

Supporting Information for

## **Nanocomposite Phosphor Consisting of $\text{CaI}_2\text{:Eu}^{2+}$ Single Nanocrystals Embedded in Crystalline $\text{SiO}_2$**

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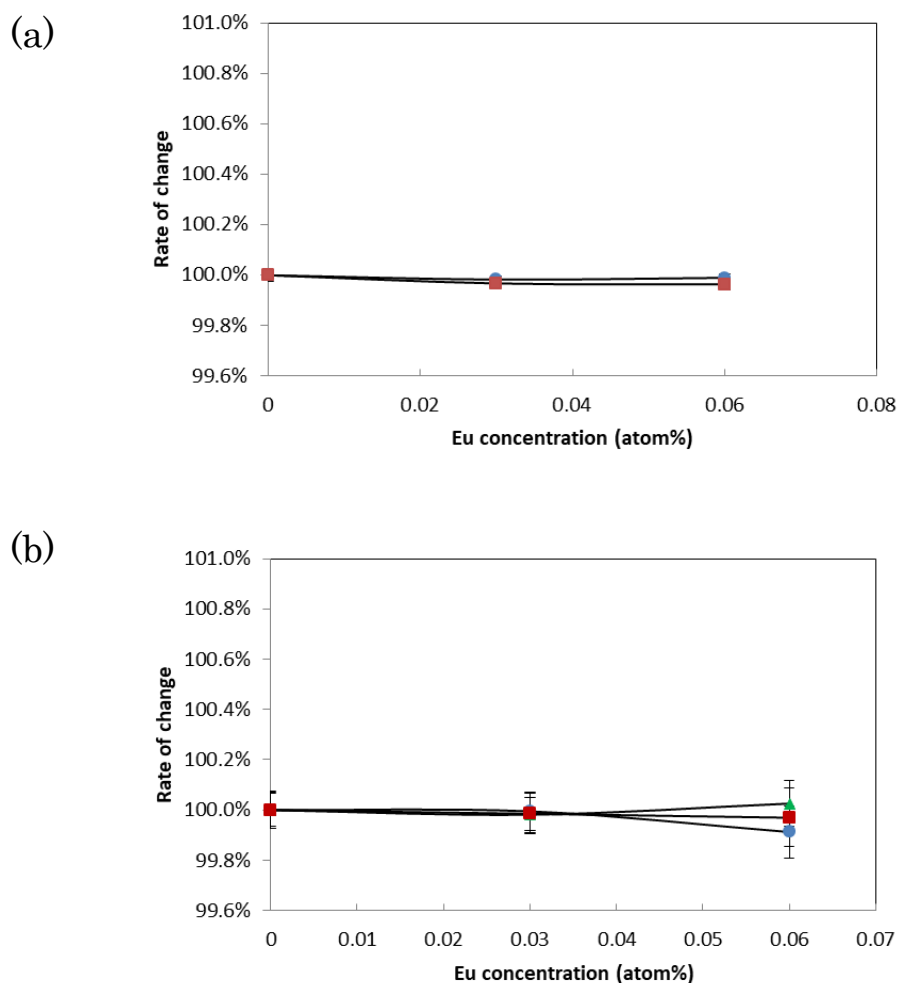
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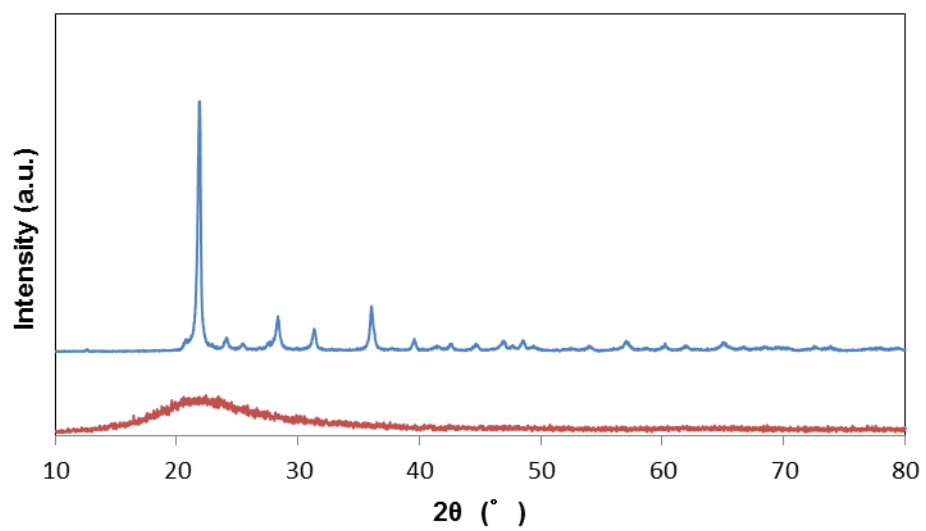
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Corresponding author;

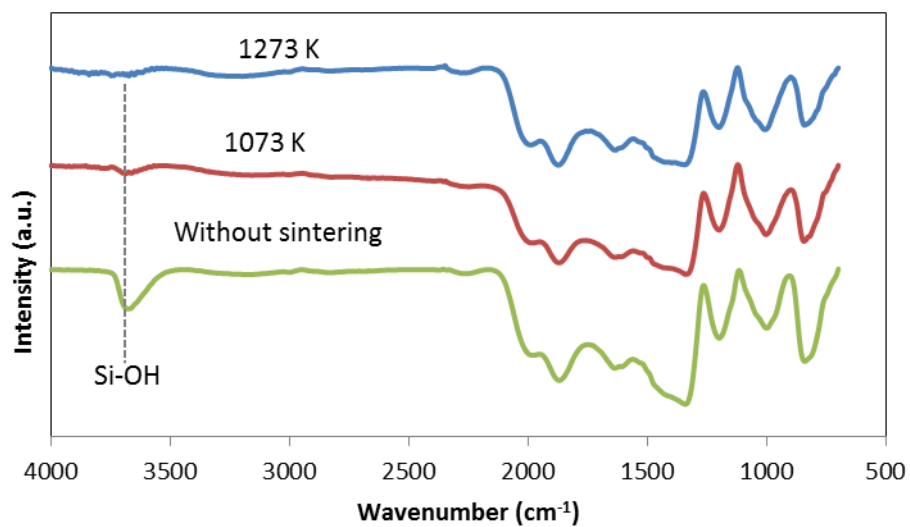
E-mail: cl\_ms@koito.co.jp



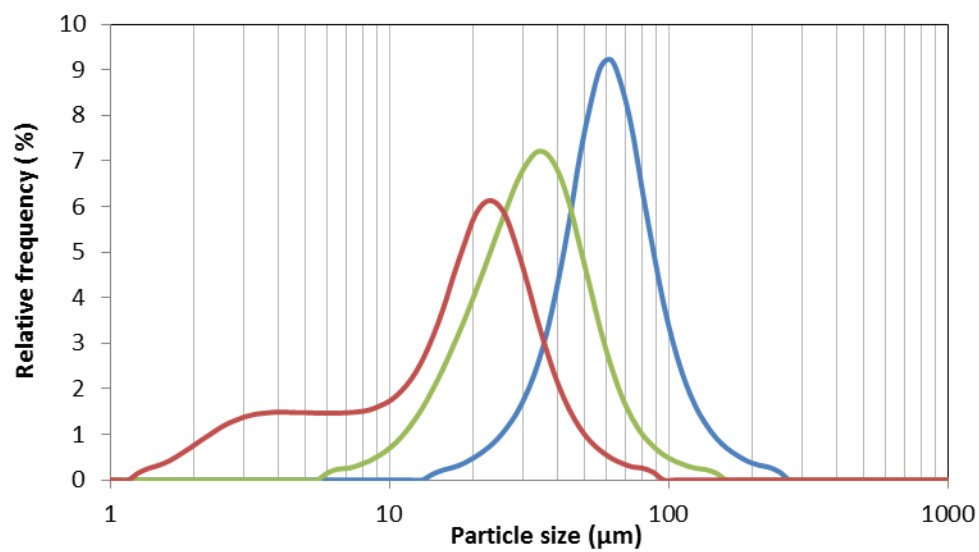
**Figure S1.** (a) Normalized lattice parameters against  $\alpha$ -cristobalite in  $(\text{CaI}_2:\text{Eu}^{2+}/\text{SiO}_2)$  ( $\text{Eu}=0$ ) along the a-axis (blue circles) and c-axis (red squares) of  $\alpha$ -cristobalite as a function of Eu content. (b) Normalized lattice parameters against  $\alpha$ - $\text{CaSiO}_3$  in  $(\text{CaI}_2:\text{Eu}^{2+}/\text{SiO}_2)$  ( $\text{Eu}=0$ ) along the a-axis (blue circles), b-axis (green triangles), and c-axis (red squares) of  $\alpha$ - $\text{CaSiO}_3$  as a function of Eu content. Eu atom% in  $(\text{CaI}_2:\text{Eu}^{2+}/\text{SiO}_2)$  were determined with inductively coupled plasma atomic emission spectroscopy.



**Figure S2.** XRD patterns of  $(\text{CaI}_2:\text{Eu}^{2+}/\text{SiO}_2)$  at sintering temperature of 1273 K (blue curve) and 1073 K (red curve).

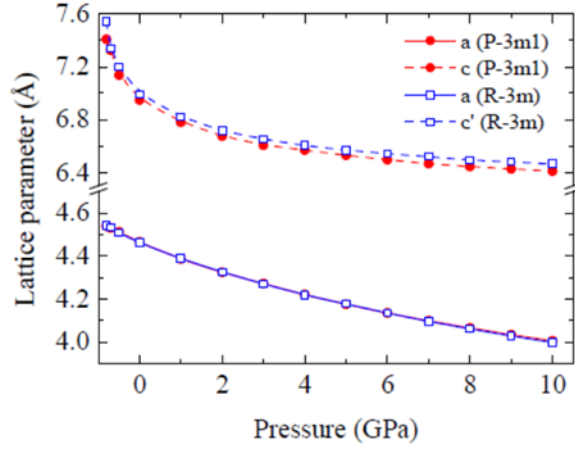


**Figure S3.** Fourier transform IR spectra of unsintered SiO<sub>2</sub> (green curve) and SiO<sub>2</sub> sintered at 1273 K (blue curve) and 1073 K (red curve) in a reducing atmosphere.

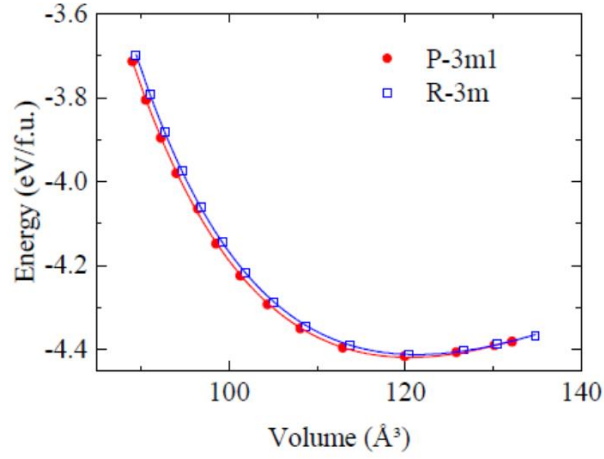


**Figure S4.** Particle size distribution curves of the SiO<sub>2</sub> raw material (green), the milled raw materials before sintering (red), and (CaI<sub>2</sub>:Eu<sup>2+</sup>/SiO<sub>2</sub>) (blue).

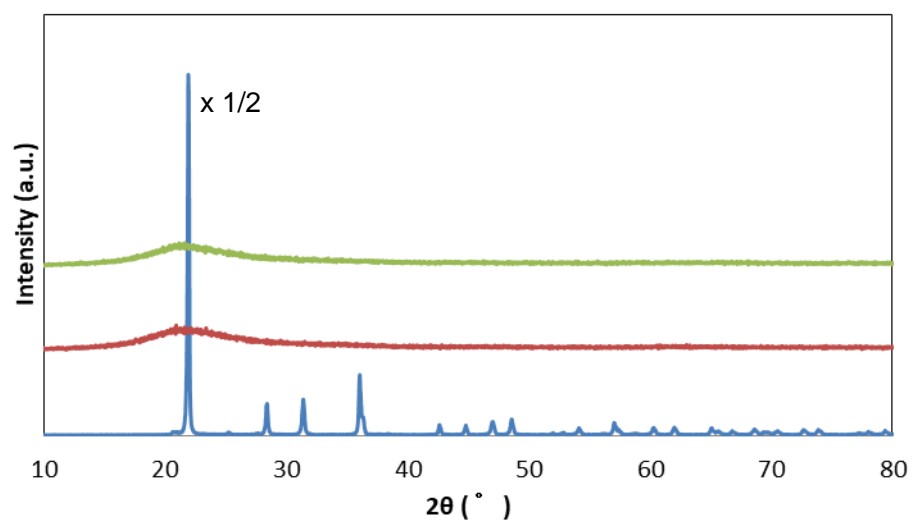
(a)



(b)



**Figure S5.** (a) Plots of lattice parameters as a function of external pressure: lattice parameter along the  $a$ -axis of  $6H\text{-CaI}_2$  (space group  $R3m$ ),  $1/3$  of the lattice parameter along the  $c$ -axis of  $6H\text{-CaI}_2$  ( $R3m$ ), lattice parameter along the  $a$ -axis of  $2H\text{-CaI}_2$  (space group  $P3m1$ ), and lattice parameter along the  $c$ -axis of  $2H\text{-CaI}_2$  ( $P3m1$ ). (b) Plots of total electron energy as a function of cell volume:  $6H\text{-CaI}_2$  ( $R3m$ ) and  $2H\text{-CaI}_2$  ( $P3m1$ ), respectively.



**Figure S6.** XRD patterns of  $\text{SiO}_2$  powder sintered at 1273 K (green curve), 1473 K (red curve), and 1623 K (blue curve).

**Table S1.** Composition (atom %) of  $(\text{CaI}_2\text{:Eu}^{2+}/\text{SiO}_2)$  and  $\text{BaMaAl}_{10}\text{O}_{17}\text{:Eu}^{2+}$  measured by inductively coupled plasma atomic emission spectroscopy combined with ion chromatography.

	Eu	Ca	Si	I	Ba	Mg	Al
$(\text{CaI}_2\text{:Eu}^{2+}/\text{SiO}_2)$	0.1	0.6	32.4	0.4	—	—	—
$\text{BaMaAl}_{10}\text{O}_{17}\text{:Eu}^{2+}$	0.65	—	—	—	2.7	3.4	33.0



**Table S2.** Composition (atom %) of each region of the (CaI<sub>2</sub>:Eu<sup>2+</sup>/SiO<sub>2</sub>) phosphor as measured by scanning electron microscopy combined with energy dispersive X-ray spectrometry.

	<b>Eu</b>	<b>Si</b>	<b>Ca</b>	<b>O</b>	<b>I</b>
<b>Nucleus at the particle center</b>	0	33.2	0	66.5	0.3
<b>Outer layer matrix</b>	0	33.0	0.2	66.1	0.7
<b>White spot in the outer layer</b>	0.6	32.1	1.0	64.1	3.2

**Table S3.** Crystallographic data for  $6H\text{-CaI}_2\text{:Eu}^{2+}$  in  $(\text{CaI}_2\text{:Eu}^{2+}/\text{SiO}_2)$  by Rietveld refinement, along with literature data for  $2H\text{-CaI}_2$ .

	$6H\text{-CaI}_2\text{:Eu}^{2+}$			$2H\text{-CaI}_2$
Eu atom % in $(\text{CaI}_2\text{:Eu}^{2+}/\text{SiO}_2)$	0	0.03	0.06	—
Space group	$R\bar{3}m$	$R\bar{3}m$	$R\bar{3}m$	$P\bar{3}m1$
Lattice parameter				
$a$	4.510(2)	4.530(1)	4.548(1)	4.49(2)
$c$	20.998(27)	21.002(12)	21.006(15)	6.975(30)

Eu atom% in  $(\text{CaI}_2\text{:Eu}^{2+}/\text{SiO}_2)$  were determined with inductively coupled plasma atomic emission spectroscopy.