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Supporting Information

Intense UV long persistent luminescence benefiting from the coexistence of Pr^{3+}/Pr^{4+} in praseodymium doped $BaLu_2Al_2Ga_2SiO_{12}$ phosphor

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Computational Details

We have employed the first-principles to perform all Spin-polarization density functional theory (DFT) calculations within the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) formulation.[1-3] We have chosen the projected augmented wave (PAW) potentials to describe the ionic cores and take valence electrons into account using a plane wave basis set with a kinetic energy cutoff of 400 eV. In all the calculation, we used 3×3×3 for the Monkhorst-Pack k-point for periodic crystal structure. The convergence threshold for energy was set at 10^{-6} eV. The equilibrium lattice constants were optimized with maximum stress on each atom within 0.05 eV/Å. The Hubbard U (DFT+U) corrections (4.78 eV) for Lu atom had been chosen.

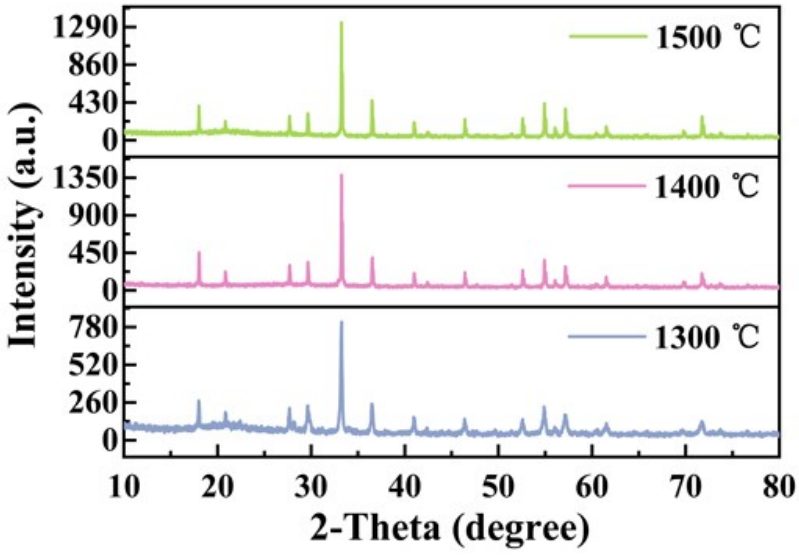

Fig. S1 XRD patterns of BLAGSO:0.04Pr^{3+} synthesized at different temperatures.

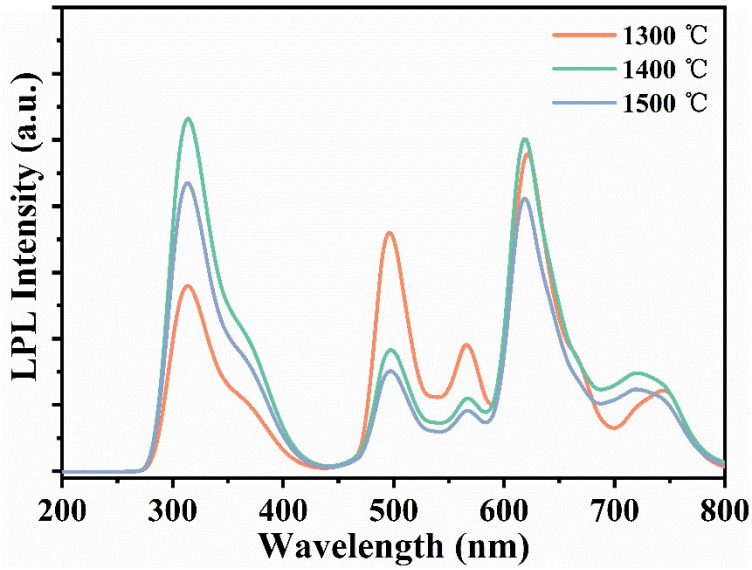

Fig. S2 The LPL spectra of BLAGSO:0.04Pr^{3+} synthesized at different temperatures.

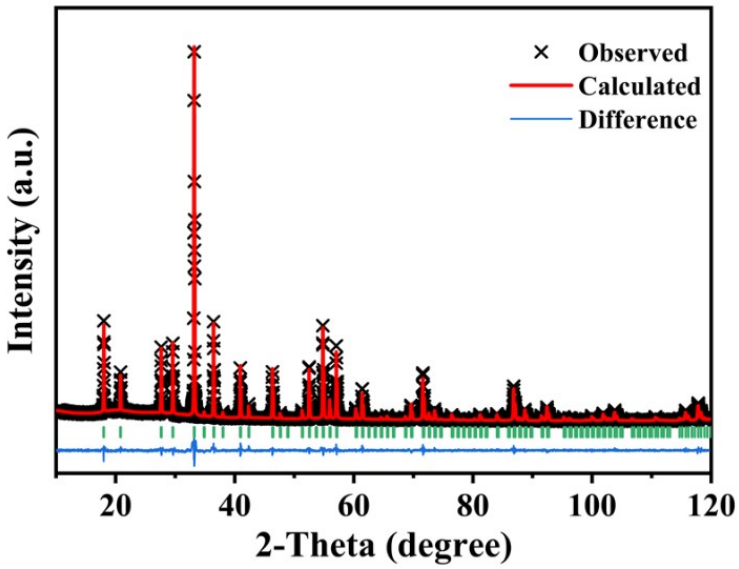

Fig. S3 XRD profile for the Rietveld refinement result of BLAGSO.

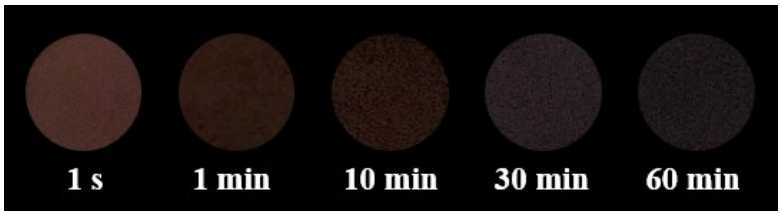

Fig. S4 The LPL images of BLAGSO:0.04Pr^{3+} taken at different afterglow time.

Table S1 Rietveld fitting results of BLAGSO and BLAGSO:0.04Pr^{3+}

Formula	BLAGSO	BLAGSO:0.04Pr^{3+}
crystal system	cubic	cubic
space group	$Ia\bar{3}d$(230)	$Ia\bar{3}d$(230)
a (Å)	12.0669	12.0786
b (Å)	12.0669	12.0786
c (Å)	12.0669	12.0786
α = β = γ (deg)	90	90
Z	8	8
V ($Å^3$)	1757.075	1762.175
Rp	0.0447	0.0452
Rwp	0.0611	0.0623
χ^2	2.849	2.969

Table S2 Atomic positions of BLAGSO

atom	site	x	y	z	Occupancy	U_{iso}
Ba1	24c	0.125	0	0.25	0.3330	0.00612
Lu1	24c	0.125	0	0.25	0.6670	0.01100
Al1	16a	0	0	0	0.5450	0.01538
Ga1	16a	0	0	0	0.4550	0.00777
Al2	24d	0.375	0	0.25	0.3033	0.02568
Ga2	24d	0.375	0	0.25	0.3634	0.01255
Si1	24d	0.375	0	0.25	0.3333	0.00456
O1	96h	-0.03879	0.04806	0.15408	1.0000	0.02588

Table S3 Atomic positions of BLAGSO:0.04Pr^{3+}

atom	site	x	y	z	Occupancy	U_{iso}
Ba1	24c	0.125	0	0.25	0.3330	0.02204
Lu1	24c	0.125	0	0.25	0.6540	0.01658
Pr1	24c	0.125	0	0.25	0.0130	0.01610
Al1	16a	0	0	0	0.5450	0.03068
Ga1	16a	0	0	0	0.4550	0.01394
Al2	24d	0.375	0	0.25	0.3033	0.00112
Ga2	24d	0.375	0	0.25	0.3634	0.00153
Si1	24d	0.375	0	0.25	0.3333	0.02567
O1	96h	-0.03656	0.04779	0.15299	1.0000	0.05205

Reference

1. P. E. Blochl, *Phys. Rev. B*, 1994, **50**, 17953-17979.

2. J. P. Perdew and K. Burke, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.

3. G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758-1775.