

Supporting Information for

Structure and luminescence properties of Dy³⁺ doped quaternary tungstate Li₃Ba₂Gd₃(WO₄)₈ for applications in wLEDs

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1-DTA analysis:

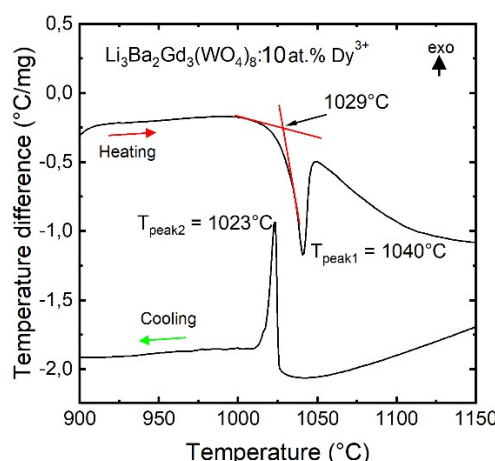


Fig.S1. Differential thermal analysis (DTA) curves for Li₃Ba₂Gd₃(WO₄)₈:10 at.% Dy³⁺

2-RAMAN and FTIR spectroscopy:

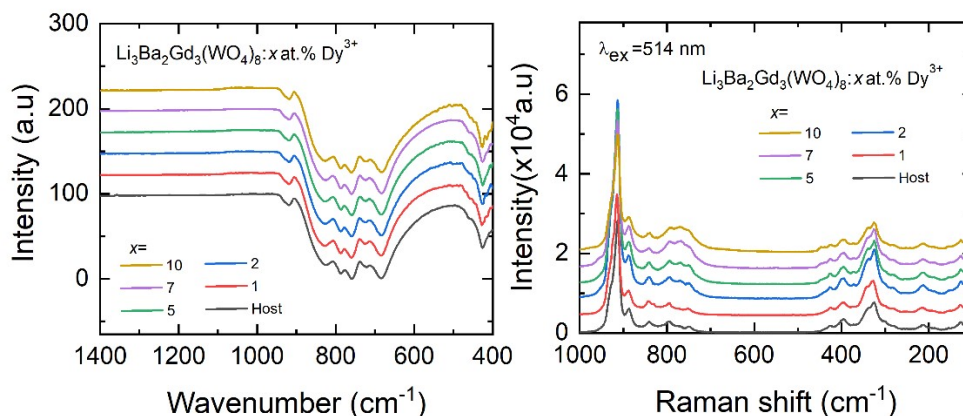


Fig.S2. (a) FTIR spectra (b) Raman spectra of Li₃Ba₂Gd₃(WO₄)₈ doped at different concentration levels of Dy³⁺ ions

3- Bandgap and electronic structure:

The Kubelka-Munk (K-M) relation is employed to evaluate the optical band gap values of the fabricated powder ³⁹:

$$F(R_{\infty}) = \frac{(1 - R_{\infty})^2}{2R_{\infty}} = K/S \quad , \quad (\text{Eq.S1})$$

where $R_{\infty} = R_{\text{sample}}/R_{\text{standard}}$; K is the absorption coefficient and S is the scattering coefficient. On the other hand, the band gap E_g of the material and the linear absorption coefficient α of the material are correlated by the Tauc equation:

$$ah\nu = C1 \times (h\nu - E_g)^{1/2} \quad , \quad (\text{Eq.S2})$$

whereby, $h\nu$ is the energy of the photon and C1 represents the proportionality constant. In the case where, the photons scatter from the surface of the material in a perfectly diffuse manner, then the value of the absorption coefficient K becomes almost equal to 2α . Assuming that S is constant with respect to the wavelength λ , the relationship between $F(R_{\infty})$ and E_g can be obtained using equations (2) and (3), as follows:

$$[F(R_{\infty})h\nu]^2 = C2 \times (h\nu - E_g) \quad , \quad (\text{Eq.S3})$$

3- Calculation of the chromaticity coordinates:

In the case of the CIE 1931-XYZ tri-chromatic system, the tri-stimulus values are defined as follow:

$$X = \int \bar{x}(\lambda)I(\lambda)d\lambda \quad , \quad (\text{Eq.S4})$$

$$Y = \int \bar{y}(\lambda)I(\lambda)d\lambda \quad , \quad (\text{Eq.S5})$$

$$Z = \int \bar{z}(\lambda)I(\lambda)d\lambda \quad , \quad (\text{Eq.S6})$$

where $\bar{x}(\lambda)$, $\bar{y}(\lambda)$, $\bar{z}(\lambda)$ are the observer's colour functions defined by the CIE $I(\lambda)$ and $I(\lambda)$ is the spectral intensity of the material. The chromaticity coordinates are determined as follows:

$$x = \frac{X}{X + Y + Z} \quad , \quad (\text{Eq.S7})$$

$$y = \frac{Y}{X + Y + Z} \quad , \quad (\text{Eq.S8})$$

$$z = \frac{Z}{X + Y + Z} \quad , \quad (\text{Eq.S9})$$

where $x + y + z = 1$, so it is sufficient to define chromaticity with two numbers, usually x and y.