Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Mechanism of upconversion luminescence enhancement in Yb^{3+}/Er^{3+} co-doped Y_2O_3 through Li^+ incorporation

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Table S1. Rietveld fitting parameters for the Li6

Atom	Site	x	y	z	Occupancy	U_{iso}
Y	8a	0.25	0.25	0.25	0.9611	0.03
Y	24d	0.9716	0	0.25	0.9763	0.00005
Li	8a	0.25	0.25	0.25	0.0389	0.03
Li	24d	0.9716	0	0.25	0.0237	0.00005
O	48e	0.3904	0.1530	0.3811	0.99	0.0001

Table S2. Rietveld fitting parameters for the Li12

Atom	Site	x	y	z	Occupancy	U_{iso}
Y	8a	0.25	0.25	0.25	0.9287	0.01204
Y	24d	0.9688	0	0.25	0.9124	0.0089
Li	8a	0.25	0.25	0.25	0.0613	0.01204
Li	24d	0.9688	0	0.25	0.0876	0.0089
O	48e	0.3908	0.1514	0.3802	0.9410	0.0097

The measured diffraction patterns of X-ray diffraction and neutron diffraction were refined by Rietveld analysis using the GSAS software.[1]

Table S3. Ratio of various oxygen species, estimated from the relative area of the fitted subpeaks.

Sample	O^{2-}(%)	O_2^{2-}/O^-	-OH/O_2(%)	CO_3^{2-}/CO_2 (%)
Li0	34.4	8.4	41.0	16.2
Li6	25.4	9.3	44.7	20.6
Li12	8.1	11.2	57.8	22.9

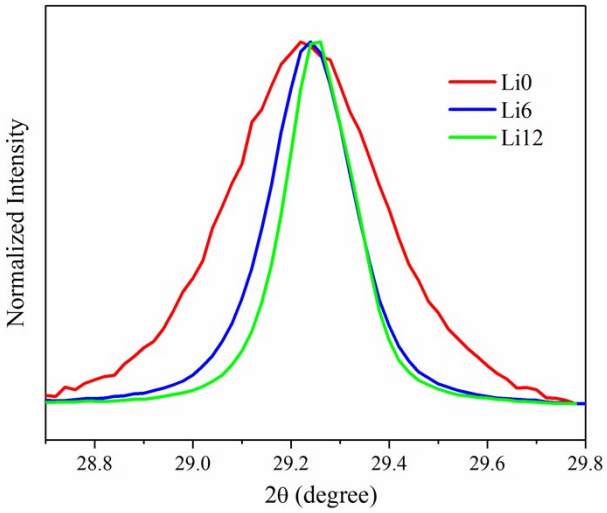

Figure S1. Dependence of the FWHM* of a given X-ray diffraction peak on Li^+ content.
*:The average crystallite size of the powders (D) was calculated by using the Scherrer's equation

$$D=\frac{K\lambda}{\beta cos\theta}$$

where K is the Scherrer's shape factor constant (0.94), λ is the wavelength of the X-ray (λ = 1.5406 Å), and β is the full-width at half maximum (FWHM), in radians, of the diffraction peak at a certain value of 2θ.

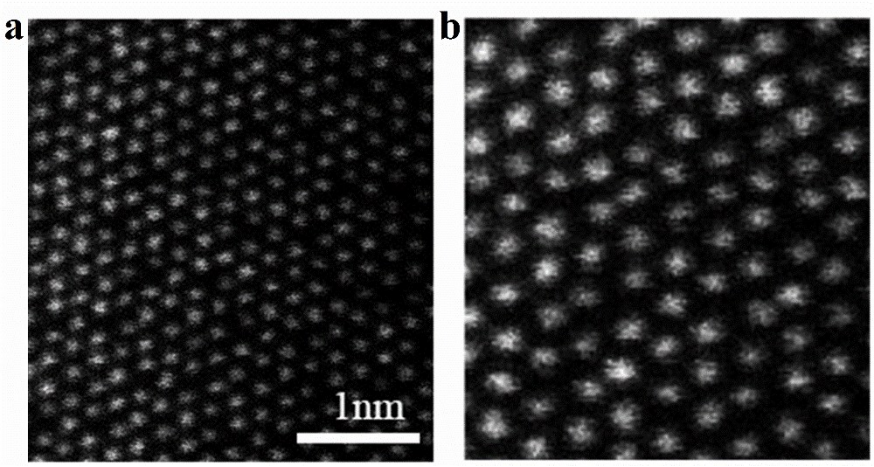

Figure S2. HAADF-STEM image from the Li12 sample (a), and (b) local enlarged view of the image in (a).

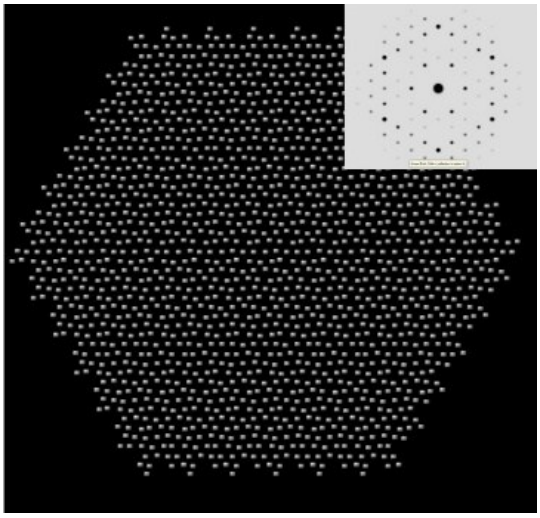

Figure S3. Arrangement of Y atoms along the [111] axis projection in the Y_2O_3 supercell. The inset shows the SAED pattern in the [111] zone axis in Y_2O_3 (by crystalmaker).

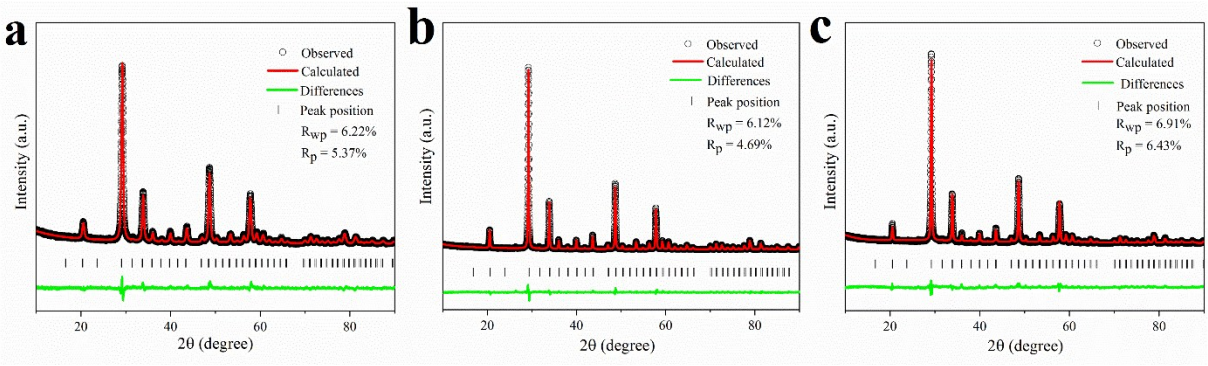

Figure S4. X-ray diffraction patterns and refinement for the samples $(Y_{1-X}Li_X)_2O_3$ with X = (a) 0.00, (b) 0.06, and (c) 0.12.

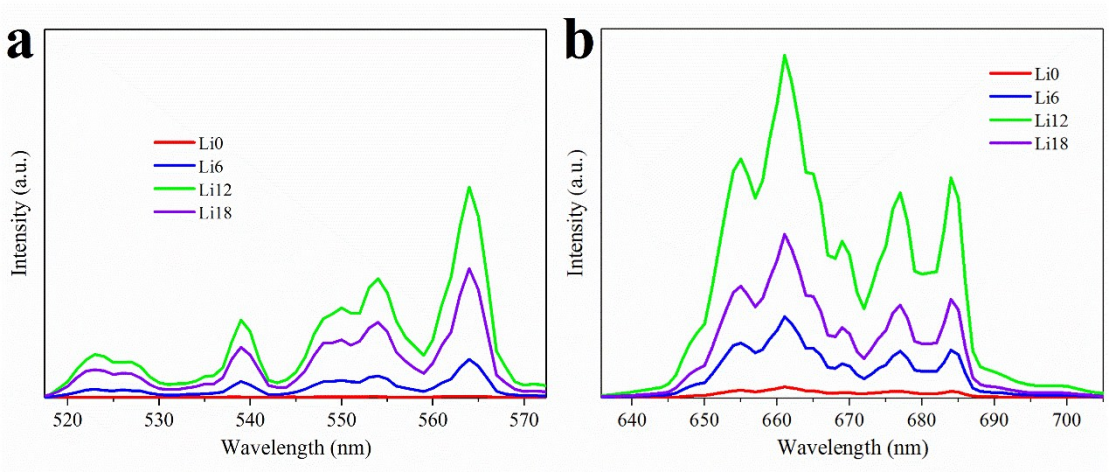

Figure S5. Magnification of room temperature upconversion spectra in (a) the green light, (b) the red light.

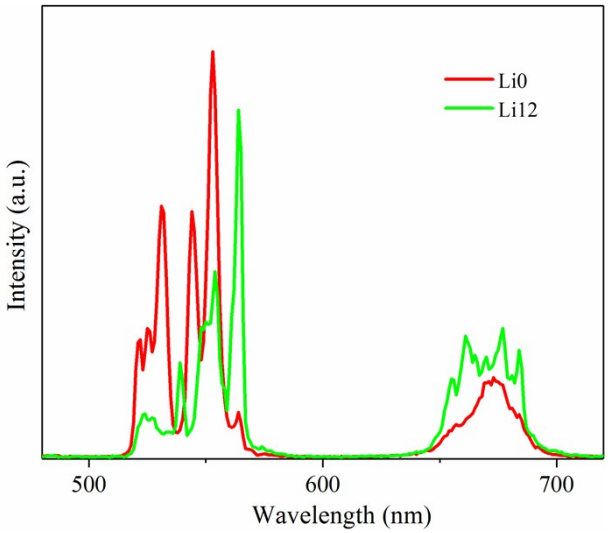

Figure S6. Room temperature upconversion spectra of $(Y_{0.98-X}Er_{0.02}Li_X)_2O_3$ powders (X = 0.00 and 0.12) under the excitation of a 980 nm CW laser with the same pump power.

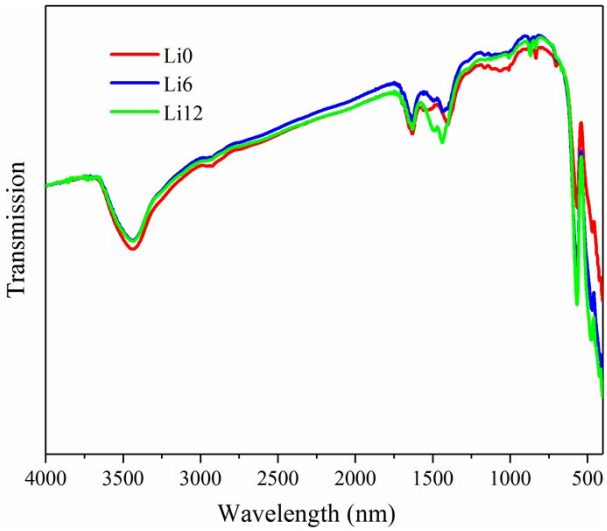

Figure S7. FT-IR spectra of the samples.

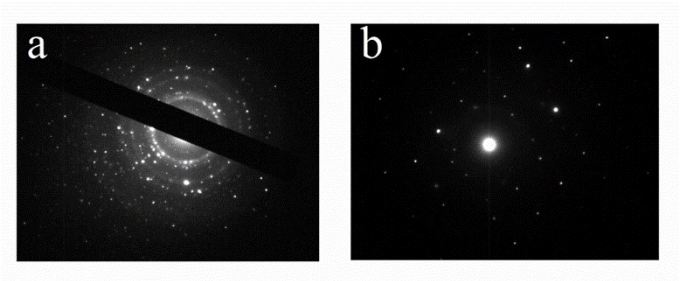

Figure S8. SAED patterns of the samples (a) Li0 and (b) Li12.

Reference

1 L. B. McCusker, R. B. Von Dreele, D. E. Cox, D. Louër and P. Scardi, Rietveld refinement guidelines, *Journal of Applied Crystallography*, 1999, **32**, 36–50.