A novel material Cs₂Rb_xAg_{1-x} In_{0.875}Bi_{0.125}Cl₆ with special blue shift

and application for white light LED devices

Xixiang Wang¹, Chen Niu², Wenjian Liao¹, Shiliang Mei³, Rongrong Hu², Yang Li⁴, Bobo Yang^{2*},

Yong Chen^{1*} and Jun Zou^{2,5,6*}

1 School of Chemistry and Environmental Engineering, Shanghai Institute of Technology, Shanghai 201418, People's Republic of China

2 School of Science, Shanghai Institute of Technology, Shanghai 201418, People's Republic of China

3 Institute for Electric Light Sources, Fudan University, Shanghai 200433, People's Republic of China

4 School of Materials Science and Engineering, Shanghai Institute of Technology, Shanghai 201418, People's Republic of China

5 National Semiconductor Lighting Application System Engineering Technology Research Center, Shanghai 201418, People's Republic of China

6 Institute of New Materials & Industrial Technology, Wenzhou University, Wenzhou 325024,

People's Republic of China

 $*\ Corresponding\ authors:\ boboyang@sit.edu.cn,\ yongchen@sit.edu.cn,\ zoujun@sit.edu.cn.$

| x value | Rb contents | Ag contents | chemical formula |
|---------|-------------|-------------|---|
| 0 | 0 | 1 | Cs2AgIne ozeBie 100Cle |
| 0.05 | 0.05 | 0.95 | Cs2Rb0.05Ag0.05In0.875Bi0.125Cl6 |
| 0.1 | 0.1 | 0.9 | $Cs_2Rb_{0.1}Ag_{0.9}In_{0.875}Bi_{0.125}Cl_6$ |
| 0.15 | 0.15 | 0.85 | Cs ₂ Rb _{0.15} Ag _{0.85} In _{0.875} Bi _{0.125} Cl ₆ |
| 0.2 | 0.2 | 0.8 | Cs2Rb0.2Ag0.8In0.875Bi0.125Cl6 |
| 0.25 | 0.25 | 0.75 | Cs2Rb0.25Ag0.75In0.875Bi0.125Cl6 |
| 0.3 | 0.3 | 0.7 | $Cs_2Rb_{0.3}Ag_{0.7}In_{0.875}Bi_{0.125}Cl_6$ |
| 0.4 | 0.4 | 0.6 | $Cs_2Rb_{0.4}Ag_{0.6}In_{0.875}Bi_{0.125}Cl_6$ |
| 0.6 | 0.6 | 0.4 | $Cs_2Rb_{0.6}Ag_{0.4}In_{0.875}Bi_{0.125}Cl_6$ |
| 0.8 | 0.8 | 0.2 | $Cs_2Rb_{0.8}Ag_{0.2}In_{0.875}Bi_{0.125}Cl_6$ |
| 1 | 1 | 0 | $Cs_2RbIn_{0.875}Bi_{0.125}Cl_6$ |

Table S1 The contents of Rb for the samples

*Each sample was intended to yield 1 mmol of product.



Fig S1 XRD image of $Cs_2Rb_xAg_{1-x}In_{0.875}Bi_{0.125}Cl_6$ (x=0, 0.2, 0.4, 0.6, 0.8, 1).



Fig S2 The EDS spectra of $Cs_2Rb_{0.2}Ag_{0.8}In_{0.875}Bi_{0.125}Cl_{6.}$



Fig S3 The XPS spectra of $Cs_2Rb_{0.2}Ag_{0.8}In_{0.875}Bi_{0.125}Cl_6$

Table S1 Summary of the EDS analysis of $Cs_2Rb_{0.2}Ag_{0.8}In_{0.875}Bi_{0.125}Cl_{6.}$

| Element | Wt% | At% |
|---------|------------|-------|
| RbL | 02.74 | 02.34 |
| BiM | 05.04 | 01.76 |
| CIK | 28.27 | 58.26 |
| AgL | 10.27 | 06.96 |
| InL | 13.55 | 08.62 |
| CsL | 40.13 | 22.06 |
| Matrix | Correction | ZAF |



Fig S4 TEM image of Cs₂Rb_{0.2}Ag_{0.8}In_{0.875}Bi_{0.125}Cl₆, from which a microcrystalline structure can be analyzed.



Fig S5 The emission spectra of Cs₂Rb_xAg_{1-x} In_{0.875}Bi_{0.125}Cl₆ (x=0, 0.2, 0.4, 0.6, 0.8, 1).



Fig S6 PL for calculation for PLQY ($Cs_2Rb_xAg_{1-x}In_{0.875}Bi_{0.125}Cl_6$, x = 0.15). The red and blue curve represent for the PL background (measured without samples in), and the black curve represent PL for sample.

According to protocol,

$$PLQY = \frac{E_B - E_A}{S_A - S_B}$$

 S_A is the blank spectrum when the vessel is filled Teflon instead of the sample. S_B is the is the peak signal of the remaining excitation source after the sample placed. E_A is the fluorescence background baseline and E_B is emission signal of the sample.



Fig S7 PL for $Cs_2Rb_{0.15}Ag_{0.85}In_{0.875}Bi_{0.125}Cl_6$ under different temperature.



Fig S8 PL spectra for $Cs_2Rb_{0.15}Ag_{0.85}In_{0.875}Bi_{0.125}Cl_6$ after being soaked in ethanol.