Supporting Information

Synergy effect of rare earth cations on local structure and PL emission in Ce$^{3+}$:REPO$_4$ (RE=La, Gd, Lu, Y) system

Congting Sun and Dongfeng Xue*

State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, China

*Corresponding author. E-mail: dongfeng@ciac.ac.cn
Fig. S1 SEM images of as-prepared Ce$^{3+}$:Gd$_x$L$_{1-x}$PO$_4$ with different Gd/Lu ratios in reactants. (A–I) SEM images of Ce$^{3+}$:Gd$_x$L$_{1-x}$PO$_4$ prepared with Gd/Lu ratios ranging from 1:9 (A), 2:8 (B), 3:7 (C), 4:6 (D), 5:5 (E), 6:4 (F), 7:3 (G), 8:2 (H), and 9:1 (I) in reactants.
**Fig. S2** Emission spectra of Ce$^{3+}$:Y$_x$Lu$_{1-x}$PO$_4$ with identical Ce$^{3+}$ concentration excited at 257 nm.
**Fig. S3** Experimental powder XRD patterns demonstrating the effect that varying initial metal precursor ratios has on the product that is produced. XRD patterns of samples obtained with different La/Lu ratios in reactants.
Fig. S4 ATR-IR spectra of Ce:La$_x$Lu$_{1-x}$PO$_4$ samples obtained with different La/Lu ratios in reactants. In hexagonal phase REPO$_4$, PO$_4^{3-}$ group crystallizes with $C_2$ symmetry, while PO$_4^{3-}$ group crystallizes with $D_{2d}$ symmetry in tetragonal phase REPO$_4$. The PO$_4^{3-}$ groups are located on $C_2$ and $T_d$-sites respectively for the $D_6^4$ and $D_{4h}$ space groups.
**Fig. S5** Emission spectra of Ce\(^{3+}\):La\(_x\)Lu\(_{1-x}\)PO\(_4\) with identical Ce\(^{3+}\) concentration excited at 257 nm (A) and 277 nm (B).
The Beer–Lambert law relates the attenuation of light to the properties of the material through which the light is traveling. According to Lambert-Beer law, the absorbance intensity of the sample is proportional to the concentration of each composition in the sample. As shown in Fig. 6A, the ATR-IR absorbance bands locates at 641 cm\(^{-1}\) for tetragonal phase, while locates at 620 cm\(^{-1}\) for hexagonal phase. In tetragonal and hexagonal mixture, these two bands coexist. Therefore, we can calculate the relative content of tetragonal and hexagonal phase by comparing the absorbance intensity of these two bands. When the Gd/Lu ratio in reactants ranges from 1.1 to 1.4, the relative absorbance intensities between the band at 641 cm\(^{-1}\) and at 620 cm\(^{-1}\) are 2.50, 2.27, 0.31, and 0. On the basis of the calculated results, we can further obtain the relative content of tetragonal and hexagonal phase in Lu\(_{1-x}\)Gd\(_x\)PO\(_4\) mixtures, that are, 71.4% tetragonal phase and 28.6% hexagonal phase for M(Gd)/M(Lu)=1.1 in reactants, 69.4% tetragonal phase and 30.6% hexagonal phase for M(Gd)/M(Lu)=1.2 in reactants, 23.4% tetragonal phase and 76.6% hexagonal phase for M(Gd)/M(Lu)=1.3 in reactants, and only hexagonal phase for M(Gd)/M(Lu)=1.1 in reactants.