

## Supporting Information

### **Luminescent Zero-Dimensional Organic Metal Halide Hybrids with Near-Unity Quantum Efficiency**

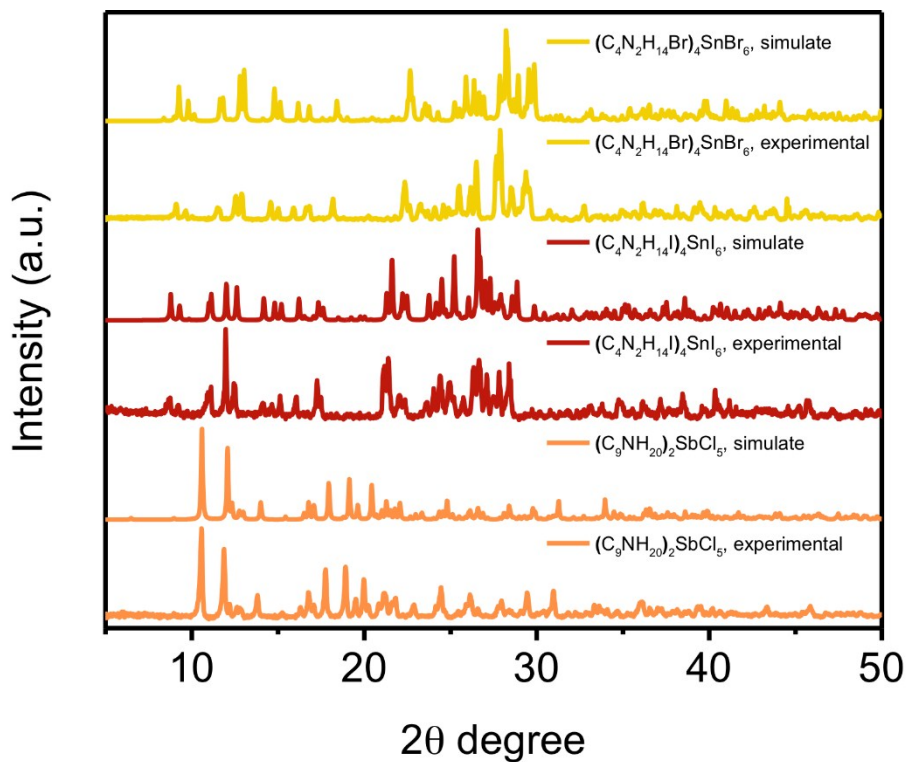
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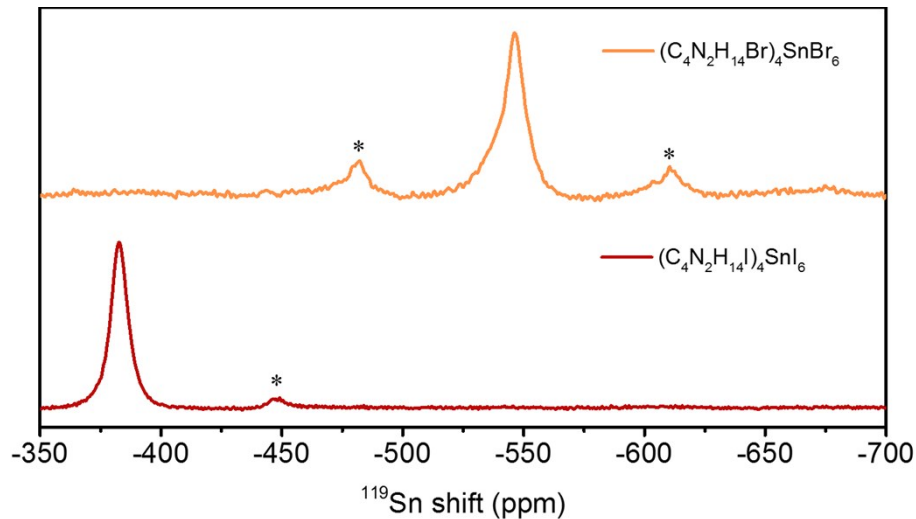
**Table S1** | Single crystal x-ray diffraction data and collection parameters. The collection was performed at a temperature of  $\sim 120$  K.

Compound	(C <sub>4</sub> N <sub>2</sub> H <sub>14</sub> Br) <sub>4</sub> SnBr <sub>6</sub>	(C <sub>4</sub> N <sub>2</sub> H <sub>14</sub> I) <sub>4</sub> SnI <sub>6</sub>	(C <sub>9</sub> NH <sub>20</sub> ) <sub>2</sub> SbCl <sub>5</sub>
Formula	[(CH <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> C <sub>2</sub> H <sub>4</sub> ] <sub>4</sub> SnBr <sub>10</sub>	[(CH <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> C <sub>2</sub> H <sub>4</sub> ] <sub>4</sub> SnI <sub>10</sub>	C <sub>18</sub> H <sub>40</sub> Cl <sub>5</sub> N <sub>2</sub> Sb
Molecular weight	1278.40 g/mol	1748.37 g/mol	583.54 g/mol
Space group	<i>P</i> -1 (# 2)	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i>	10.2070(4) Å	10.7464(7) Å	8.7562(2) Å
<i>b</i>	10.6944(4) Å	10.8924(7) Å	27.2439(5) Å
<i>c</i>	18.5996(6) Å	11.1796(7) Å	10.64230(2) Å
$\alpha$	94.043(3)°	64.2658(7)°	90.0000°
$\beta$	102.847(3)°	80.1825(7)°	97.354(2)°
$\gamma$	97.904(3)°	72.8331(7)°	90.0000°
<i>V</i>	1949.89(12) Å <sup>3</sup>	1124.94(12) Å <sup>3</sup>	2518.02(8) Å <sup>3</sup>
<i>Z</i>	2	1	4
$\rho_{\text{calc.}}$	2.177 g/cm <sup>3</sup>	2.581 g/cm <sup>3</sup>	1.539 g/cm <sup>3</sup>
$\mu$	10.922 mm <sup>-1</sup>	7.448 mm <sup>-1</sup>	1.633 mm <sup>-1</sup>
Data collection range	2.815° < $\theta$ < 34.220°	1.986° < $\theta$ < 29.408°	2.782° < $\theta$ < 31.981°
Reflections collected	57392	14019	32635
Independent reflections	11532	5710	8177
Parameters refined	540	165	395
Restraints	240	0	174
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub>	0.0651 <sup>a</sup> , 0.0511 <sup>b</sup>	0.0178, 0.0349	0.0418, 0.0542
Goodness-of-fit on <i>F</i> <sup>2</sup>	0.9933	1.078	0.9984

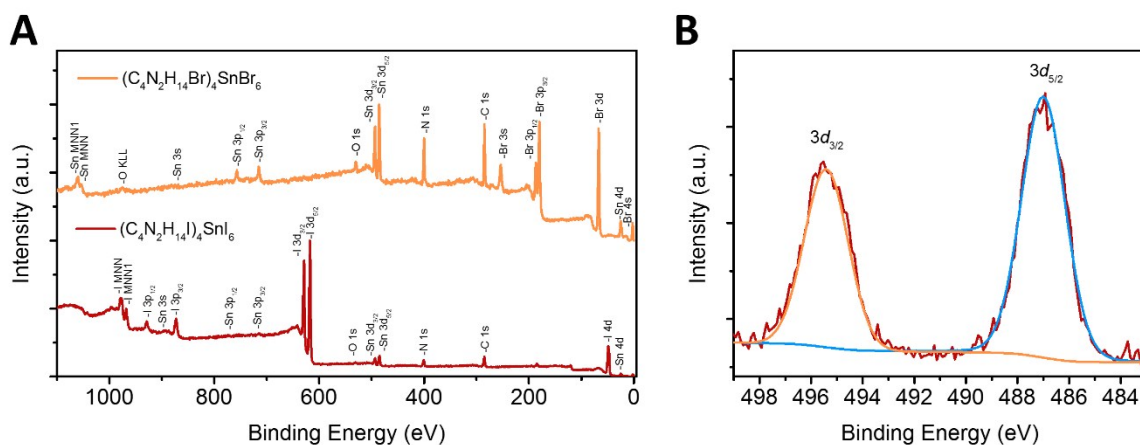
<sup>a)</sup>  $R_1 = \sum \|F_o\| - \|F_c\| / \sum \|F_o\|$ . <sup>b)</sup>  $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ .



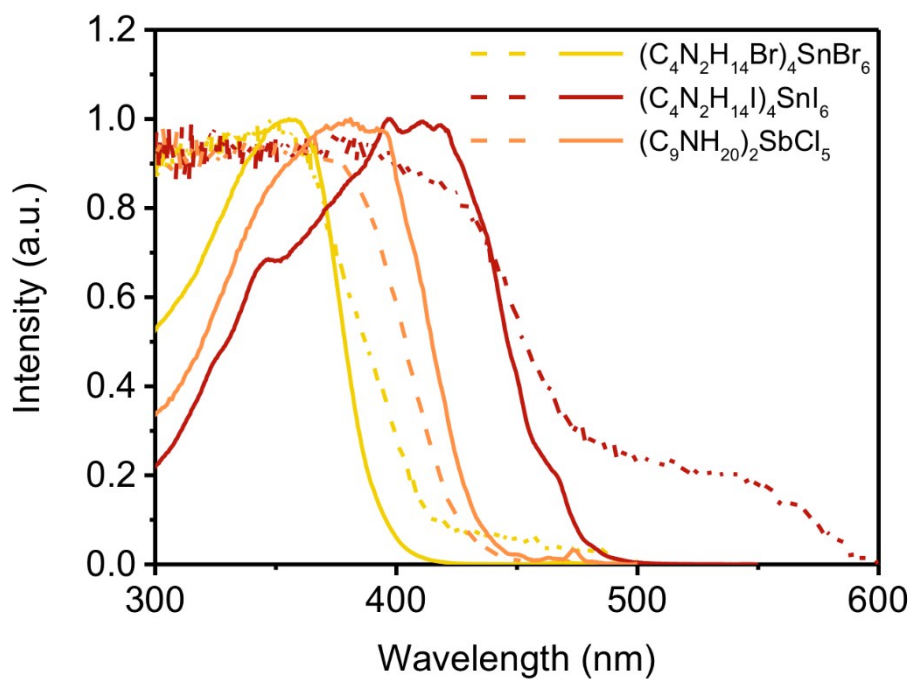
**Figure S1.** PXRD of powder 0D organic metal halide hybrids as well as their simulated results.



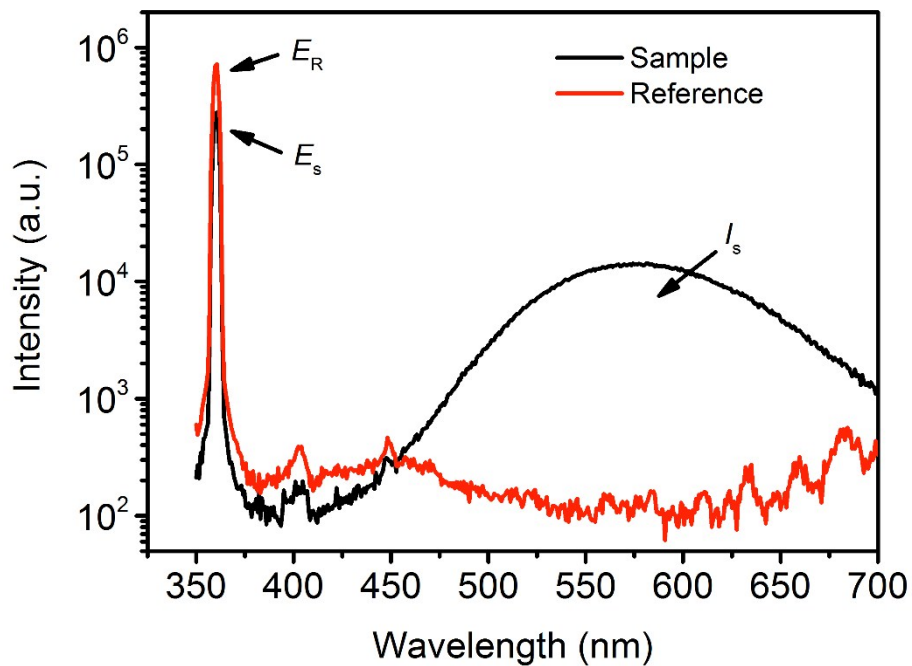
**Figure S2.**  $^{119}\text{Sn}$  MAS NMR spectra of 0D organic tin halide hybrids recorded at room temperature spinning at 12 kHz. Spinning sidebands are indicated with asterisks.



**Figure S3.** X-ray photoelectron spectroscopy (XPS) of 0D organic tin halide hybrids: (a) survey spectra of two 0D organic tin halide hybrids, and (b) high resolution Sn spectra in  $(C_4N_2H_{14}Br)_4SnBr_6$ .

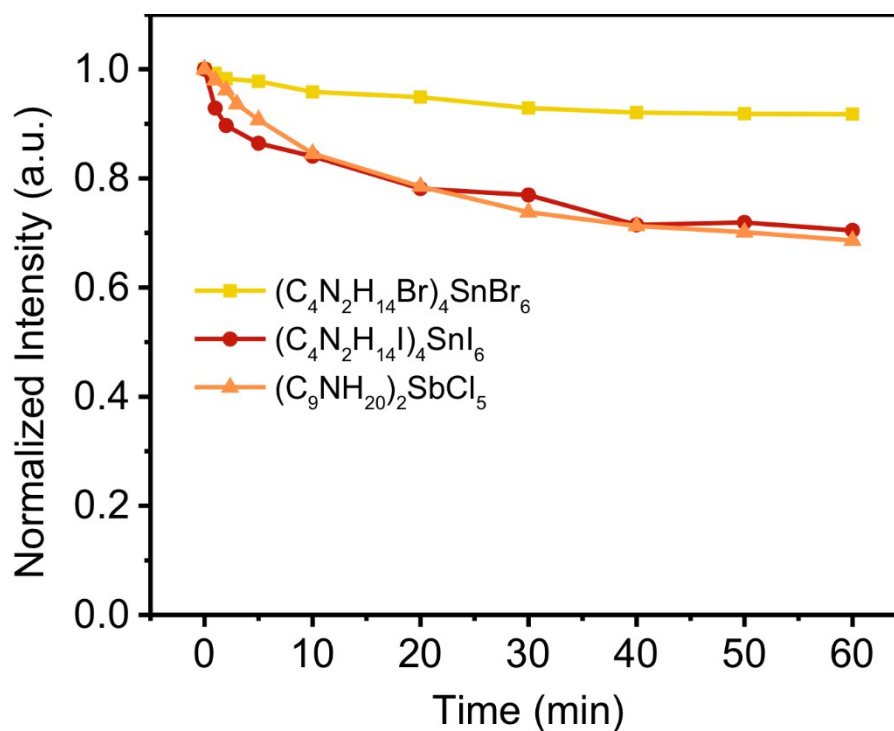


**Figure S4.** Absorption (dash line) and excitation (solid line) spectra of 0D organic metal halide hybrids recorded at room temperature.

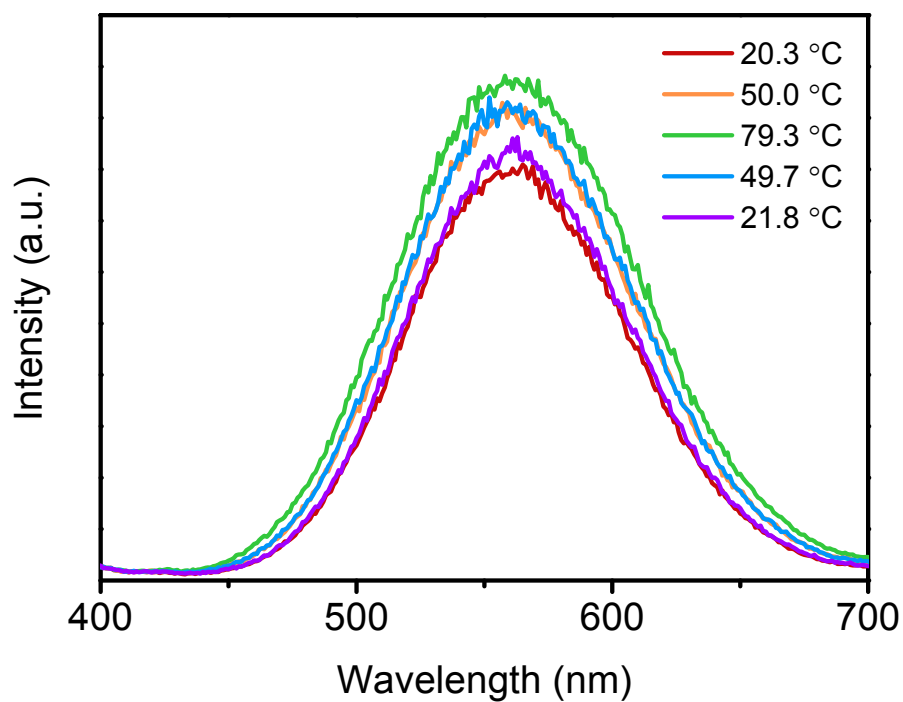


**Figure S5.** Excitation line of reference and emission spectrum of  $(C_4N_2H_{14}Br)_4SnBr_6$  collected by an integrating sphere. The PLQE was calculated by the equation:

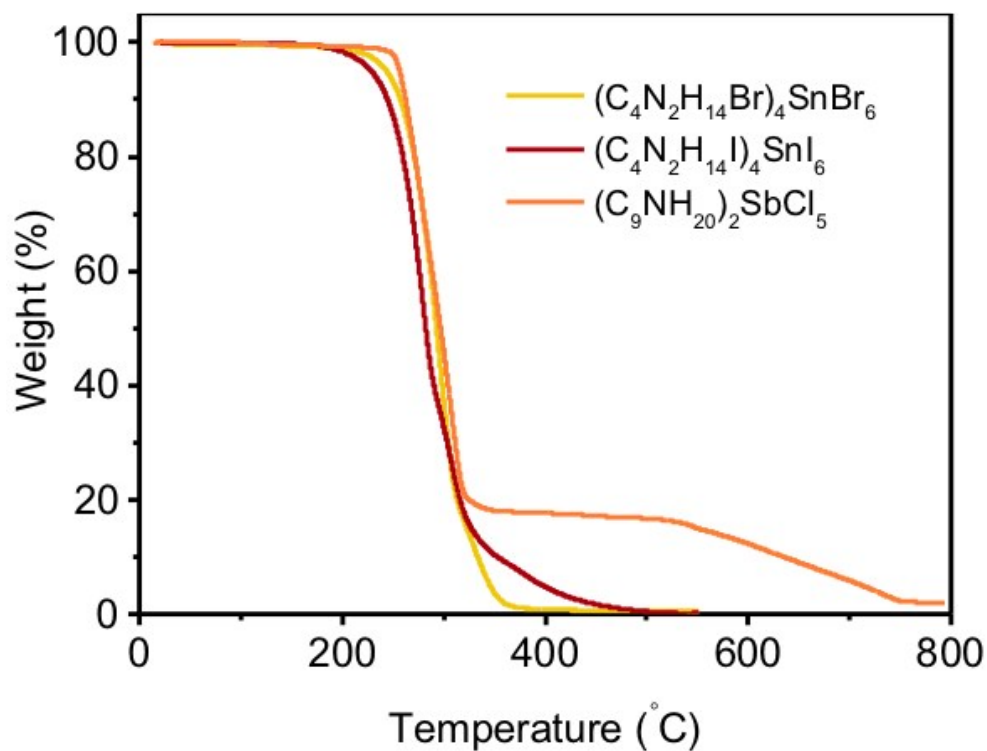
$$\eta_{QE} = I_s / (E_R - E_S)$$



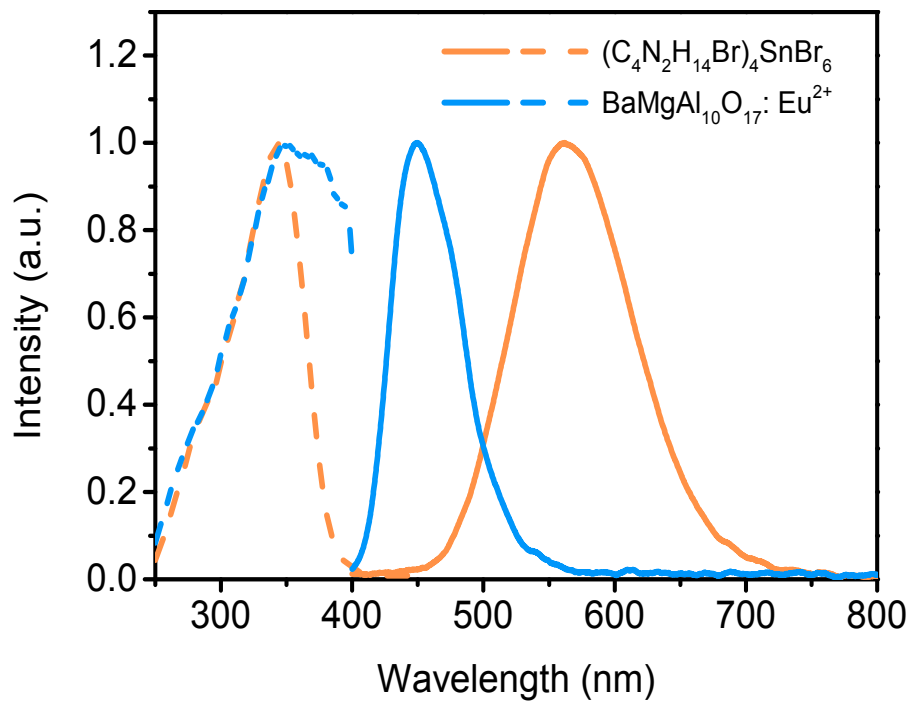
**Figure S6.** Photostability of 0D organic metal halide hybrids under continuous illumination using a high-power mercury lamp ( $150 \text{ mW/cm}^2$ ).



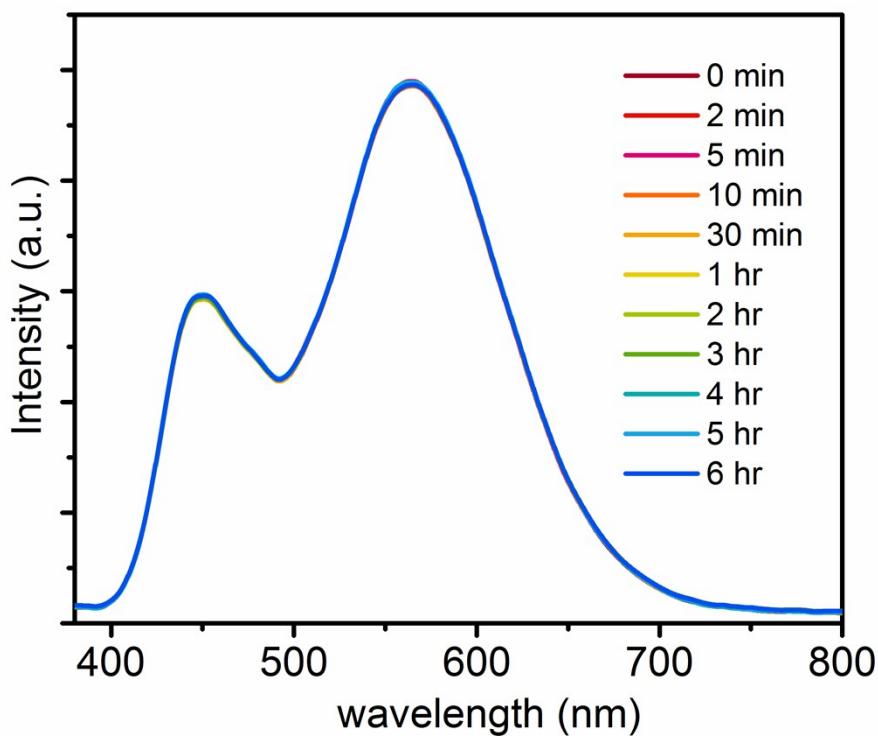
**Figure S7.** Temperature dependent photoluminescence of  $(C_4N_2H_{14}Br)_4SnBr_6$ .



**Figure S8.** TGA of Sn based 0D organic metal halide hybrids.



**Figure S9.** The normalized excitation (dash lines) and emission (solid lines) spectra of  $\text{BaMgAl}_{10}\text{O}_{17}:\text{Eu}^{2+}$  and  $(\text{C}_4\text{N}_2\text{H}_{14}\text{Br})_4\text{SnBr}_6$  phosphors.



**Figure S10.** Emission spectra of a white LED continuously operated in air for more than six hours with a brightness of  $\sim 400 \text{ cd/m}^2$ .