

Supporting Information

A novel efficient broadband near-infrared phosphor $\text{LiGaGe}_2\text{O}_6:\text{Cr}^{3+}$ with
EQE enhancement and spectral tuning by Sc^{3+} - Ga^{3+} substitution for NIR
pc-LED application

Jiaqi Fan ^{a,1}, Weiyang Zhou ^{a,1}, Jilin Zhang ^b, Peichan Chen ^c, Qi Pang ^c, Liya Zhou ^c,
Chunyan Zhou ^d, Xinguo Zhang ^{a*□}

^a NMPA Key Laboratory for Research and Evaluation of Drug Metabolism, Guangdong
Provincial Key Laboratory of New Drug Screening, School of Pharmaceutical Sciences, Southern
Medical University, Guangzhou, 510515, China

^b Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of
Education of China), College of Chemistry and Chemical Engineering, Hunan Normal University,
Changsha, 410081, China

^c School of Chemistry and Chemical Engineering, Guangxi University, Nanning 530004, China

^d College of Pharmaceutical Science, Guangxi Medical University, Nanning, 530021, China

Corresponding author. *E-mail address:* panzer@smu.edu.cn (X.G. Zhang);

● ¹ These authors contributed equally to this work.
Corresponding author. *E-mail address:* panzer@smu.edu.cn (X.G. Zhang);

Table S1. Refinement parameters of LiGaGe₂O₆: 0.06Cr³⁺ sample from the Rietveld Structure

Analysis						
Formula		LiGa _{0.94} Cr _{0.06} Ge ₂ O ₆				
Space group		P12 ₁ /c ₁ (No.14) - monoclinic				
Cell parameters		$a = 9.8013(1) \text{ \AA}$, $b = 8.7147(1) \text{ \AA}$, $c = 5.3511(0) \text{ \AA}$, $\beta = 108.91^\circ$ $V = 432.40(9) \text{ \AA}^3$, $Z = 4$				
Reliability factors		$R_{wp} = 7.81 \%$, $R_p = 5.35 \%$				
Atom	Site	x	y	z	occupancy	$U (\text{Å}^2)$
Li1	4e	0.270	0.0233	0.217	1.0	0.0059(24)
Ga1	4e	0.2510	0.65557	0.2103	0.94	0.0057(6)
Cr1	4e	0.2510	0.65557	0.2103	0.06	0.0057(6)
Ge1	4e	0.04622	0.3433	0.2690	1.0	0.0112(7)
Ge2	4e	0.55205	0.8424	0.2297	1.0	0.0082(6)
O1	4e	0.8586	0.3337	0.1552	1.0	0.0048(24)
O2	4e	0.1117	0.5257	0.2723	1.0	0.040(5)
O3	4e	0.1108	0.2883	0.5909	1.0	0.027(4)
O4	4e	0.3651	0.8298	0.1014	1.0	0.018(4)
O5	4e	0.6285	1.0085	0.3841	1.0	0.0055(24)
O6	4e	0.6103	0.6977	0.4684	1.0	0.018(4)

Table S2 Transition energy and crystal field parameter of Li(Ga_{0.94-y}Sc_y)Ge₂O₆: 0.06Cr³⁺

y	D_{dis}	${}^4T_{2g}$ (cm ⁻¹)	ΔE (cm ⁻¹)	ΔS (cm ⁻¹)	Dq (cm ⁻¹)	$\Delta E/Dq$	Dq/B	B (cm ⁻¹)
0	0.0455	15313	5962.6	3265.7	1368.0	4.358	2.221	615.9
0.1	0.0431	15220	6055.8	3244.3	1359.8	4.453	2.154	631.3
0.2	0.0417	15083	6193.6	3206.5	1347.9	4.595	2.056	655.6
0.3	0.0409	14947	6328.9	3182.9	1335.5	4.739	1.961	681.0
0.4	0.0398	14815	6461.7	3159.8	1323.5	4.882	1.872	706.9
0.5	0.0386	14706	6570.7	3145.1	1313.3	5.003	1.798	730.4
0.6	0.0377	14577	6699.3	3135.6	1300.9	5.153	1.709	761.2
0.7	0.0368	14492	6783.8	3142.0	1292.1	5.250	1.654	781.1
0.8	0.0348	14430	6846.5	3130.5	1286.5	5.321	1.614	797.1
0.94	0.0333	14388	6888.1	3122.5	1282.6	5.370	1.586	808.7

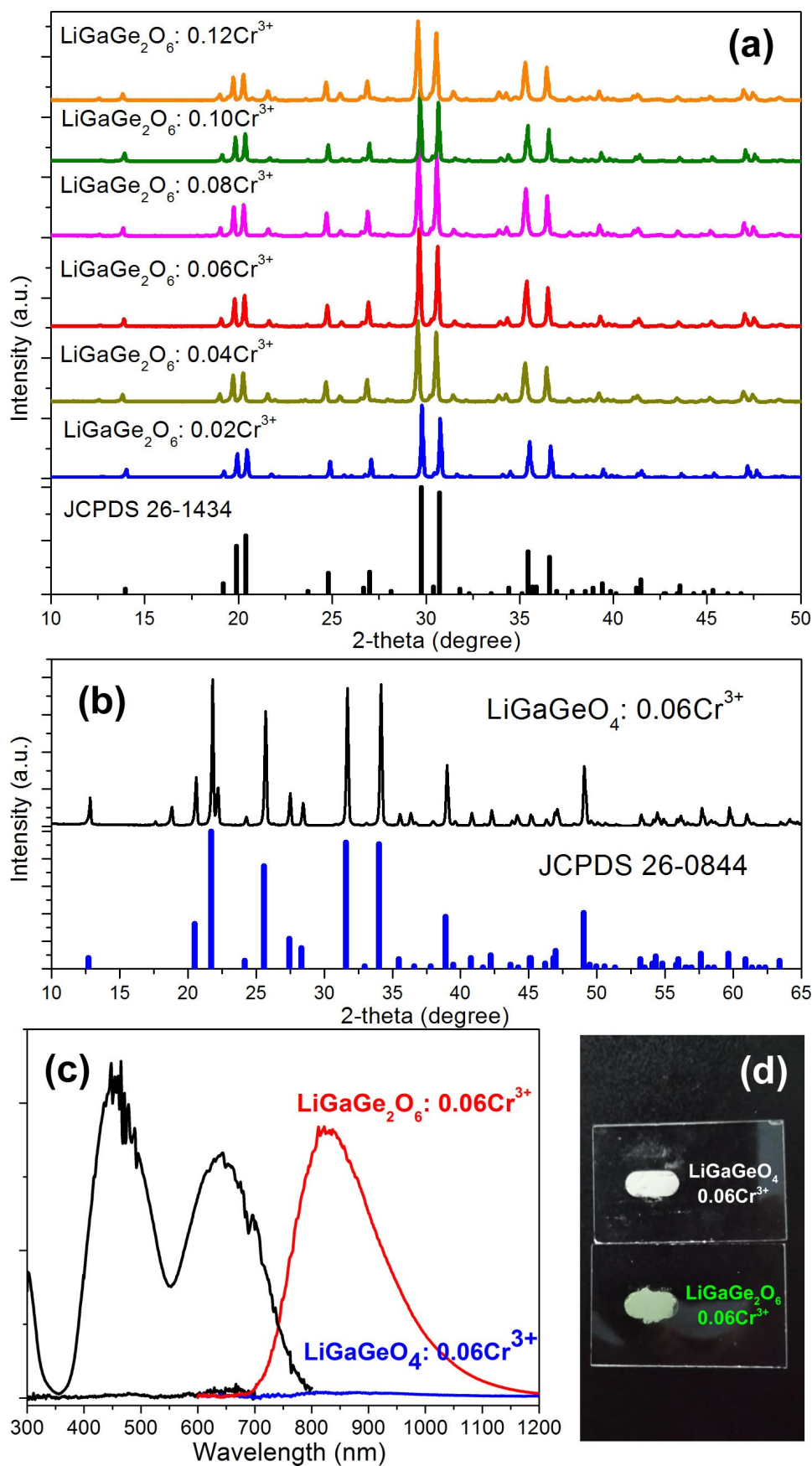


Fig.S1 XRD patterns of $\text{LiGaGe}_2\text{O}_6: x\text{Cr}^{3+}$ (a) and $\text{LiGaGeO}_4: \text{Cr}^{3+}$ (b) and the corresponding PL/PLE comparison (c) with sample picture (d)

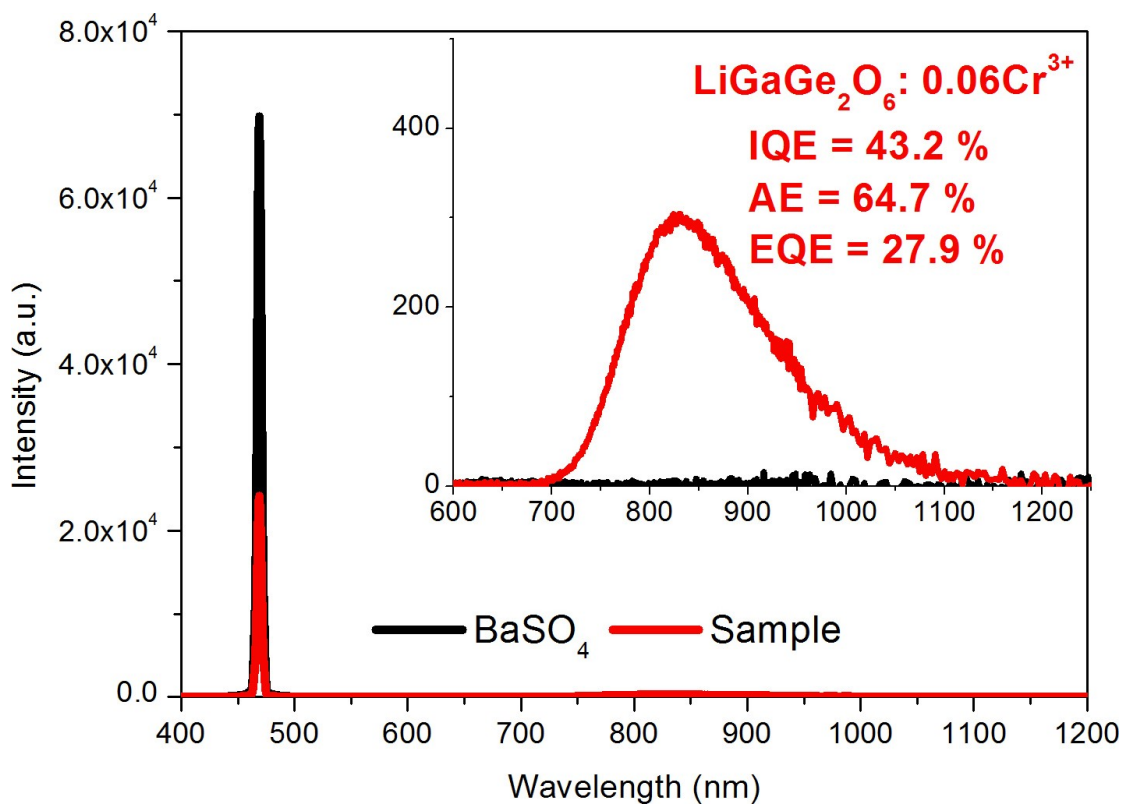


Figure S2. QY measurement spectra of LiGaGe₂O₆: 0.06Cr³⁺

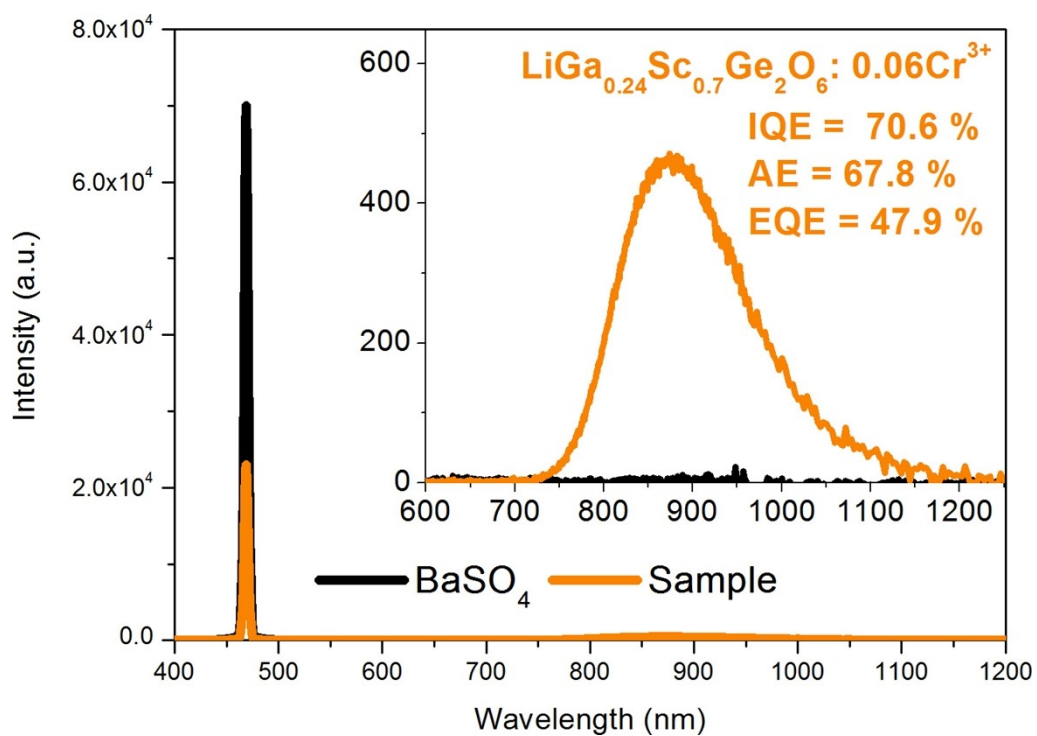


Figure S3. QY measurement spectra of Li(Ga_{0.24}Sc_{0.7})Ge₂O₆: 0.06Cr³⁺

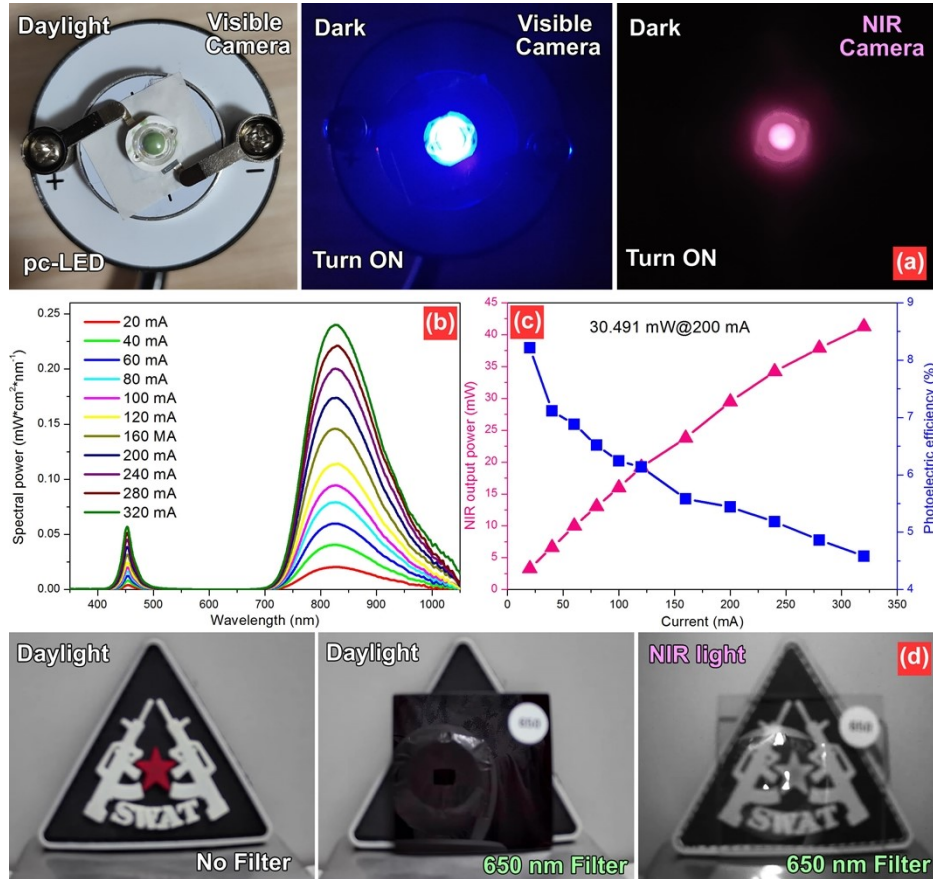


Figure S4. Electroluminescence spectra of the fabricated pc-NIR-LED device that combines a 460 nm InGa_n blue LED chip with LiGa_{0.94}Ge₂O₆: 0.06Cr³⁺ NIR phosphor under a forward bias of 20~320 mA (a); Output power and photoelectric conversion efficiency variation of pc-NIR-LED with different currents (b); The working and nonworking state of LED device (c); Visible images and NIR images with and without 650 nm filter and under the fabricated NIR pc-LED lamp (d).