

Supporting Information for
Synthesis and strong near-infrared fluorescence of
 $\text{LiLa}_{1-x}\text{Nd}_x(\text{PO}_3)_4$ nanocrystals with high doping
concentration

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Experimental Section

Chemicals. HNO₃ (GR, 65-68%), CH₄N₂O (AR) and ammonia solution (GR, 25-28%) were obtained from Aladdin Chemistry Co., Ltd. Urea while LiNO₃ (99%), Nd(NO₃)₃ · 6H₂O (99.9%), La(NO₃)₃ · 6H₂O (99.9%) and NH₄H₂PO₄ (98%) was provided by Alfa Aesar.

Preparation of LLNP nanocrystals. In this work, the LLNP nanocrystals were synthesized via combustion method. Taking LiNd(PO₃)₄ nanocrystals as an example, CH₄N₂O was added into 20mL aqueous solution containing 2mmol LiNO₃ and 2mmol Nd(NO₃)₃ under agitation. Then the solution of 8mmol NH₄H₂PO₄ in 10 mL deionized water was added into above solution dropwise after the pH was adjusted. After drying to honeycomb in blast oven at 80°C, the precursor was treated at 750°C for 10min following combustion reaction. The collected product was washed and dried at 60°C for 48h under vacuum.

Characterization. The X-ray diffraction (XRD) patterns of the samples were measured on a Bruker D8 Advance X-ray powder diffractometer with graphite monochromatized Cu Ka radiation ($k_{\alpha}=0.15405$ nm). The Fourier transform infrared (FT-IR) spectra was obtained on a Shimadzu IRPrestige-21 FT-IR spectrophotometer in the wavenumber range of 400~4000cm⁻¹ at a resolution of 2cm⁻¹, on a pressed pellet of the powdered sample dispersed in KBr. The morphologies were characterized by a JEOL JEM-3010 transmission electron microscope (TEM) under a 300 kV working voltage. The emission spectra and luminescence decay times of all the samples were measured by full-featured steady state/transient fluorescence spectrometer FLS920 from Edinburgh Instruments.

Table S1 Crystal data and structure refinement for NdP₅O₁₄, LiNdP₄O₁₂ and

Empirical formula	LiNd(PO ₃) ₄		
	NdP ₅ O ₁₄	LiNdP ₄ O ₁₂	LiNd(PO ₃) ₄
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space Group	P21/a	I2/a	C2/c
Cell parameters	a=13.03Å,	a=13.25Å,	a=16.487Å,
	b=9.001Å,	b=7.008Å,	b=7.043Å,
	c=8.768Å,	c=9.844Å,	c=9.754Å,
	β=90.48°	β=90.1°	β=126.46°
Volume(Å ³)	1028.3	914.1	910.9
Z	4	4	4
Density(g/cm ⁻³)	3.38	3.393	3.406
JCPDS	24-0782	29-0812	34-0003
d _{min(Nd-Nd)} (Å)	5.192	5.62	5.644
c (10 ²¹ cm ⁻³)	3.88	4.37	4.39
τ (μs)	110	120	120
σ (10 ⁻¹⁹ cm ²)	2.5	3.2	3.2
ref	1, 2	3, 4, 5	6, 7

Table S2 FT-IR spectral data (cm^{-1}) and band assignments for $\text{LiNd}(\text{PO}_3)_4$

Wavenumber	Assignment
1310, 1240	$\nu_{\text{as}}(\text{PO}_2)$
1149, 1083, 1067	$\nu_{\text{s}}(\text{PO}_2)$
1012, 932	$\nu_{\text{as}}(\text{POP})$
812, 754, 735, 685	$\nu_{\text{s}}(\text{POP})$
596, 575, 560, 522	$\delta(\text{PO}_2)$
474, 457, 436	$\delta(\text{POP})$

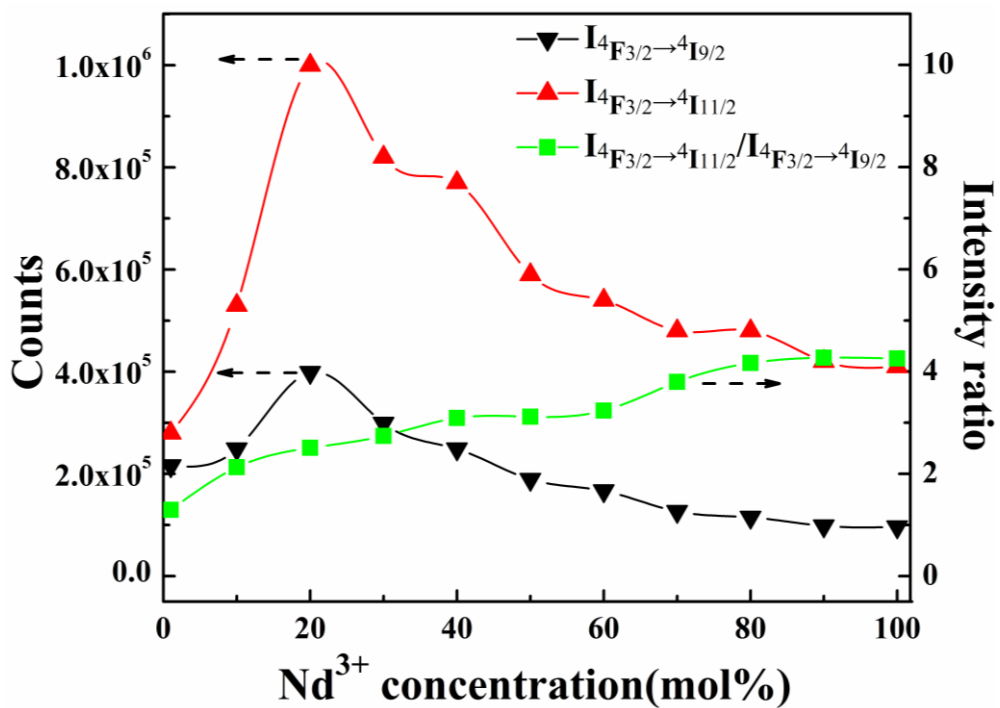


Fig.S1 Emission intensities (⁴F_{3/2}→⁴I_{11/2} and ⁴F_{3/2}→⁴I_{9/2}) of LiLa_{1-x}Nd_x(PO₃)₄ nanocrystals and their ratio dependence on the Nd³⁺ doping concentration

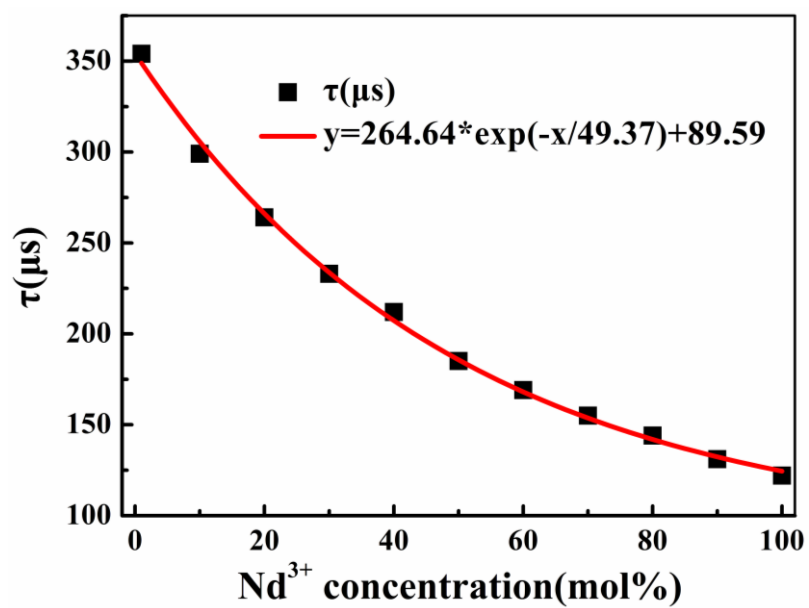


Fig.S2 The curve of fluorescence lifetimes (τ) dependence on Nd^{3+} concentration in $\text{LiLa}_{1-x}\text{Nd}_x(\text{PO}_3)_4$ nanocrystals

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