Tailored Luminescence Output of Bi^{3+} Doped $BaGa_2O_4$ Phosphor with the Assistant of the Introduction of Secondary Cations Sr^{2+} Ions

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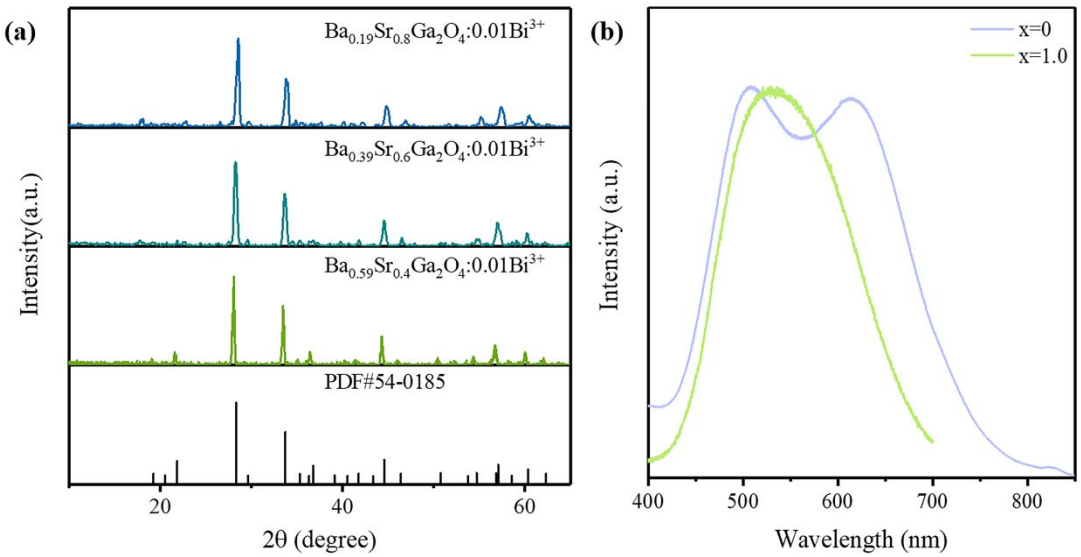

Figure S1. *(a) XRD patterns of* $Ba_{1-x}Sr_xGa_2O_4:0.01Bi^{3+}$ *(x=0.4, 0.6 and 0.8) phosphors and the standard data of* $BaSrGa_4O_8$*. (b) The normalized PL spectra of* $Ba_{1-x}Sr_xGa_2O_4:0.01Bi^{3+}$ *(x=0 and 1.0) phosphors, respectively.*

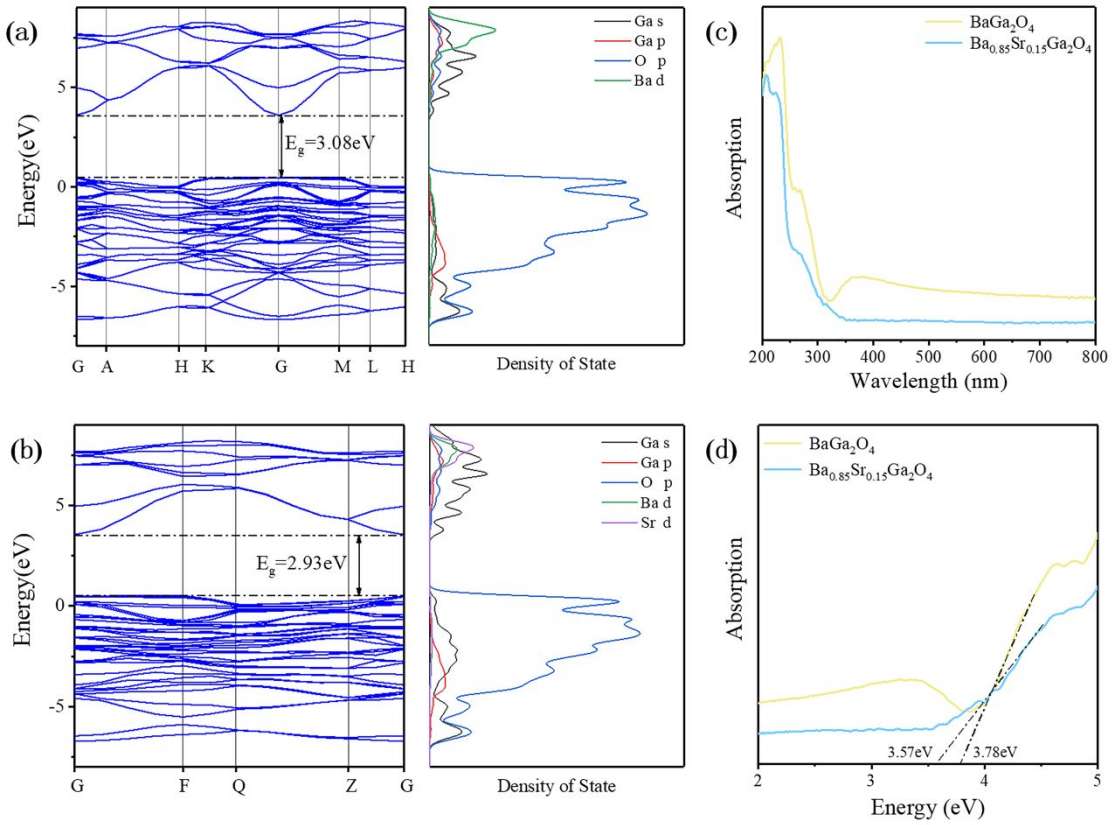

Figure S2. *Electronic band structure and the corresponding PDOS of $BaGa_2O_4$ (a), and $Ba_{0.85}Sr_{0.15}Ga_2O_4$ (b), respectively. (c) Optical absorption spectra and (d) Kubelka-Munk plots with extrapolation of the band gap for pure $BaGa_2O_4$ and $Ba_{0.85}Sr_{0.15}Ga_2O_4$, respectively.*

The calculated electronic band structure of pure $BaGa_2O_4$ possesses a direct band gap at the *G* point of Brillouin zone (E_g= ~3.08eV), where the O 2*p* orbit*, and* the Ba 4*d* and Ga 4*s* orbit contributes to the valence band maximum (VBM) and conduction band minimum (CBM) of $BaGa_2O_4$ host, respectively. Meanwhile, the calculated band gap decreases to be ~2.93eV (Figure S2b) of $Ba_{0.85}Sr_{0.15}Ga_2O_4$, for the contribution of the 4*d* orbit of Ba and 4*s* orbit of Ga as well as the 3*d* orbit

of Sr to the CBM of the host matrix. The decreased band gap is further confirmed with the absorption spectra of the $BaGa_2O_4$ and $Ba_{0.85}Sr_{0.15}Ga_2O_4$, respectively in Figure S2c, where all the phosphors exhibit an effective absorption in the range of ultraviolet light. The band gap can be obtained using the following equation:

$$F(R) = (1-R)^2/2R$$

$$[F(R) \times h\upsilon]^2 = A(h\upsilon - E_g) \quad (1)$$

where $F(R_\infty)$ is the Kubelka-Munk function, $h\upsilon$ is the photon energy, R represent the reflection parameters, A is a proportionality constant and E_g stands for the optical band gap. The E_g values of $BaGa_2O_4$ host and $Ba_{0.84}Sr_{0.15}Ga_2O_4$ are estimated to be about 3.78 eV and 3.57 eV by extrapolating linear portion of $[F(R) \times h\upsilon]^2 = 0$ in Figure S2d.

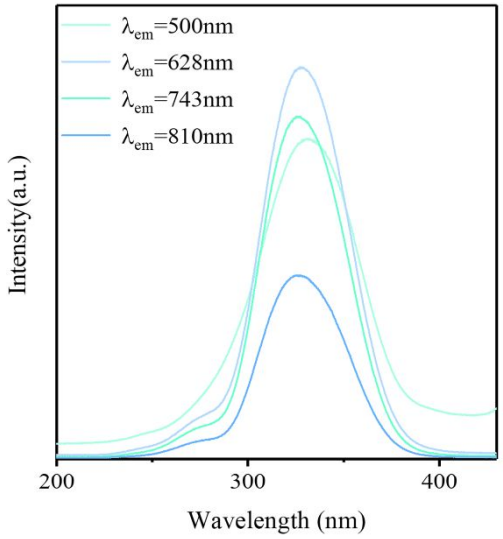

Figure S3. *PLE spectra of $Ba_{0.94}Sr_{0.05}Ga_2O_4$:0.01$Bi^{3+}$ phosphor monitored at 500, 628, 743 and 800 nm emission.*

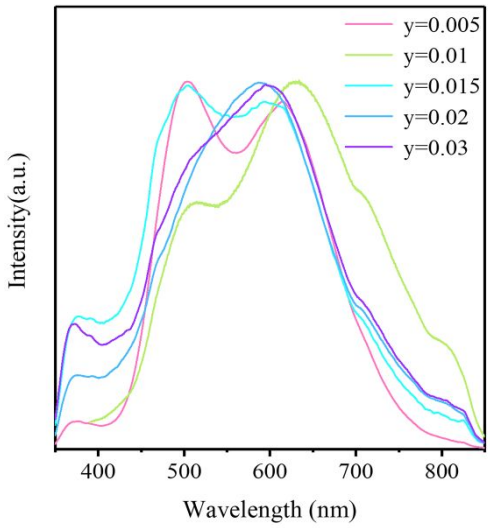

Figure S4. *Normalized PL spectra of $Ba_{0.94}Sr_{0.05}Ga_2O_4$: yBi^{3+} (y=0.005, 0.010, 0.015, 0.020, 0.030) phosphors under 320 nm excitation.*

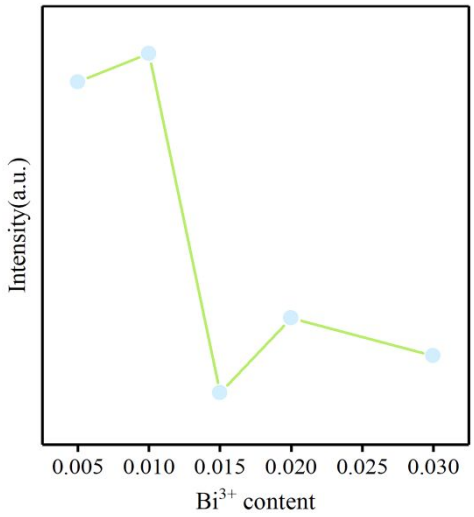

Figure S5. *The emission intensity in $Ba_{0.94}Sr_{0.05}Ga_2O_4$: yBi^{3+} (y=0.005, 0.010, 0.015, 0.020, 0.030) phosphors as a function of Bi^{3+} concentration.*

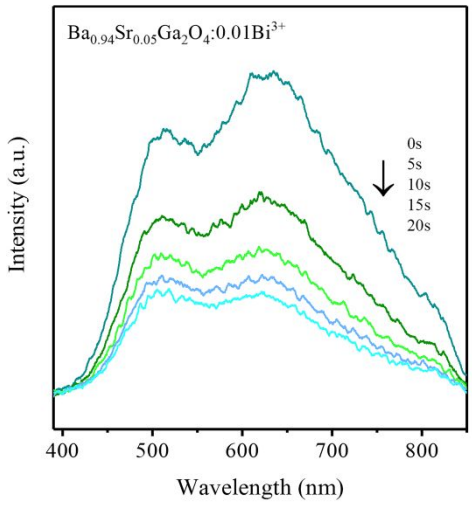

Figure S6. *LPL spectra of* $Ba_{0.94}Sr_{0.05}Ga_2O_4:0.01Bi^{3+}$.