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Supporting Information

Highly efficient and thermally stable broadband Cr³⁺-activated double borate phosphor for near-infrared light-emitting diodes

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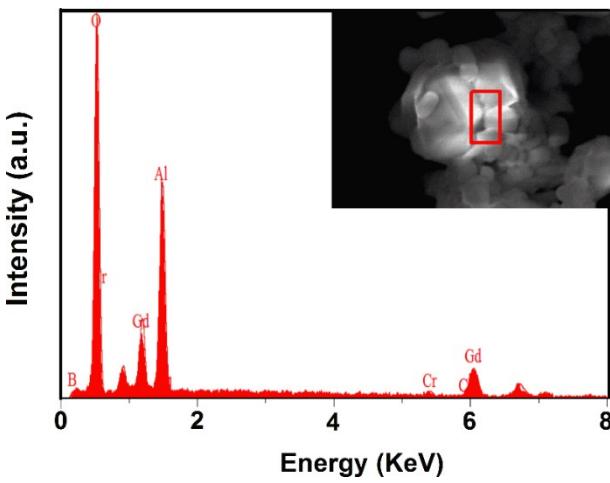


Fig. S1. EDS spectrum of the GAB: Cr³⁺ (1.0 at.%) sample.

Table S1. Crystallographic data determined from Rietveld refinement for GdAl_{2.99}Cr_{0.01}(BO₃)₄ and GdAl₃(BO₃)₄ crystals.

Formula	GdAl _{2.99} Cr _{0.01} (BO ₃) ₄	GdAl ₃ (BO ₃) ₄
Crystal system	Trigonal	Trigonal
Space group	<i>R</i> 32	<i>R</i> 32
a(Å)	9.3107(6)	9.3014(7)
b(Å)	9.3107(6)	9.3014(7)
c(Å)	7.2612(4)	7.2571(7)
V(Å ³)	545.12	543.74
α (°)	90	90
β (°)	90	90
γ (°)	120	120
<i>R</i> _p (%)	6.56	—
<i>R</i> _{wp} (%)	4.56	—
χ^2	2.68	—

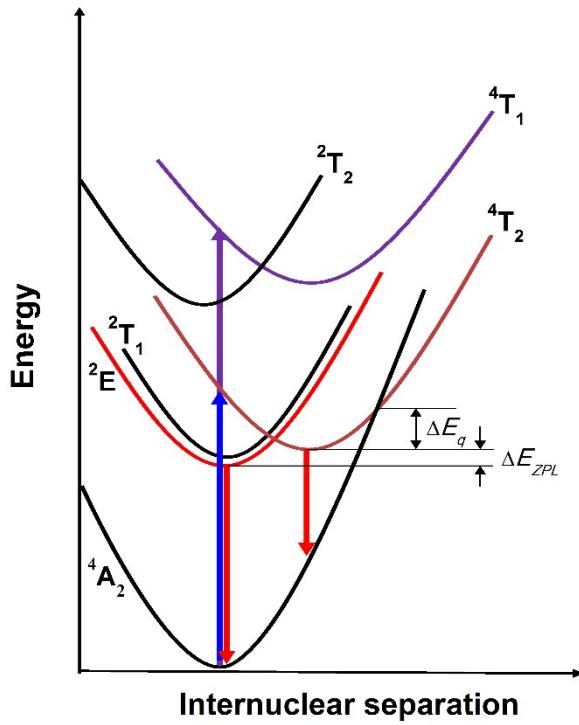


Fig. S2. Configurational coordinate diagram of Cr^{3+} ions in GAB crystal. ΔE_a is the activation energy, ΔE_{ZPL} is the energy gap between ^2E (^2G) and the $^4\text{T}_2$ (^4F) ZPL.

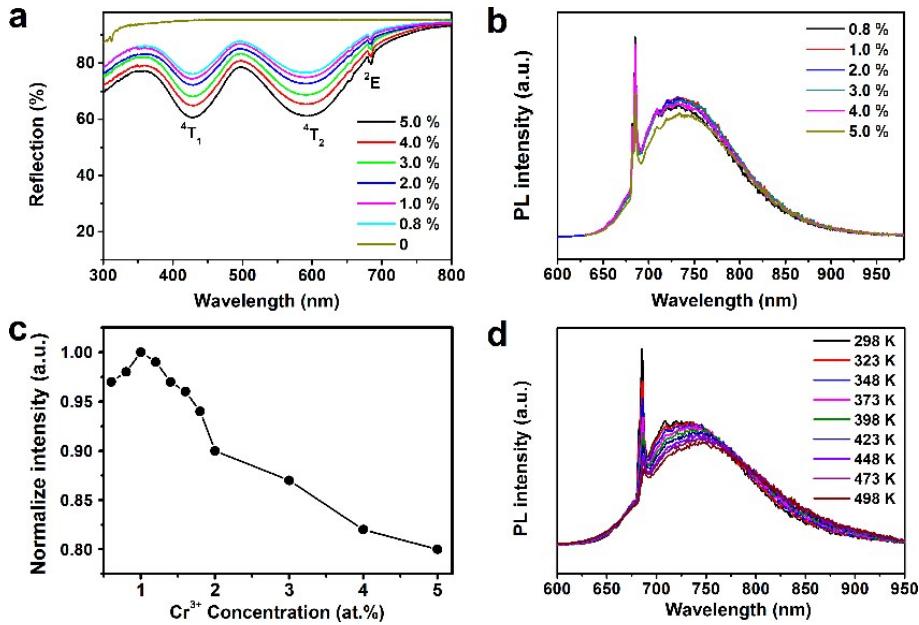


Fig. S3. (a) Diffuse reflection spectra and (b) PL spectra of GAB: Cr^{3+} samples with Cr^{3+} doping concentrations of 0.8–5.0 at.% ($\lambda_{\text{ex}} = 426$ nm). (c) The Cr^{3+} concentration dependent normalized PL intensity. (d) Temperature-dependent emission spectra of GAB: Cr^{3+} (1.0 at.%) upon excitation at 426 nm.

Table S2. Several key optical parameters of Cr³⁺-activated phosphors.

Phosphor	Emission range	PL QY(%)	$I_{423\text{ nm}} / I_{298\text{ K}} (\%)$	Ref.
GdAl ₃ (BO ₃) ₄ :Cr ³⁺	650-1000 nm	91	100	This work
LiInSi ₂ O ₆ :Cr ³⁺	700-1100 nm	75	77	¹
Ca ₃ Sc ₂ Si ₃ O ₁₂ :Cr ³⁺	650-1000 nm	92.3	97.4	²
Ga ₂ O ₃ :Cr ³⁺	650-900 nm	92.4	~85	³
Na ₃ AlF ₆ :Cr ³⁺	640-850 nm	~75	~71	⁴
Ca ₂ LuZr ₂ Al ₃ O ₁₂ :Cr ³⁺ , Yb ³⁺	650-1100 nm	~77	~60	⁵
ScBO ₃ :Cr ³⁺	650-1000 nm	~73	51	⁶
La ₃ Ga ₅ GeO ₁₄ :Cr ³⁺ , Pr ³⁺	650-1400 nm	~39	15	⁷
La ₃ Ga ₅ GeO ₁₂ :Cr ³⁺	650-950 nm	35	~60	
Gd ₃ Sc _{1.42} Al _{0.5} Ga ₃ O ₁₂ :8%Cr ³⁺	650-1000 nm	91	86	⁸
La ₃ Sc ₂ Ga ₃ O ₁₄ :Cr ³⁺	650-1400 nm	~8	20	⁹
Y/Gd/Lu ₃ Sc ₂ Ga ₃ O ₁₂ : Cr ³⁺	650-1100 nm	~60	~93	
Mg ₃ Ga ₂ GeO ₈ :Cr ³⁺	650-1200 nm	~35	~55	¹⁰
K ₃ Ga/AlF ₆ :Cr ³⁺	650-1000 nm	—	~40	¹¹
La ₂ MgZrO ₆ :Cr ³⁺	650-1200 nm	~58	~30	¹²
Y ₃ Ga ₅ O ₁₂ : Cr ³⁺	600-1000 nm	~46	—	¹³
Gd ₃ Ga ₅ O ₁₂ : Cr ³⁺	600-1000 nm	~30	—	
LaMgGa ₁₁ O ₁₉ :Cr ³⁺	650-1000 nm	82.6	~87	¹⁴

Supplementary Discussion: The D_q parameter is obtained from the peak energy of the $^4A_2 \rightarrow ^4T_2$ transition, while Racah parameters B and C can be estimated by the following equations:¹⁵

$$E(^4T_2 - ^4A_2) = 10D_q \quad (1)$$

$$\frac{B}{D_q} = \frac{(\Delta E/D_q)^2 - 10(\Delta E/D_q)}{15(\Delta E/D_q - 8)} \quad (2)$$

$$3.05C = E(^2E) - 7.9B + 1.8B^2/\Delta E \quad (3)$$

where $\Delta E = [E(^4T_1) - E(^4T_2)]$ is the difference between the energies of the 4T_1 and 4T_2 states and $E(^2E)$ is the energy of the 2E state. The value of 4T_1 , 4T_2 and 2E are estimated to be 23470, 16730 and 14598 cm^{-1} from the excitation and emission bands, respectively. Based on equations (1) - (3), the values of B , C and D_q/B were calculated to be 675 cm^{-1} , 3197 cm^{-1} and 2.48, respectively.

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