Supporting Information for

One-dimensional lead-free halide with near-unity greenish-yellow light emission

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Table S1. Comparison of photoluminescence quantum efficiency (PLQY) values of the greenish-yellow luminescence of halide perovskites and relevant materials.

Materials	Electronic dimension	Emission peak [nm]	PLQY [%]	Pros and cons	Ref.
$(KC)_2MnCl_4$	0D	518	7.79	Weak PL	1
$(C_9NH_{20})_6Pb_3Br_{12}$	0D	522	12	toxic	2
$[Bzmim]_3SbCl_6$	0D	525	87.5	toxic	3
$C_3Bi_2I_9$	0D	545	0.018	Weak PL	4
$[KC_2]_2[Cu_4I_6]$	1D	540	97.8	stable, nontoxic	this work

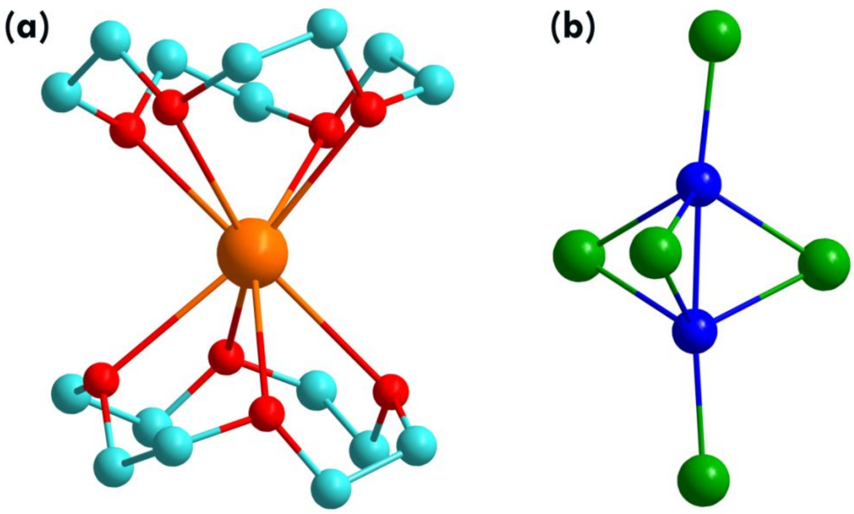

Figure S1. Crystal structure of $[(12\text{-crown-}4)_2K]^+$ ions and two adjacent inorganic CuI_4 units. (orange: potassium atoms; green: iodine atoms; blue: copper atoms; red: oxygen; aqua: carbon atoms; hydrogen atoms were hidden for clarity).

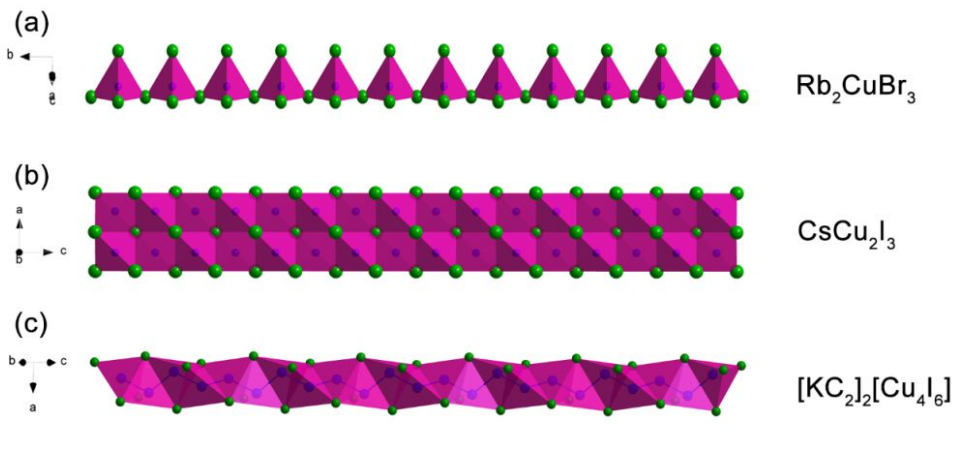

Figure S2. individual copper iodide chain in the different 1D copper(I)-based halides. The green spheres are halide atoms (bromine in Rb_2CuBr_3, iodine in $CsCu_2I_3$ and $[KC_2]_2[Cu_4I_6]$), and the blue spheres are cooper atoms.

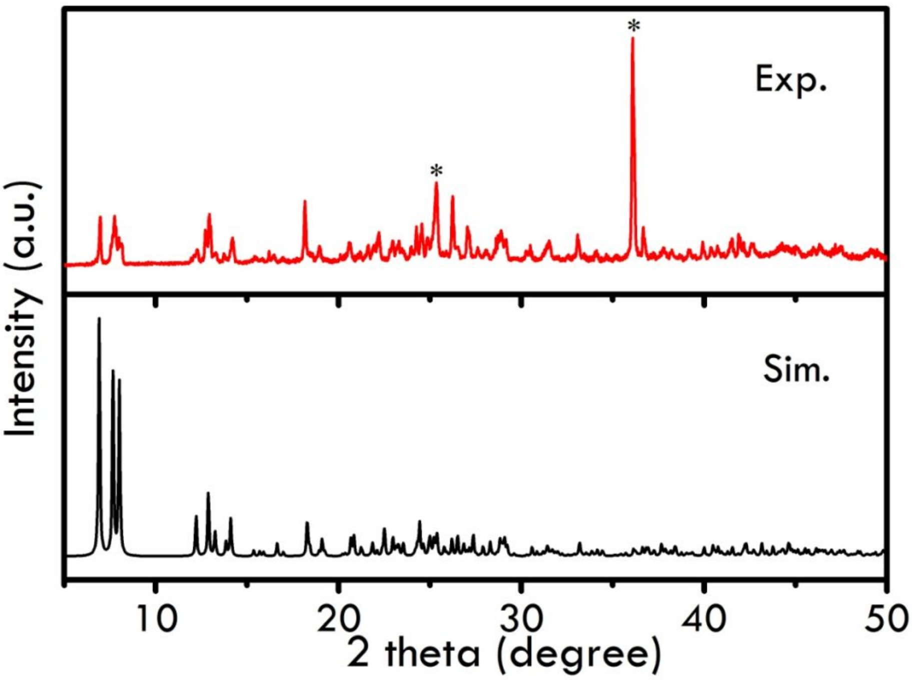

Figure S3. PXRD pattern of $[KC_2]_2[Cu_4I_6]$ as well as the simulated results. The marked peaks are attributed to potassium iodide.

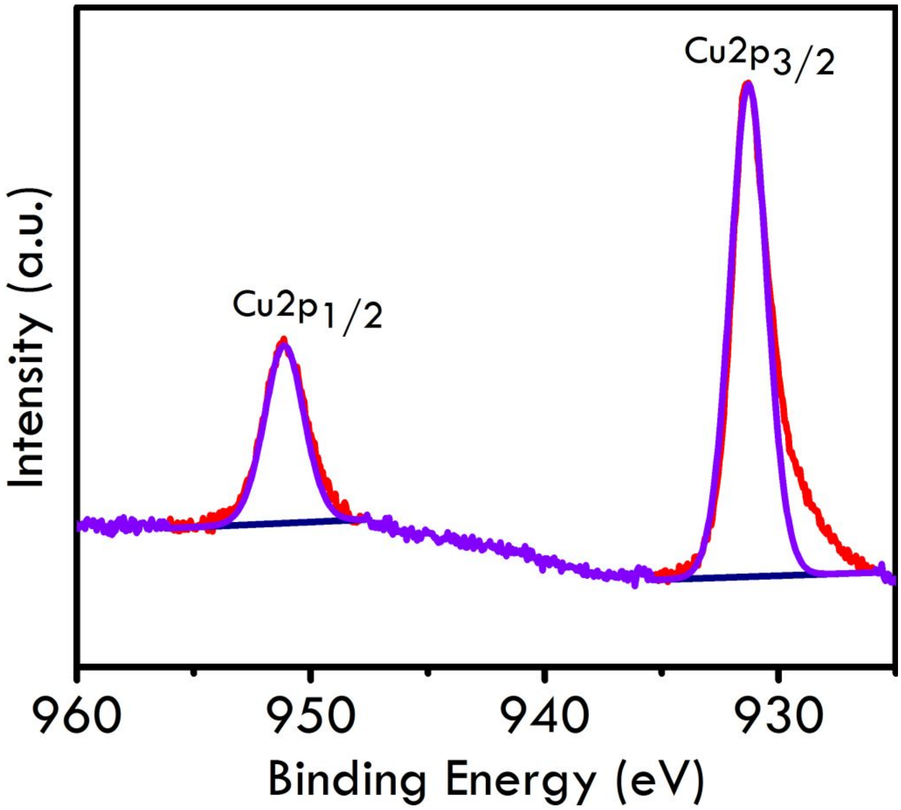

Figure S4. XPS analysis of $[(12\text{-crown-}4)_2K]_2[Cu_4I_6]$.

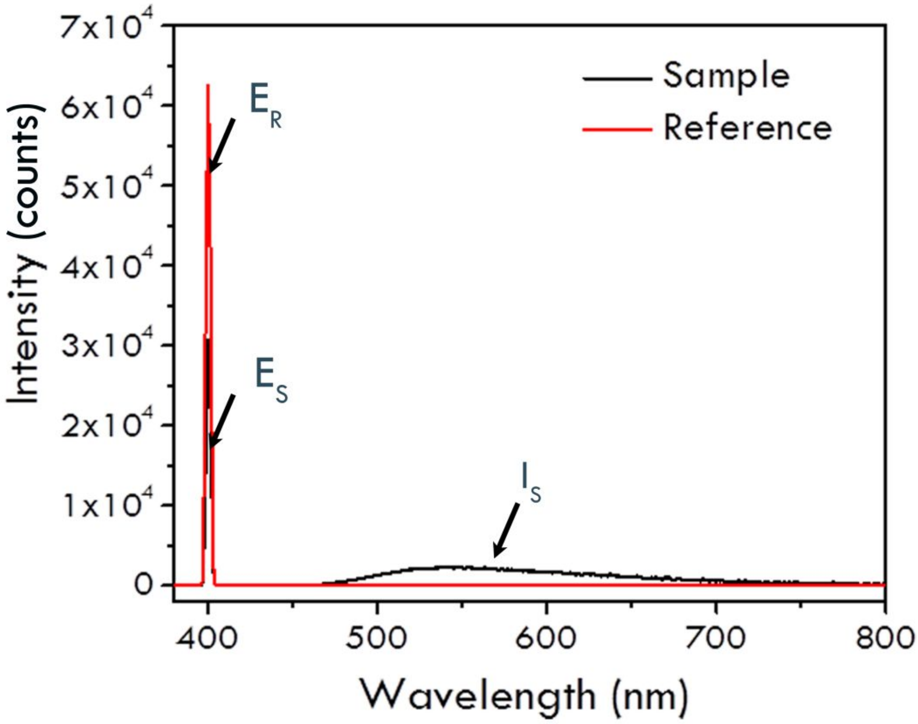

Figure S5. Excitation line of reference (400 nm) and emission spectrum of bulk crystals collected by an integrating sphere system. The PLQY was calculated based on the equation: $\eta_{QE} = I_S/(E_R - E_S)$, which I_S represents the luminescence emission spectrum of the sample, E_R is the spectrum of the excitation light from the empty integrated sphere (without the sample), and E_S is the excitation spectrum for exciting the sample. Control samples, $BaMgAl_{10}O_{17}:Eu^{2+}$ and $[K(18\text{-crown-}6)]_2SbCl_5$, were measured using this method to give PLQE of 93% and 54% , respectively, which are close to the literature reported values.[5]

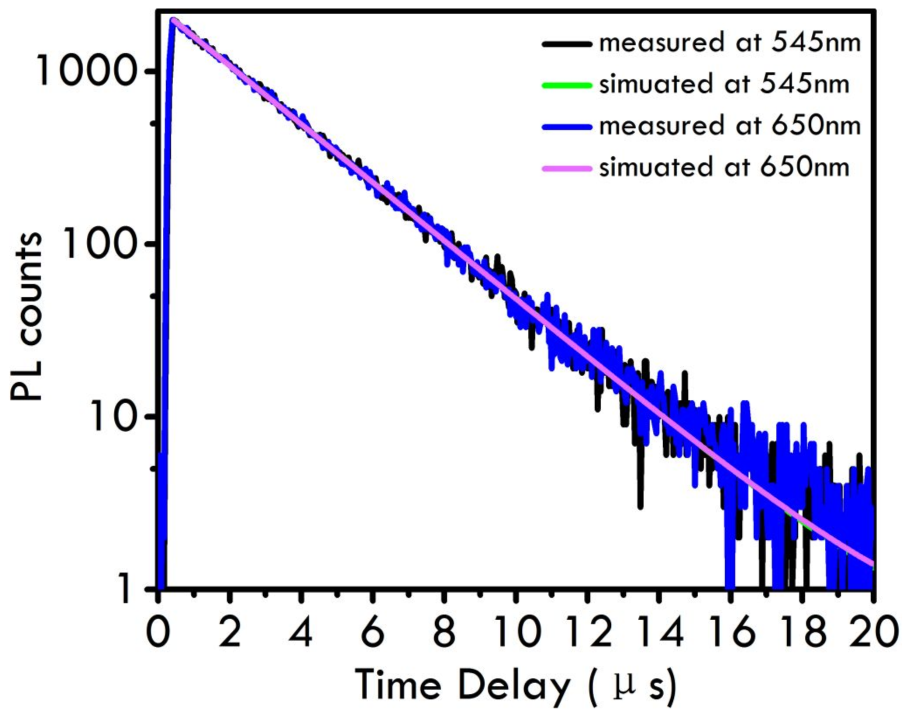

Figure S6. Time-resolved photoluminescence decay of $[KC_2]_2[Cu_4I_6]$ monitored at 545 nm and 650 nm.

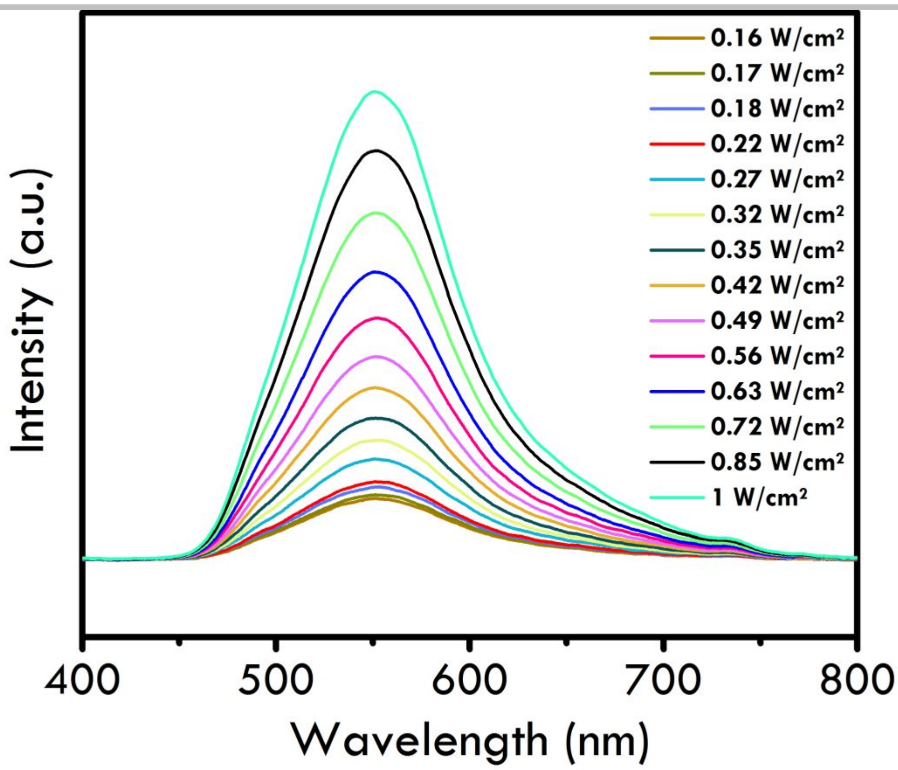

Figure S7. Emission spectra at different excitation powers.

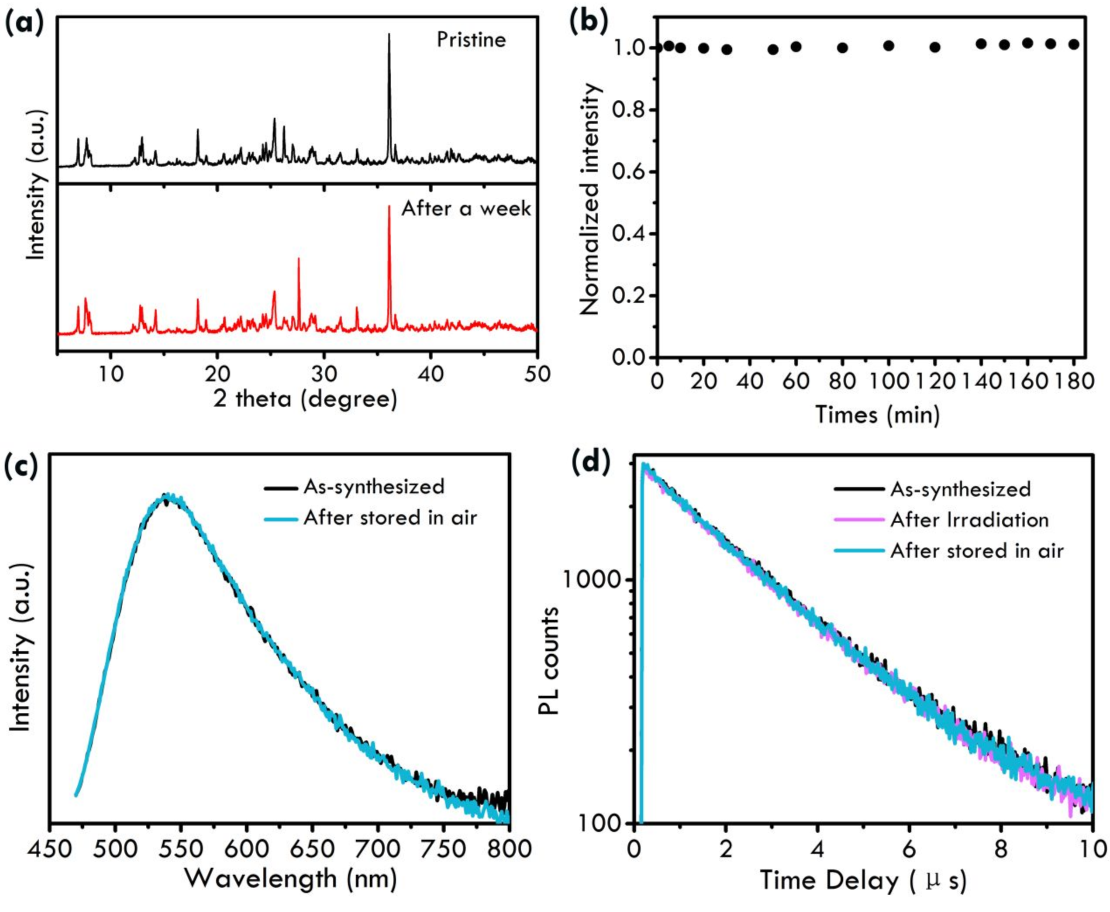

Figure S8. (a) The structural stability of $[KC_2]_2[Cu_4I_6]$. (b) The photostability of $[KC_2]_2[Cu_4I_6]$ of different irradiation time with a 350W xenon lamp. (c) Emission spectra of pristine sample and sample stored in air for a week. (d) PL lifetime of pristine sample, sample radiated for 3 hours and sample stored in air for a week sample monitored at 545 nm.

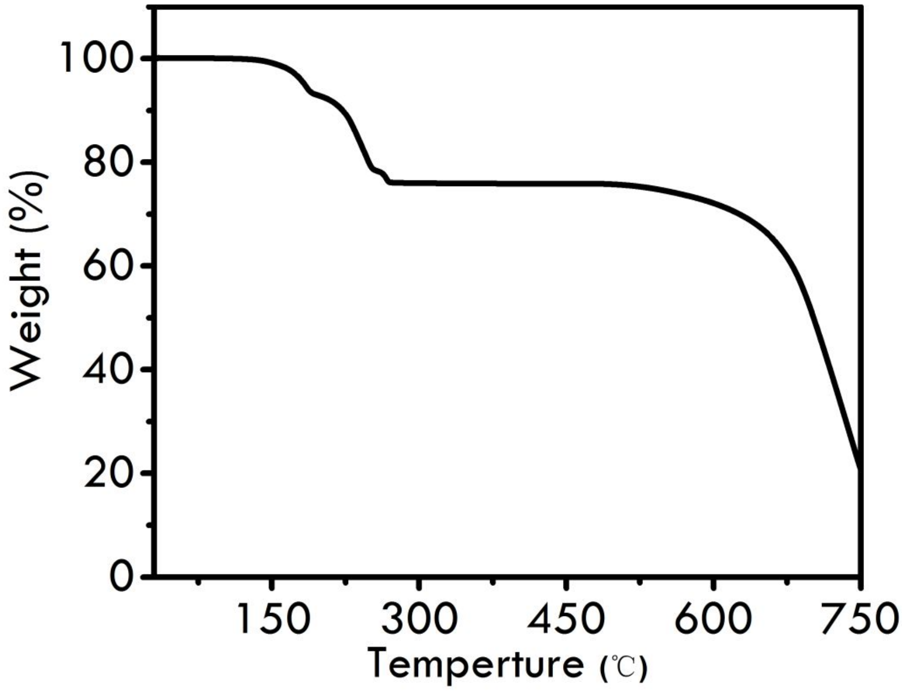

Figure S9. Thermogravimetric analysis (TGA) of $[KC_2]_2[Cu_4I_6]$. The sample begins to decompose at about 140 °C.

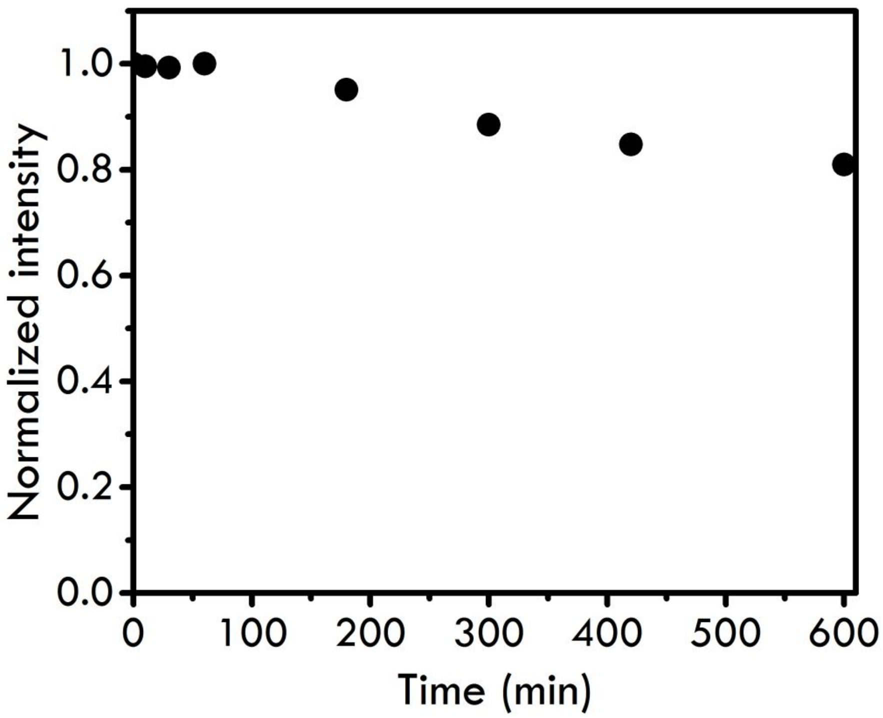

Figure S10. PL spectra of the WLED measured at different working time.

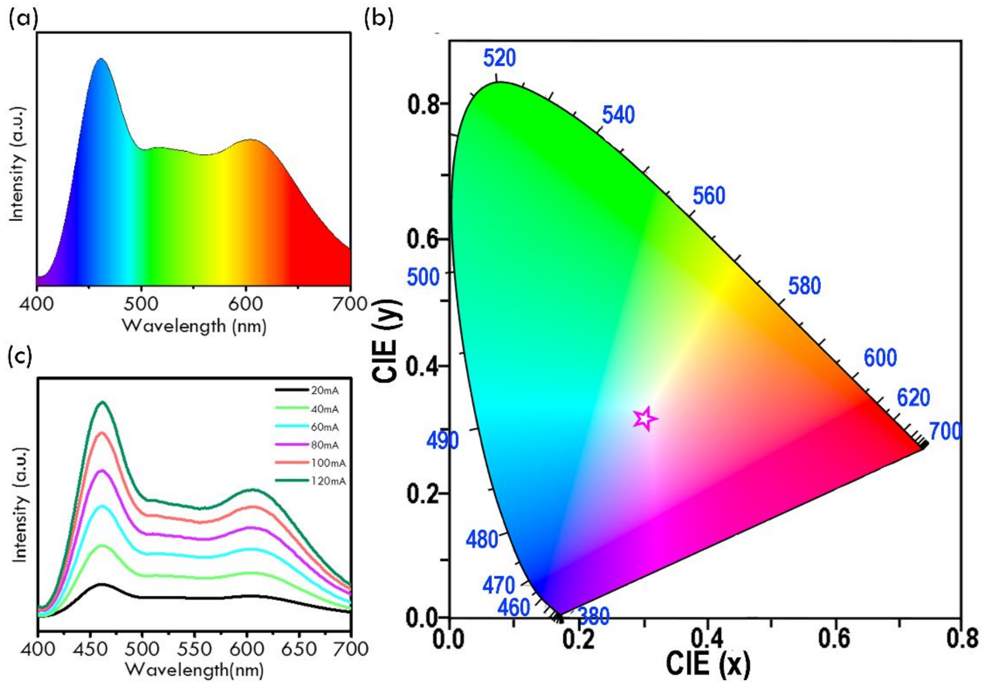

Figure S11. (a) Luminescence spectra from $[KC_2]_2[Cu_4I_6]$-based white light-emitting diodes (LEDs) excited with a 450 nm blue chip. (b) CIE coordinates corresponding to white-LED device (pink star). (c) The emission spectra of white-LED device at different driving currents.

References

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