

**A Novel High-efficiency Near-infrared Phosphor $Mg_{0.9}Ta_2Zn_{2.1}O_8:Cr^{3+},Yb^{3+}$ for
Spectroscopy Applications**

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Supplementary Note 1:

The decay curve of MTZO: x Cr $^{3+}$ ($0.004 \leq x \leq 0.014$) phosphors is shown in Figure 3f, and its lifetime increases with the increase of Cr $^{3+}$ content, which properly promotes the energy transfer between Cr $^{3+}$ ions and can be fitted by the following formula:[1]

$$I = A \exp\left(-\frac{t}{\tau}\right) \quad (1)$$

where I denotes the emission intensity at time t , A is a constant, and τ represents the lifetime. All the decay curves follow a single exponential function, indicating that there is only one kind of emission center, which is consistent with the substitution of Mg $^{2+}$ by Cr $^{3+}$ in the host.

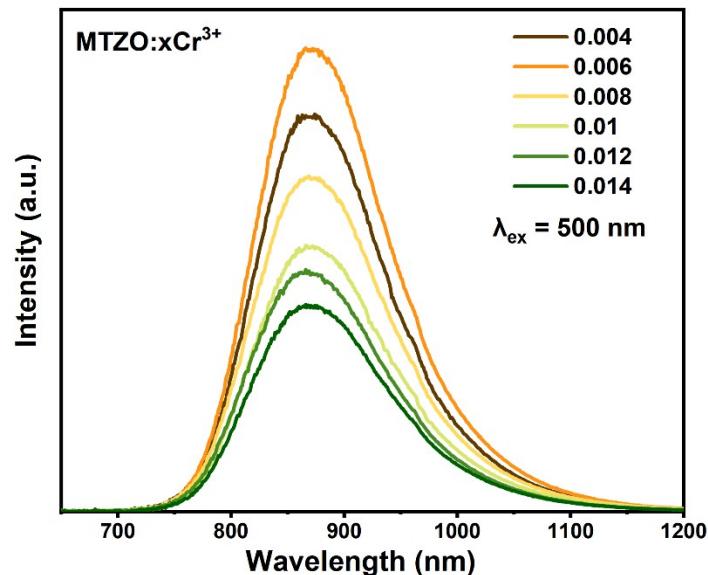


Fig. S1 Concentration-dependent PL spectra of MTZO: x Cr $^{3+}$ ($x = 0.004$ to 0.014).

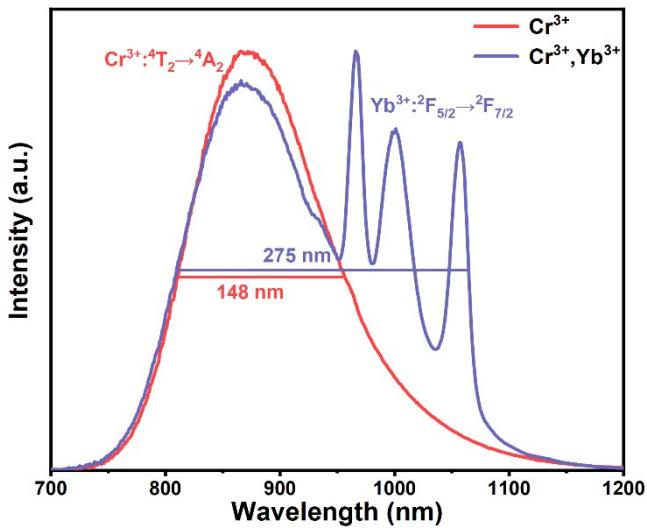


Fig. S2 the FWHM of Cr^{3+} emission and the combined peak of $\text{Cr}^{3+}\text{-Yb}^{3+}$ emission in MTZO.

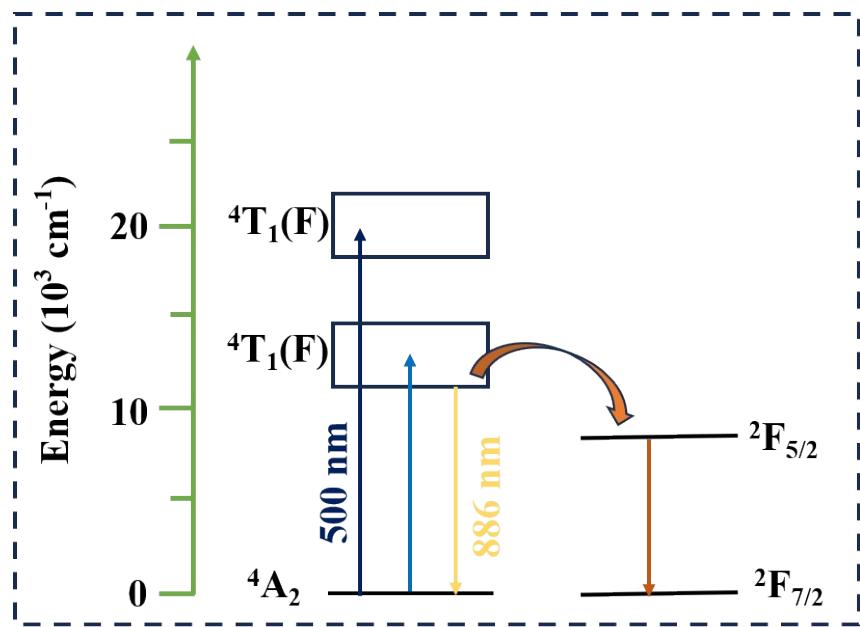


Fig. S3 Schematic representation of the energy transfer from the Cr^{3+} to Yb^{3+} ions.

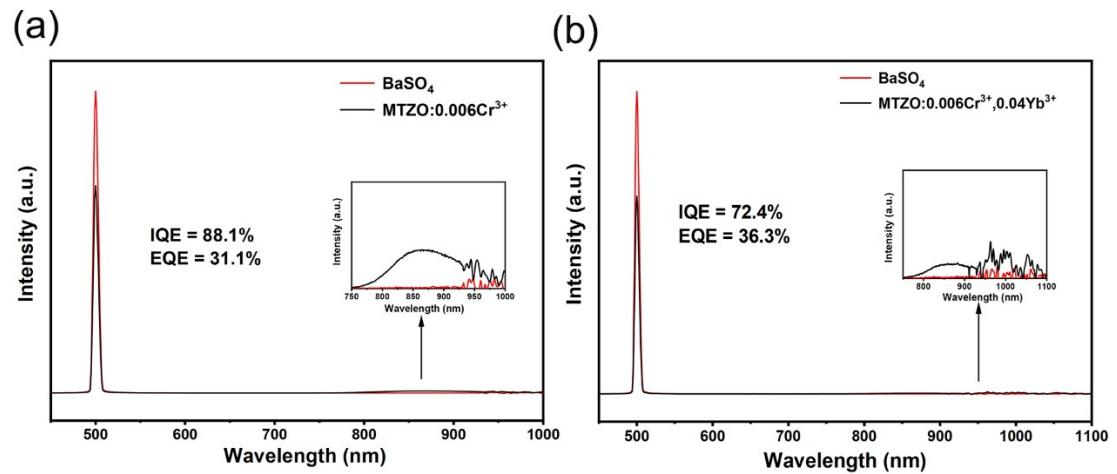


Fig. S4 Quantum yield (QY) of the sample MTZO:0.006Cr³⁺ and MTZO:0.006Cr³⁺,0.04Yb³⁺.

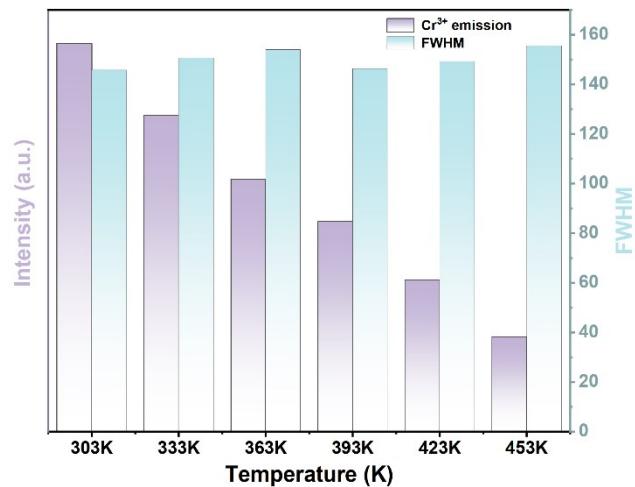


Fig. S5 The FWHM of Cr³⁺ emission and the combined peak of Cr³⁺-Yb³⁺ emission in MTZO.

Table S1. Crystallographic data of MTZO:Cr³⁺ and MTZO:Cr³⁺,Yb³⁺.

Compound	MTZO:Cr ³⁺	MTZO: Cr ³⁺ ,Yb ³⁺
Crystal system	Monoclinic	Monoclinic
Space group	C 2/c	C 2/c
a (Å)	19.01420	19.02620
b (Å)	5.88345	5.88628
c (Å)	5.20010	5.20192
V [Å ³]	581.726793	582.577589
α [°]	90	90
β [°]	90.2041	90.2080
γ [°]	90	90
Rwp [%]	5.38	6.32
Rp [%]	7.05	8.15
Mg _{0.9} Ta ₂ Zn _{2.1} O ₈	Z = 4	

Table S2. Atomic position of the MTZO:Cr³⁺ sample

Atom	Site	X	Y	Z	Occ.
O1	8f	0.19405	0.35572	0.37058	1.000
O2	8f	0.18155	0.10382	0.94254	1.000
O3	8f	0.05704	0.39366	0.06638	1.000
O4	8f	0.05972	0.14926	0.59066	1.000
Zn1	4e	0.00000	0.64072	0.25000	0.194
Zn2	8f	0.27997	0.15159	0.26672	1.000
Mg1	4e	0.00000	0.64072	0.25000	0.806
Ta1	8f	0.11482	0.16186	0.24100	0.994
Cr1	8f	0.11482	0.16186	0.24100	0.006

Table S3 Atomic position of the MTZO:Cr³⁺,Yb³⁺.

Atom	Site	X	Y	Z	Occ.
O1	8f	0.19405	0.35572	0.37058	1.000
O2	8f	0.18155	0.10382	0.94254	1.000
O3	8f	0.05704	0.39366	0.06638	1.000
O4	8f	0.05972	0.14926	0.59066	1.000
Zn1	4e	0.00000	0.64393	0.25000	0.528
Zn2	8f	0.28070	0.15152	0.28359	1.000
Mg1	4e	0.00000	0.64393	0.25000	0.472
Ta1	8f	0.11514	0.16222	0.24766	0.988
Cr1	8f	0.11514	0.16222	0.24766	0.006
Yb1	8f	0.11514	0.16222	0.24766	0.04

[1] B. Zheng, J. Yan, J. Li, Y. Wang, X. Yang, W. Li, Sr₈MgSc(PO₄)₇:Eu²⁺ phosphor: d–f transition driven applications for solid-state lighting and extreme environment multimode sensing investigations, Inorganic Chemistry Frontiers, (2025).