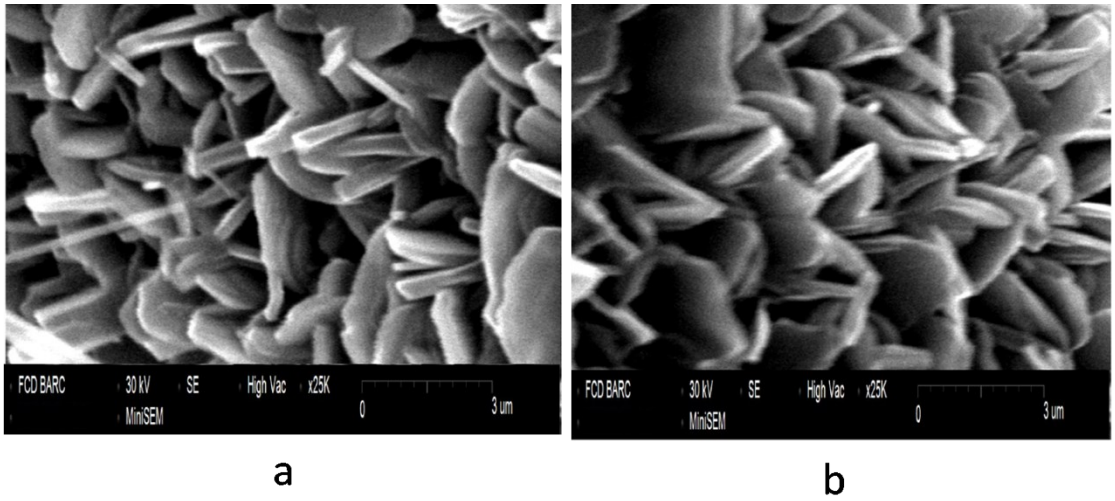


**Figure S1:** SEM images of a) $NaMgF_3$and b) $Eu^{3+}_{0.01}$ $Li^{+}_{0.005}$:$NaMgF_3$

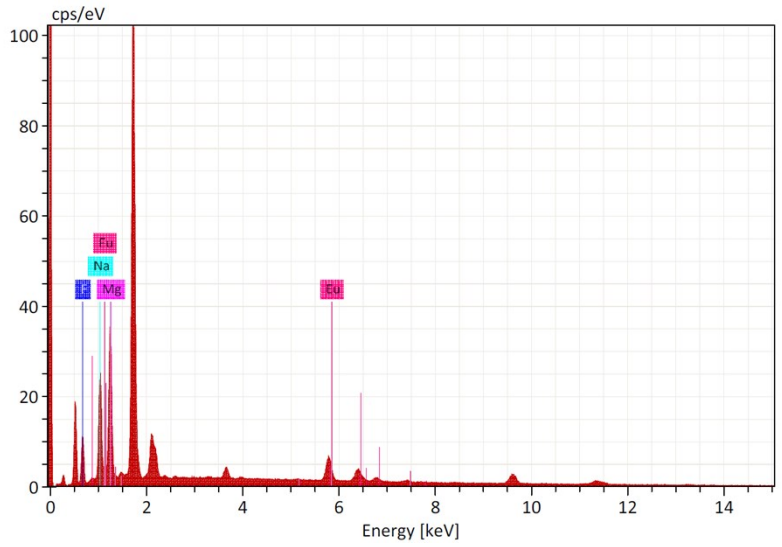


**Figure S2:** Elemental study of 0.5 mol % $Eu^{3+}$ doped $NaMgF_3$ by EDX.

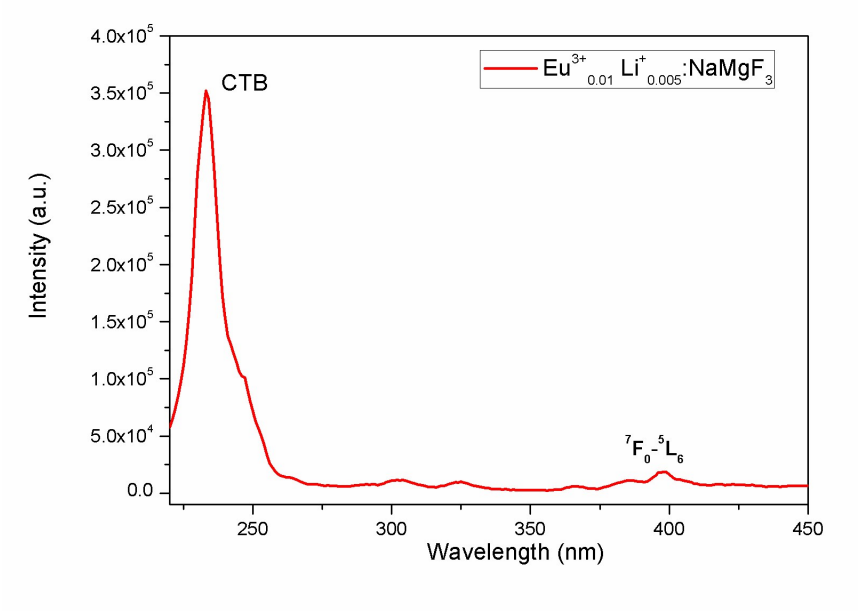


**Figure S3.** Excitation spectra of $Eu^{3+}_{0.01}$ $Li^{+}_{0.005}$:$NaMgF_3$ at an emission wavelength of 615 nm

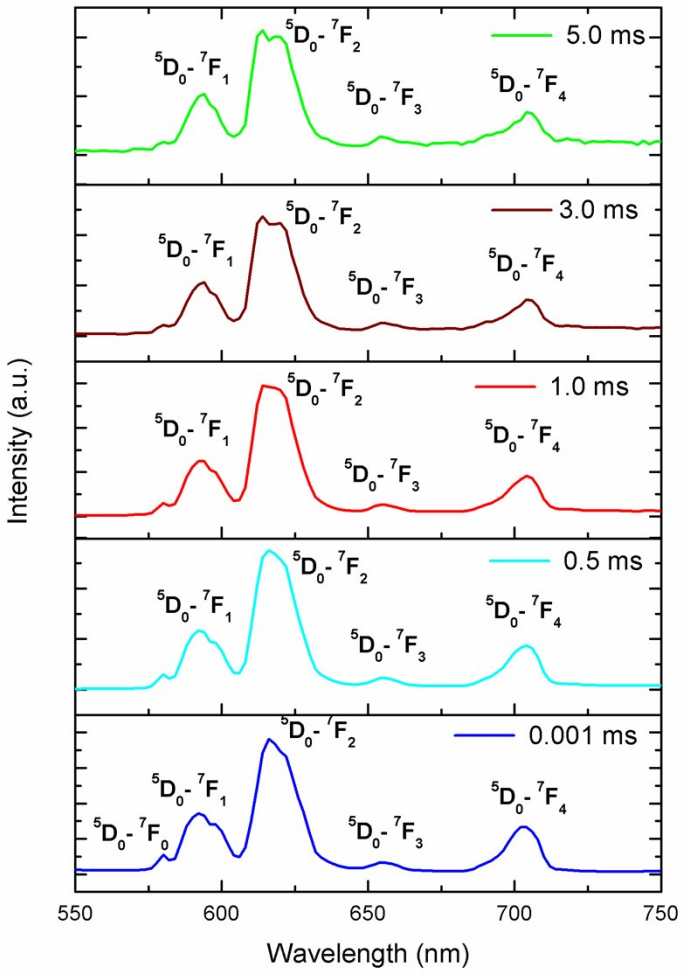


**Figure S4:** TRES spectra of 1 mol % $Eu^{3+}$ doped $NaMgF_3$ compound at different delay time.