Electronic supplementary information

Highly efficient and thermally stable broadband near-infrared emitting garnet Ca$_3$Sc$_2$Ge$_3$O$_{12}$:Cr$^{3+}$, Ce$^{3+}$ for multiple pc-LED applications

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Fig. S1 Diffuse reflectance spectra (DRS) of CSGG:xCr\(^{3+}\) (x = 0, 0.14).

(1) The band gap \((E_g)\) values of the host can be evaluated by the Kubelka-Munk equations:

\[
F(R) = \frac{(1 - R)^2}{2R} \quad (S1)
\]

\[
[F(R) \times h\nu]^2 = A(h\nu - E_g) \quad (S2)
\]

where \(F(R)\) represents the absorption, \(R\) is the reflectance (%), and \(h\nu\) is the incident photon energy, \(A\) is a constant, \(E_g\) is the bandgap value. Based on the DRS, the \(E_g\) values of CSGG hosts were determined to be 5.53 eV.
**Fig. S2** Tanabe-Sugano diagram for a Cr$^{3+}$ ion in octahedral coordination. Dq/B value of Cr$^{3+}$ in GSGG are marked in the Figure.
**Fig. S3** Variation of the shift of the diffraction peak on the (420) crystal plane with increasing doping of Cr$^{3+}$. 
Fig. S4 Concentration-dependent emission spectra of CSGG:xCr³⁺ (x = 0.01, 0.04, 0.08, 0.10, 0.14, 0.18, 0.20) phosphors. The upper inset shows the integral emission intensity under different Cr³⁺ doping concentrations.
Fig. S5 Relationship between log (I/x) and log x of GSGG:xCr^3+

The mechanism can be obtained using the following formula:

$$\log \left( \frac{I}{x} \right) = A - \frac{\theta}{3} \log x$$

Where I is the emission intensity, x is the concentration of the activator ions above the quenching concentration, β and K are constant for the same excitation conditions. The θ = 3 represents the interaction type of the energy transfer between the nearest-neighboring ions, while θ = 6, 8, and 10 represent dipole-dipole, dipole-quadrupole, and quadrupole-quadrupole interactions, respectively.
Fig. S6 Decay curves of CSGG:xCr$^{3+}$ phosphor under different Cr$^{3+}$ doping concentrations.
Fig. S7 The emission spectra of CSGG:xCr$^{3+}$, 0.04Ce$^{3+}$ (x = 0-0.18) in the NIR range.
Fig. S8 DRS of CSGG host, CSGG:0.14Cr\(^{3+}\), 0.16Ce\(^{3+}\), and CSGG:0.04Ce\(^{3+}\).
Fig. S9 XRD Rietveld refinement of (a) CSGG:0.14Cr$^{3+}$, 0.02Ce$^{3+}$, (b) CSGG:0.14Cr$^{3+}$, 0.16Ce$^{3+}$, and (c) CSGG:0.14Cr$^{3+}$, 0.20Ce$^{3+}$. 

- (a) CSGG:0.14Cr$^{3+}$, 0.02Ce$^{3+}$: $R_w = 9.3\%$, $R_r = 6.9\%$
- (b) CSGG:0.14Cr$^{3+}$, 0.16Ce$^{3+}$: $R_w = 9.1\%$, $R_r = 7.2\%$
- (c) CSGG:0.14Cr$^{3+}$, 0.20Ce$^{3+}$: $R_w = 9.8\%$, $R_r = 6.7\%$
Fig. S10 Decay curves of CSGG:0.14Cr\textsuperscript{3+} phosphors at different temperatures.
Fig. S11 The PL spectrum and corresponding Gaussian fitting of CSGG:0.14Cr$^{3+}$ phosphor recorded at (a) 25 °C, (b) 100 °C, (c) 150 °C, and (d) 250 °C.
Fig. S12 Temperature-dependent excitation spectra of CSGG:0.14Cr$^{3+}$. 
Fig. S13 (a) Variable temperature spectra of $\ln([I_0/I] - 1)$ versus $1/kT$ were plotted.

(b) Fitting FWHM curve with temperature.

$\Delta E = 0.18$ eV

$y = 0.01656 + 0.55815x$

$\hbar \omega = 0.030$ eV

$S = 3.38$
### Table S1. Main parameters of processing and refinement results of CSGG:0.14Cr$^{3+}$, yCe$^{3+}$ ($y = 0.02, 0.16, 0.20$).

<table>
<thead>
<tr>
<th>CSGG:Cr$^{3+}$</th>
<th>$y = 0.02$</th>
<th>$y = 0.16$</th>
<th>$y = 0.20$</th>
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<tbody>
<tr>
<td>Space group</td>
<td>$Ia3d$</td>
<td>$Ia3d$</td>
<td>$Ia3d$</td>
</tr>
<tr>
<td>$a=b=c$, Å</td>
<td>12.500594(235)</td>
<td>12.502334(264)</td>
<td>12.506791(160)</td>
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<tr>
<td>$V$, Å$^3$</td>
<td>1953.403(110)</td>
<td>1954.219(124)</td>
<td>1956.310(75)</td>
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<tr>
<td>$\alpha = \beta = \gamma$, $^\circ$</td>
<td>90$^\circ$</td>
<td>90$^\circ$</td>
<td>90$^\circ$</td>
</tr>
<tr>
<td>$R_{wp}$, %</td>
<td>9.3</td>
<td>9.1</td>
<td>9.8</td>
</tr>
<tr>
<td>$R_p$, %</td>
<td>6.9</td>
<td>7.2</td>
<td>6.7</td>
</tr>
<tr>
<td>$\chi^2$</td>
<td>2.401</td>
<td>2.386</td>
<td>2.391</td>
</tr>
</tbody>
</table>

### Table S2. Selected bond length (Å) of CSGG:0.14Cr$^{3+}$, yCe$^{3+}$ ($y = 0.02, 0.16, 0.20$).

<table>
<thead>
<tr>
<th></th>
<th>$y = 0.02$</th>
<th>$y = 0.16$</th>
<th>$y = 0.20$</th>
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</thead>
<tbody>
<tr>
<td>$8 \times \text{Ca—O}$</td>
<td>$4 \times 2.4370$ (2)</td>
<td>$4 \times 2.42306$ (4)</td>
<td>$4 \times 2.40094$ (4)</td>
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<tr>
<td></td>
<td>$4 \times 2.50086$ (5)</td>
<td>$4 \times 2.50684$ (3)</td>
<td>$4 \times 2.51506$ (5)</td>
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<tr>
<td>Average bond length</td>
<td>2.47192</td>
<td>2.46495</td>
<td>2.45800</td>
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<td>$D^*$</td>
<td>1.41%</td>
<td>1.70%</td>
<td>2.32%</td>
</tr>
</tbody>
</table>

(*lattice distortion index $D = \frac{1}{n} \sum_{i=1}^{n} \frac{|d_{i}-d_{av}|}{d_{av}}$)