Electronic Supplementary Information for "Exciton diffusion in solid solutions of luminescent lanthanide β-diketonates"

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Elemental Analysis. The C, H, N content of TBALn $(TTA)_4$ are determined by an Elementar *Vario EL III* elemental analyzer. The results are listed in Table S1. For ICP-AES analysis of lanthanide ions, about 30 mg of lanthanide complex solid solution is digested in a mixture of 5 mL 12 M nitric acid and 1 mL of 30% hydrogen peroxide while heated. After complete dissolution of the lanthanide complex, the solution is further heated to decompose hydrogen peroxide until bubbling is ceased. The solution is cooled to room temperature and diluted with DI water to 100 mL. The concentrations of Eu^{3+} and other lanthanide ions in the solution are determined by a Leeman Labs Profile Spec ICP-AES spectrometer. The results are listed in Table S2.

Tabel S1. Elemental analysis results of the pure complexes*

Pure complexes	C (%)	H (%)	N (%)
$TBAEu(TTA)_4$	44.67(45.08)	4.04(4.10)	1.09(1.09)
$TBALa(TTA)_4$	45.37(45.55)	4.18(4.14)	1.04(1.11)
$TBAGd(TTA)_4$	44.80(44.90)	4.14(4.08)	0.93(1.09)

*Theoretical value in parentheses

Table S2. ICP-AES analysis results of the doped-complexes

Solid solutions	C_{Eu} (μg/mL)	C_M (μg/mL)	$n_{Eu} : n_M$
$TBAEu_{0.2}La_{0.8}(TTA)_4$	8.397	26.78	0.22 : 0.78
$TBAEu_{0.6}La_{0.4}(TTA)_4$	24.31	12.80	0.63 : 0.37
$TBAEu_{0.8}Gd_{0.2}(TTA)_4$	34.65	7.746	0.82 : 0.18

Infrared spectroscopy. Infrared absorption (IR) spectra of the samples are collected by a Nicolet Magna IR-750B Fourier transform infrared spectrometer. For the studies, each sample is mixed with spectroscopic grade KBr powder in a 1:10 ratio (w/w) and pressed to a 1-mm-thick pellet. Measurement for each sample is repeated for 32 times for a spectral resolution of 4 cm^{-1}. A few representative spectra are shown in Fig. S1.

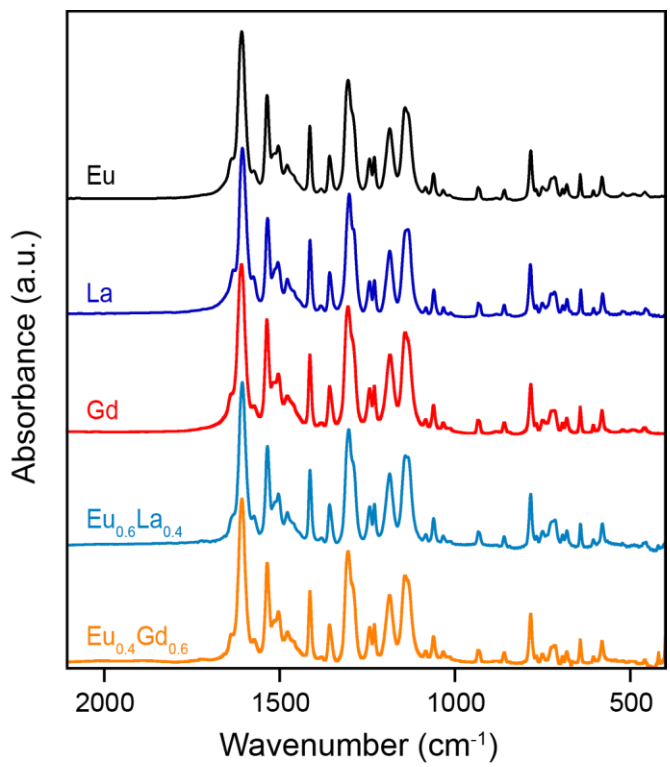

Fig. S1. Representative infrared spectra of a few pure complexes and their solid solutions.

X-ray powder diffraction. X-ray powder diffraction (XRD) patterns are collected by a Rigaku D/MAX 2400 X-Ray diffractometer using the Cu K_α radiation (1.541 Å). A few representative spectra are shown in Fig. S2.

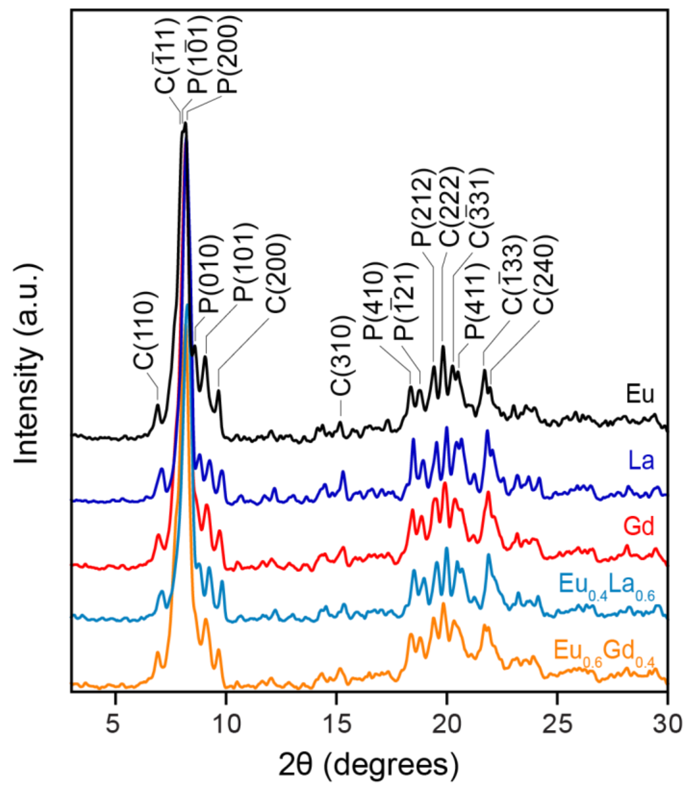

Fig. S2. Representative X-ray powder diffraction patterns of a few pure complexes and their solid solutions. The diffraction pattern of $TBAEu(TTA)_4$ are indexed to the two isomorphs in space groups *C*2/*c* (labeled as C) and *P*2/*n* (labeled as P). The other diffraction patterns can be indexed in the same way.

Ratio of intersystem crossing (ISC) rates. To find out the ratio, we rely on the fact that for all Eu_xM_{1-x} solid solutions with $x \geq 0.2$, all triplet excitons would transfer their energy to Eu^{3+}. As such, the Eu^{3+} emission intensity from a Eu_xM_{1-x} solid solutions ($x \geq 0.2$) may write

$$I = A\left[x\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} + (1-x)\Gamma_{\mathrm{ISC}}^{\mathrm{M}}\right] = A\left[x\left(\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} - \Gamma_{\mathrm{ISC}}^{\mathrm{M}}\right) + \Gamma_{\mathrm{ISC}}^{\mathrm{M}}\right],$$

in which A is a constant and the Γ terms are ISC rates as defined in the main text. A linear regression for the I-x relation ($x \geq 0.2$) gives a slope $k = A\left(\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} - \Gamma_{\mathrm{ISC}}^{\mathrm{M}}\right)$ and intercept $b = A\Gamma_{\mathrm{ISC}}^{\mathrm{M}}$. We may therefore derive the ISC rate ratio $\Gamma_{\mathrm{ISC}}^{\mathrm{M}}/\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} = b/(k+b)$. The linear fittings for Eu_xGd_{1-x} and Eu_xLa_{1-x} are shown in Fig. S3. Based on the fitting, we determine that $\Gamma_{\mathrm{ISC}}^{\mathrm{Gd}}/\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} = 0.84$ and $\Gamma_{\mathrm{ISC}}^{\mathrm{La}}/\Gamma_{\mathrm{ISC}}^{\mathrm{Eu}} = 0.37$.

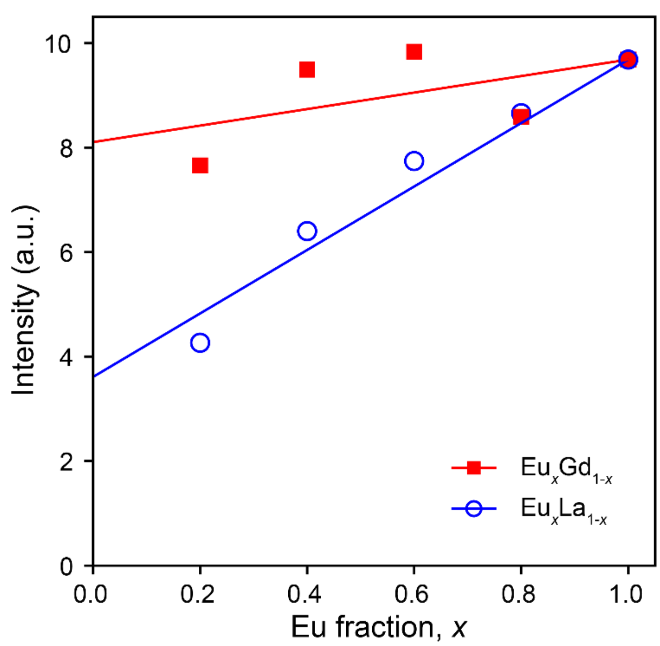

Fig. S3. Dependence of Eu^{3+} emission intensities on x, for various Eu_xLa_{1-x} and Eu_xGd_{1-x} solid solutions ($x \geq 0.2$). Straight lines are linear regressions of the data points.