

Support information

Broadband near-infrared luminescence in cubic pyrophosphate

$\text{Al}_{0.5}\text{Ta}_{0.5}\text{P}_2\text{O}_7$: Cr^{3+} phosphor for multi-functional applications

Long Chen^a, Jiyou Zhong^{a,*}, Jiajun Wu^a and Weiren Zhao^{a,b*}

^aSchool of Physics and Optoelectronic Engineering, Guangdong University of Technology, Guangzhou 510006, China. E-mail: zhongjiyou@126.com; zwren123@126.com.

^bGuangdong Provincial Key Laboratory of Information Photonics Technology, Guangdong University of Technology Guangzhou, 510006, China.

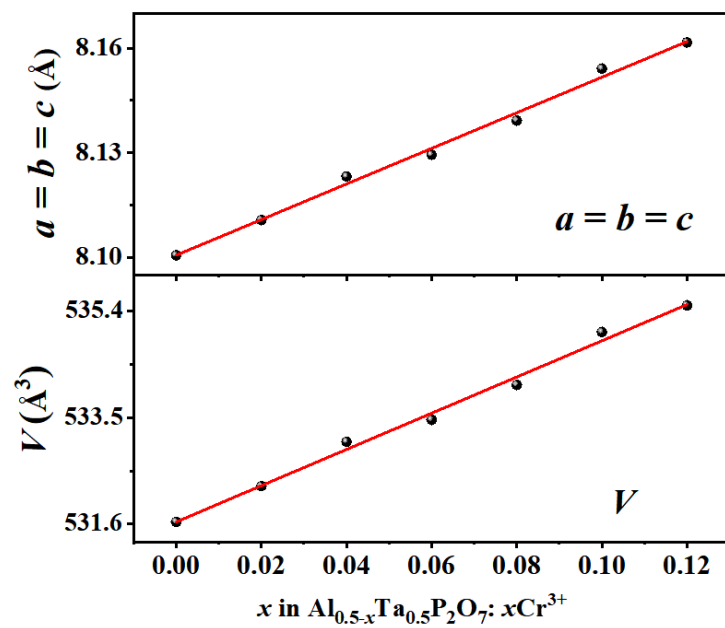


Fig. S1 The refined lattice parameters as a function of Cr^{3+} concentration.

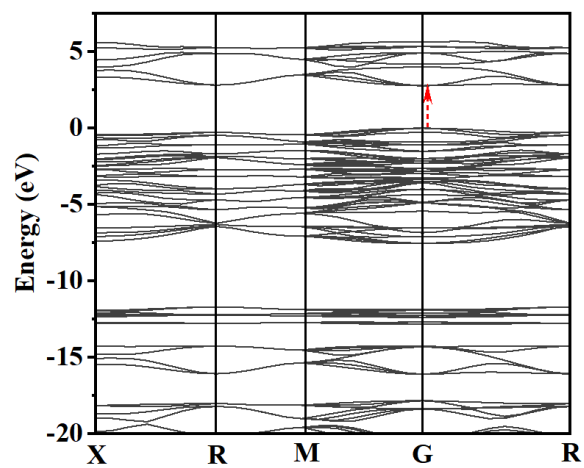


Fig. S2 DFT-calculated electronic band structure of $\text{Al}_{0.5}\text{Ta}_{0.5}\text{P}_2\text{O}_7$.

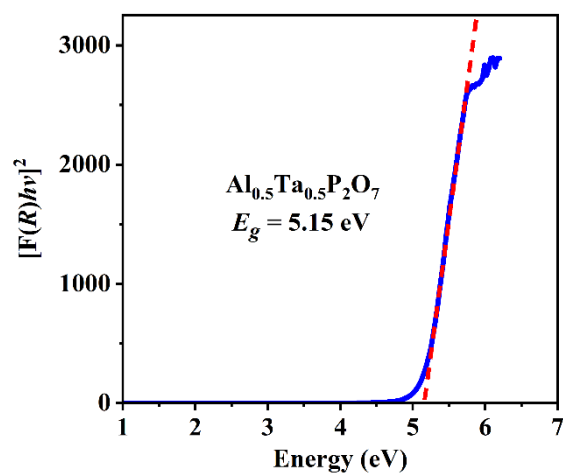


Fig. S3 The optical band gap (E_g) calculated based on Kubelka-Munk equation.

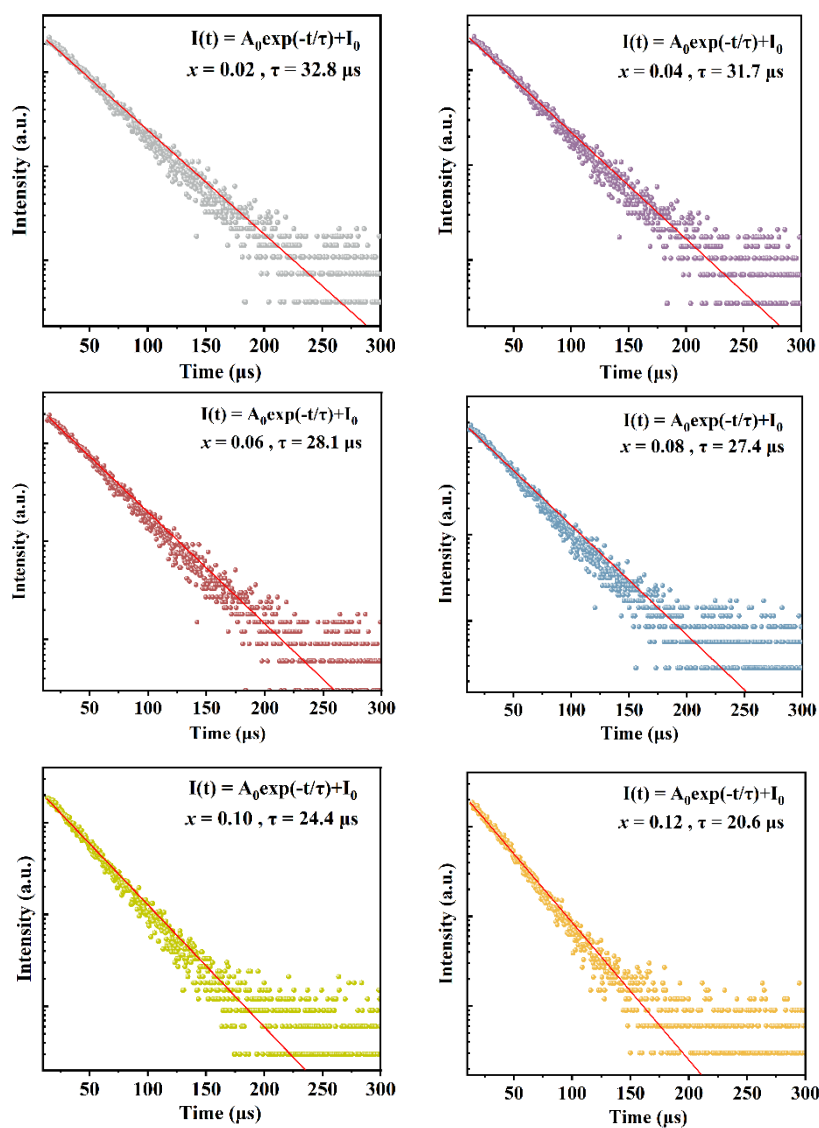


Fig. S4 Decay curves and the fitted lifetimes of $\text{Al}_{0.5-x}\text{Ta}_{0.5}\text{P}_2\text{O}_7: x\text{Cr}^{3+}$ ($x = 0.02, 0.04, 0.06, 0.08, 0.10,$ and 0.12) phosphors.

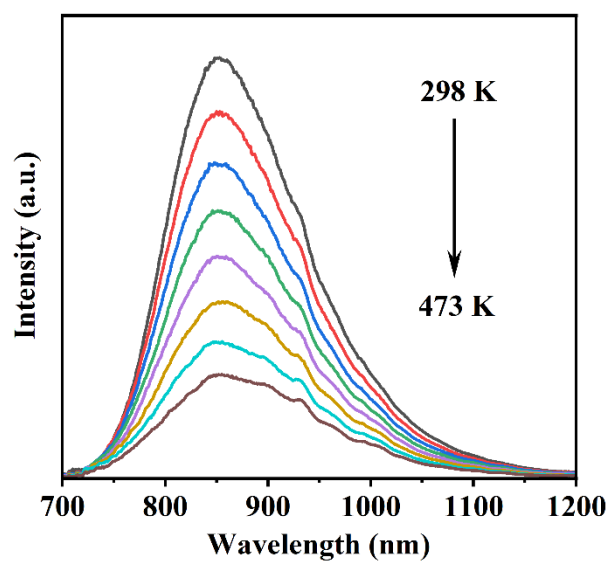


Fig. S5 Temperature-dependent PL spectra of $\text{Al}_{0.44}\text{Ta}_{0.5}\text{P}_2\text{O}_7: 0.06\text{Cr}^{3+}$.

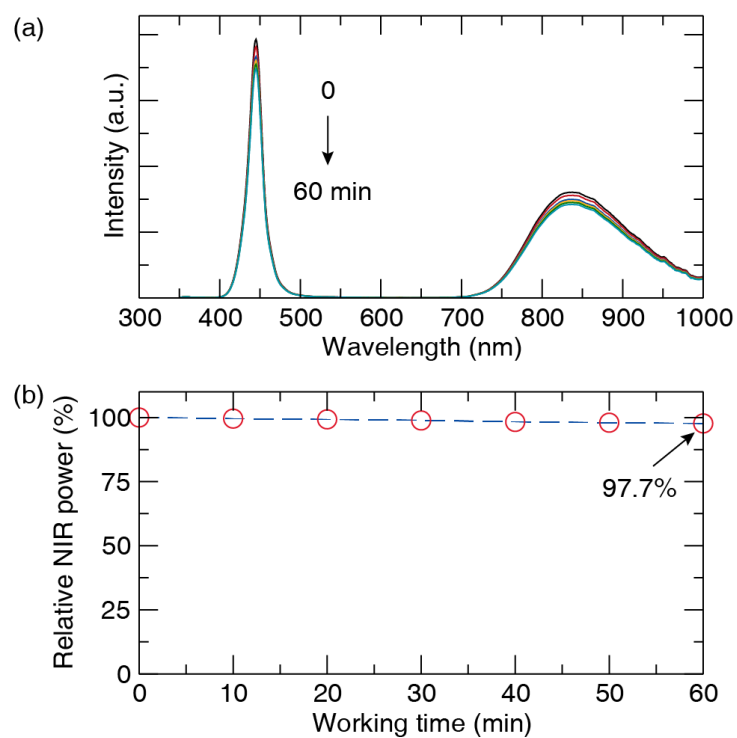


Fig. S6 (a) Time-dependent EL spectra of NIR pc-LED device under 100 mA driving current. (b) Relative NIR output power as a function of working time.

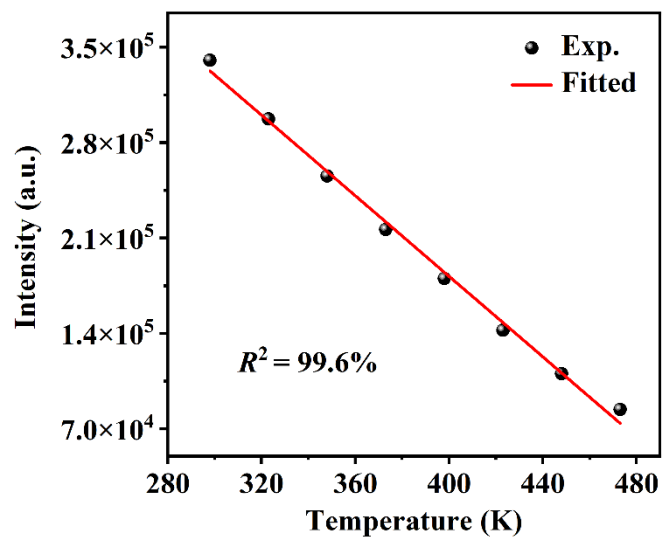


Fig. S7 Linearly fitting the relationship between emission intensity and temperature.

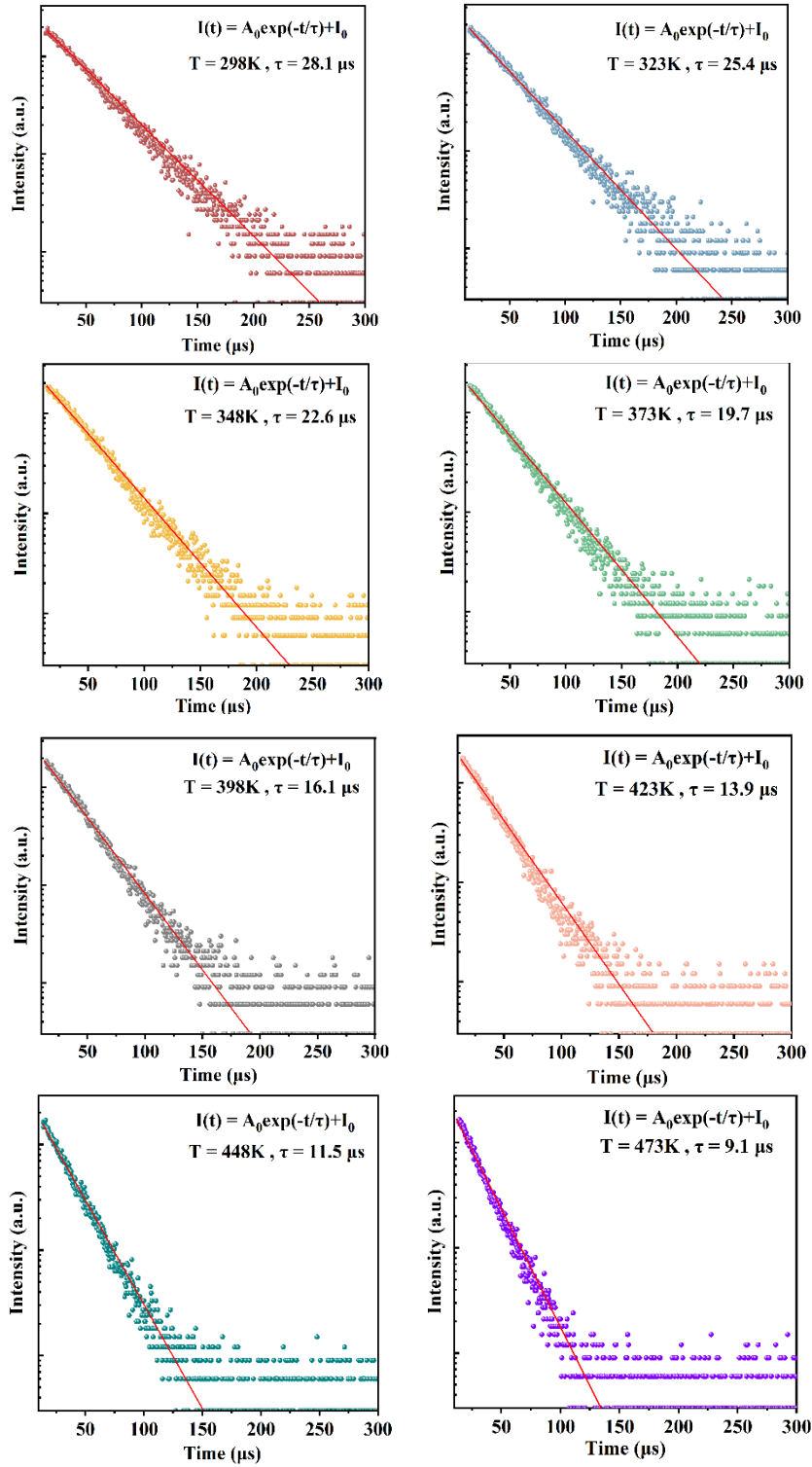


Fig. S8 Decay curves and the fitted lifetimes of $\text{Al}_{0.44}\text{Ta}_{0.5}\text{P}_2\text{O}_7: 0.06\text{Cr}^{3+}$ phosphors in temperature range of 298 – 473 K.

Table S1. The refined atomic positions of $\text{Al}_{0.5}\text{Ta}_{0.5}\text{P}_2\text{O}_7$.

Atom	Site	x	y	z	Occ.	Ueq
Al(1)	4b	0.5000	0.5000	0.5000	0.5	0.0068
Ta(1)	4b	0.5000	0.5000	0.5000	0.5	0.0053
P(1)	8c	0.1054	0.1054	0.1054	1	0.0051
O(1)	24d	0.0550	0.2733	0.0760	1	0.0097
O(2)	4a	0	0	0	1	0.0105

Table S2. The detailed parameters of NIR output power, NIR photoelectric conversion efficiency, and LED input power under different driven currents.

Current (mA)	LED input power (mW)	NIR output power (mW)	NIR photoelectric conversion efficiency (%)
25	67.61	2.983	4.919
50	139.7	5.613	4.345
75	215.5	7.849	3.833
100	294.8	9.705	3.403
125	377.5	11.17	2.963
150	463.4	12.25	2.67
175	552.8	13.02	2.329
200	645.3	13.31	2.065