## **Supporting Information**

## Defects induced changes in the Electronic structures of MgO and their correlation with the optical properties: A special case of electron-hole recombination from the conduction band

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## 1. Instrumentation:

RIGAKU Miniflex-600 diffractometer operating in the Bragg-Brentano focusing geometry has been used for Powders XRD of the samples where Cu-K $\alpha$  radiation ( $\lambda$ = 1.5406Å) has been used as X-ray source. The instrument was operated at 40 kV voltage and 30 mA current. The XRD pattern has been taken from 20° to 80° 20 range with scan rate of 1°/minute. Reflectancemode absorbance spectrum was recorded with a UV–Visible spectrophotometer (Ocean Optics USB3900 Miniature Fiber Optic Spectrometer) using Halogen light source HL 2000. PL data were recorded on an Edinburgh CD-920 unit which is equipped with M 300 monochromators. F-900 software provided by Edinburgh Analytical Instruments, UK was used for the data acquisition and analysis. Emission spectra for a particular sample was recorded with a Xenon flash with a frequency of 100 Hz. Multiple Scans (at least five) were taken to minimize the fluctuations in peak intensity and maximize S/N ratio. Fluorescence lifetime measurements were based on well established Time-correlated single-photon counting (TCSPC) technique. The MgO compounds were excited with 250 nm laser pulses provided by the frequency-doubled output of the Nd:YAG pumped, OPO laser-regenerative amplifier operating at a 10 Hz repetition rate.



Figure S1. Excitation spectra of Mg-600 at  $\lambda_{em} = 540$  nm



Figure S2. Decay profiles of the MgO-600 nanoparticles at  $\lambda_{ex} = 250$  nm and at different emission wavelength viz. a) 605 nm, b) 680 nm & c) 850 nm



Figure S3. TRES at 2µs - TRES at 20µs



Figure S4. TRES at 20 µs - TRES at 40 µs



Figure S5. TRES at 100 µs - TRES at 300 µs



Figure S6. TRES at 300  $\mu s$  - TRES at 600  $\mu s$ 



**Figure S7.** TRES at 800 µs



Figure S8. Gaussian Fit of TRES in the Figure 7f



Figure S9. Gaussian Fit of TRES in the Figure 7g

 Table S1: Lifetime values of MgO-600 nanoparticles at different emission wavelength and their respective contributions.

Wavelength	τ
(nm)	(µs)
390	11.22
450	13.54
490	212.2
540	82.48
605	15.09
680	362
850	13.23