Electronic Supplementary Information

Investigation of multicolor emitting $Cs_3GdGe_3O_9:Bi^{3+},Eu^{3+}$ phosphors via energy transfer for WLED

Fengfeng Chi[ae*], Zhangchao Ji[a], Qian Liu[b], Bin Jiang[c], Bing Wang[d], Jie Cheng[a], Bin Li[a], Shengli Liu[a*] and Xiantao Wei[e]

Corresponding authors

E-mail: ffchi@mail.ustc.edu.cn (F. Chi); liusl@njupt.edu.cn (S. Liu)

[a] *New Energy Technology Engineering Laboratory of Jiangsu Province & School of Science, Nanjing University of Posts and Telecommunications, Nanjing 210023, China*

[b] *College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China*

[c] *College of Electronic and Information Engineering, West Anhui University, Lu'an 237012, China*

[d] *Institute for Computational Materials Science, Joint Center for Theoretical Physics (JCTP),School of Physics and Electronics, Henan University, Kaifeng, 475004, China*

[e] *School of Physical Sciences, University of Science and Technology of China, Hefei 230026, China*

Experimental

S1 Synthesis of samples

A series of $Cs_3GdGe_3O_9$ (CGGO)、$Cs_3Gd_{1-x}Ge_3O_9$:$x$$Bi^{3+}$ (x = 0.01, 0.03, 0.05, 0.07, 0.01, 0.15) and $Cs_3Gd_{1-y}Ge_3O_9$:0.05Bi^{3+},$y$$Eu^{3+}$ (y = 0.01, 0.03, 0.05, 0.1, 0.15, 20) were synthesized by the common high temperature solid-state reaction. The raw materials were Cs_2CO_3、Gd_2O_3、GeO_2、Bi_2O_3 and Eu_2O_3 with the purity of 99.99%. First, the raw materials were weighed according to stoichiometric ratios. Next, the ingredients were placed on the agate mortar and ground fully to mix well. Then, the well-mixed raw materials were sintered in a muffle furnace at 1000 °C for 6 hours. Finally, the cooled sample was ground again for further measurements.

S2 Characterization

X-ray diffraction (XRD) was performed on a Rigaku Smartlab 9 kW instrument using Cu $K\alpha$ radiation (λ = 1.54056 Å) with a test range of 20º-50º. The X-ray photoelectron spectroscopy (XPS) analysis of phosphor was conducted on a Thermo Scientific ESCALAB 250 Xi instrument. The diffuse reflectance spectrum (DRS) of CGGO and CGGO:0.05Bi^{3+} samples were determined by a spectrophotometer (Shimadzu, SOLID 3600) using a $BaSO_4$ based integrating sphere. Photoluminescence emission spectra, excitation spectra, and fluorescence lifetime decay curves were tested using an Edinburgh FLS1000 fluorescence spectrometer. Meanwhile, the emission spectra at different temperatures of phosphors were measured in the Edinburgh FLS1000 with heating and warming functions. CIE coordinates are derived from emission spectral data and the CIE 1931 standard colorimetric system.

S3 Computation details

The density-functional theory (DFT) calculations of the structure and electronic properties were carried out by employing the Vienna *ab initio* Simulation Package (VASP). [1] The unit cell of $Cs_3GdGe_3O_9$ contains 64 atoms. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was employed as exchange-correlation function. [2, 3] Cs ($5s^25p^66s^1$), Gd ($5p^65d^16s^2$), Ge ($3d^{10}4s^24p^2$), and O ($2s^22p^4$) were treated as valence electrons, and their interactions with the cores were

described by the projector-augmented-wave (PAW) approach. The plane wave cutoff energy was set to 500 eV. The electronic convergence criteria set to 10^{-5} eV and the Hellmann-Feynman forces on atoms were less than 0.02 eV/Å. A 2 × 5 × 3 *k*-points grids were used to relax the geometric structure.

References

[1] J. P. Perdew, K. Burke, M. Ernzerhof. Generalized gradient approximation made simple. ***Physical review letters***, 77 (1996) 3865.

[2] G. Kresse, J. Furthmüller. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. ***Computational materials science***, 6 (1996) 15-50.

[3] G. Kresse, J. Furthmüller. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. ***Physical review B***, 54 (1996) 11169.

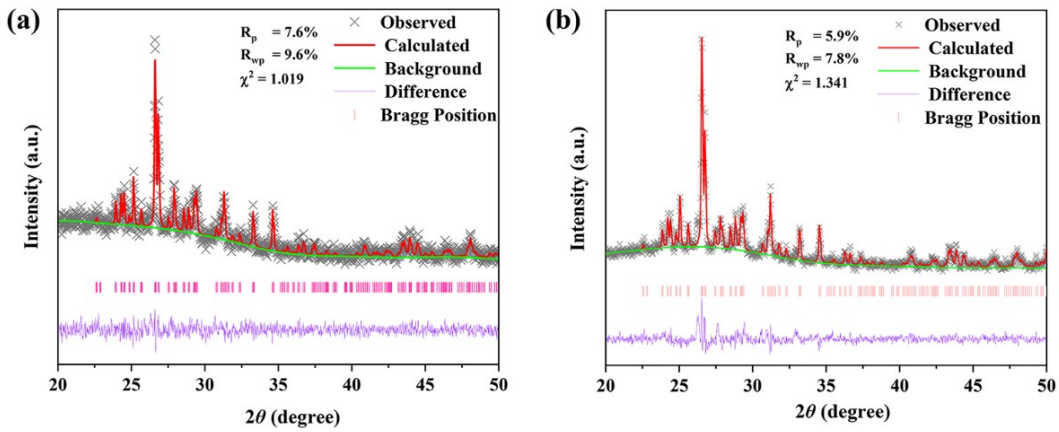

Fig. S1 The Rietveld refinement results of CGGO and CGGO:0.05Bi^{3+}, 0.1Eu^{3+} samples.

Table S1 CIE chromaticity coordinates for CGGO:0.05Bi^{3+},Eu^{3+} phosphors.

Eu^{3+} content	**CIE (x, y)**
0	(0.1678, 0.1568)
0.01	(0.1900, 0.1643)
0.03	(0.2343, 0.1839)
0.05	(0.3154, 0.2369)
0.1	(0.4311, 0.2692)
0.15	(0.5077, 0.3069)
0.2	(0.5931, 0.3251)

Table S2 The values of CIE coordinates and CCT for WLED driven by different currents.

Current (mA)	**CIE**	**CCT (K)**
20	(0.352, 0.3626)	4783
40	(0.3495, 0.3667)	4898
60	(0.3426, 0.3645)	5132
80	(0.3386, 0.3659)	5281
100	(0.3354, 0.3697)	5402
120	(0.3318, 0.371)	5533