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Electronic Supplementary Information

Enhanced Photoelectric Performance in Cu-Bi Double Halide Perovskite Single Crystals

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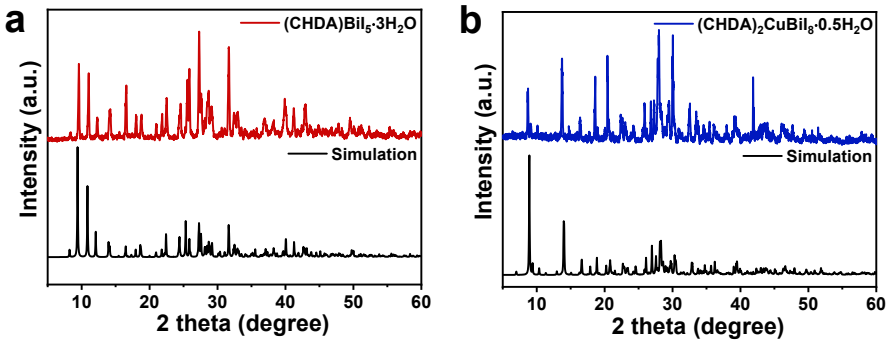

Fig. S1 Powder XRD patterns of a) $(CHDA)BiI_5 \cdot 3H_2O$ and b) $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$ powders, respectively.

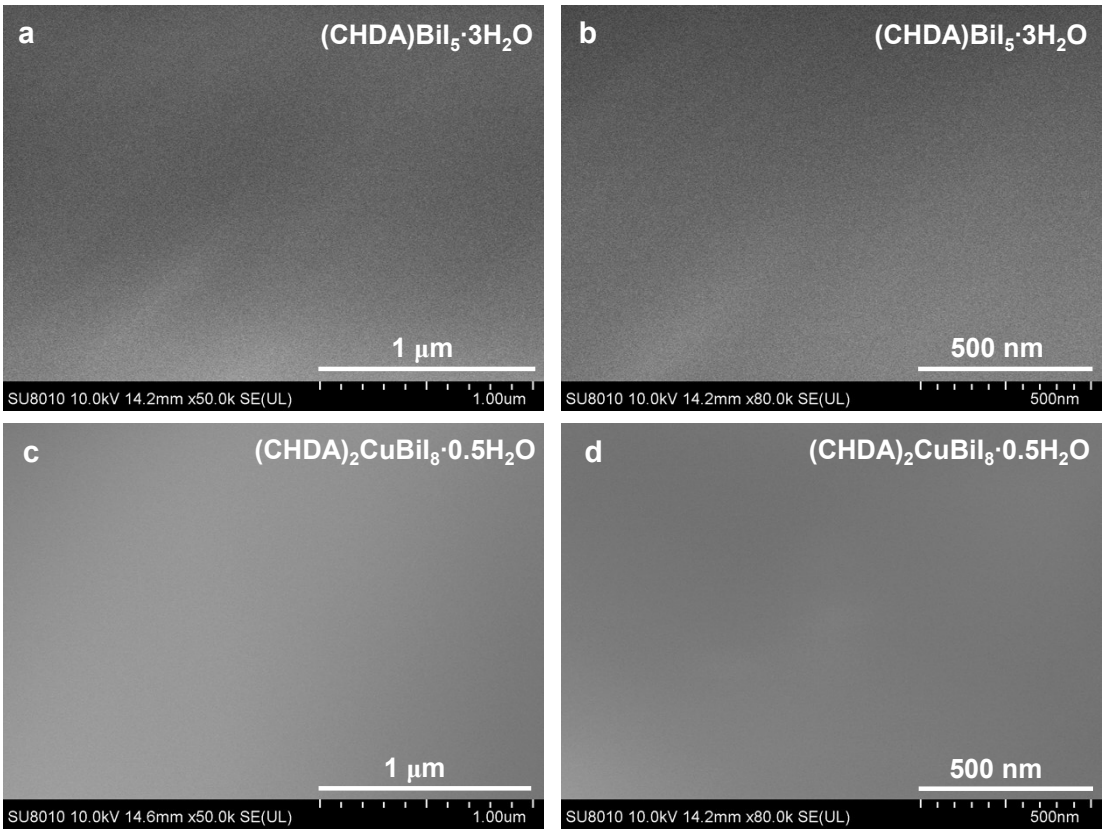

Fig. S2 SEM images of a, b) $(CHDA)BiI_5 \cdot 3H_2O$ and c, d) $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$ SCs, respectively.

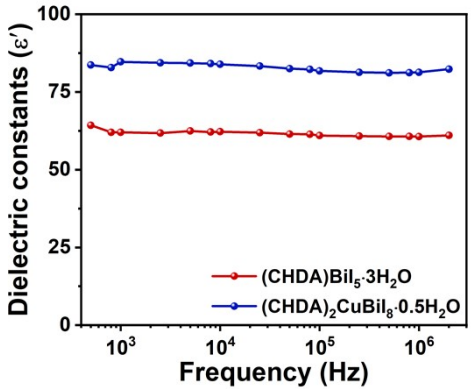

Fig. S3 The frequency dependent dielectric curves of the $(CHDA)BiI_5{\cdot}3H_2O$ and $(CHDA)_2CuBiI_8{\cdot}0.5H_2O$ SCs. It should be pointed out that the devices used to measure the relative dielectric constant adopts a parallel structure, as same as that in subsequent photodetectors. The calculation method is proposed in the references reported, previously.[1-3]

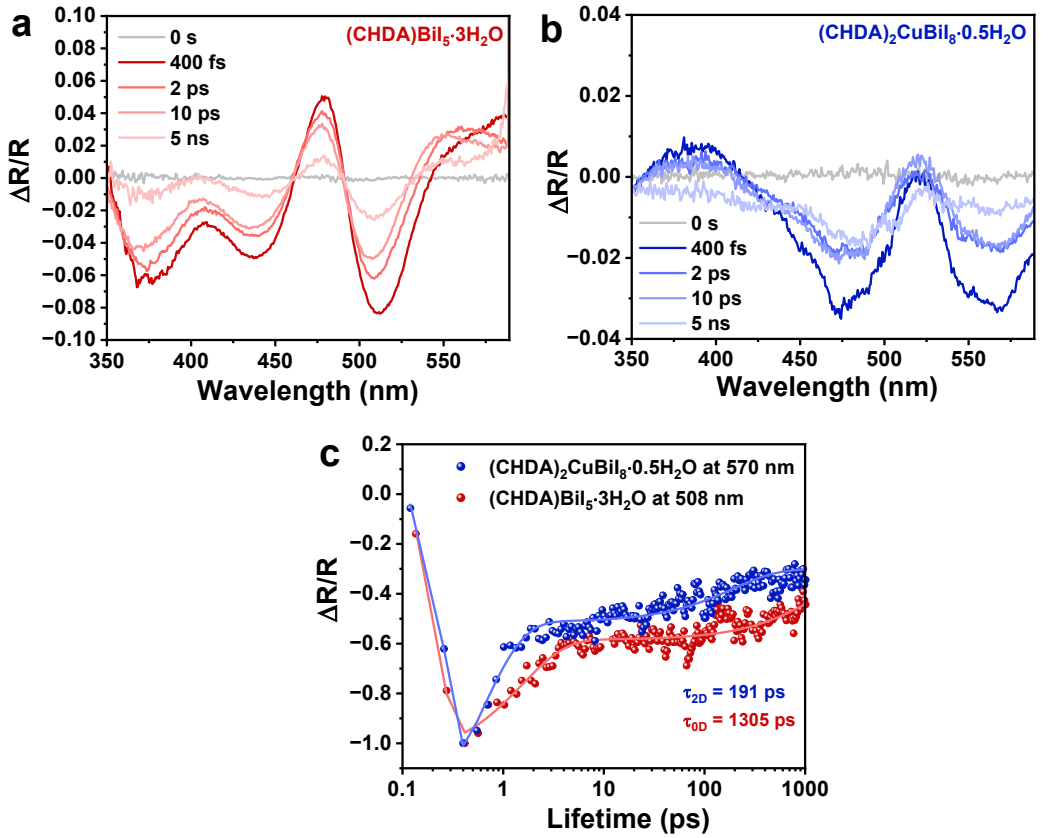

Fig. S4 The TR spectra of a) the $(CHDA)BiI_5{\cdot}3H_2O$ and b) $(CHDA)_2CuBiI_8{\cdot}0.5H_2O$ SCs. c) TR kinetic fit of $(CHDA)BiI_5{\cdot}3H_2O$ and $(CHDA)_2CuBiI_8{\cdot}0.5H_2O$ SCs recorded at 508 and 570 nm, respectively.

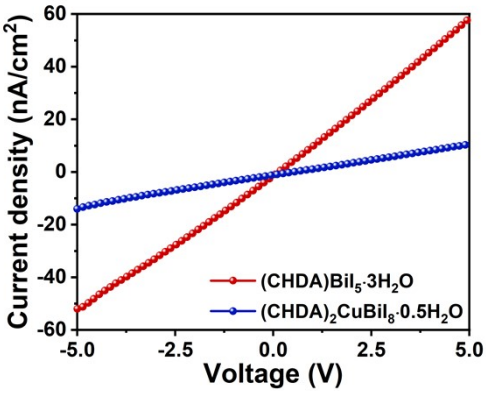

Fig. S5 *i-v* curves of the (CHDA)BiI_5·$3H_2O$ and $(CHDA)_2CuBiI_8$·$0.5H_2O$ SC photodetectors measured in the dark.

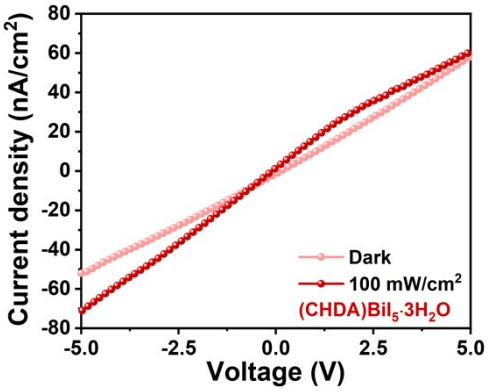

Fig. S6 *i-v* curves of the (CHDA)BiI_5·$3H_2O$ SC photodetector measured in the dark and under white LED illumination with 100 mW cm^{-2}.

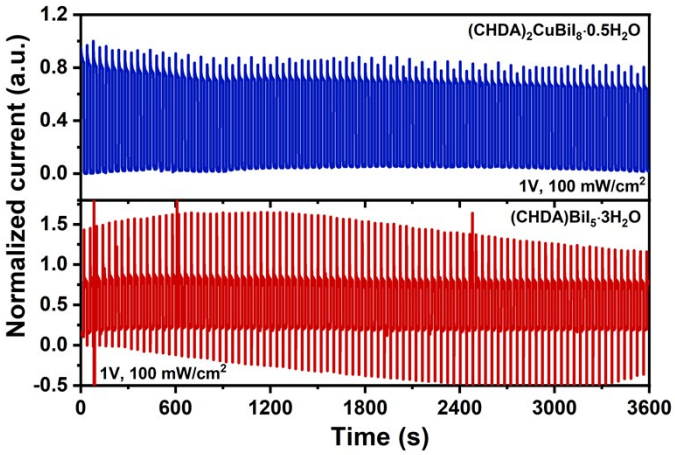

Fig. S7 The on/off switching cycles of the photocurrent of the unencapsulated $(CHDA)BiI_5 \cdot 3H_2O$ and $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$ SC photodetectors, during 60 min continuous operation under chopped white LED illumination (20 s on, 20 s off) with 100 mW cm^{-2} at 1 V.

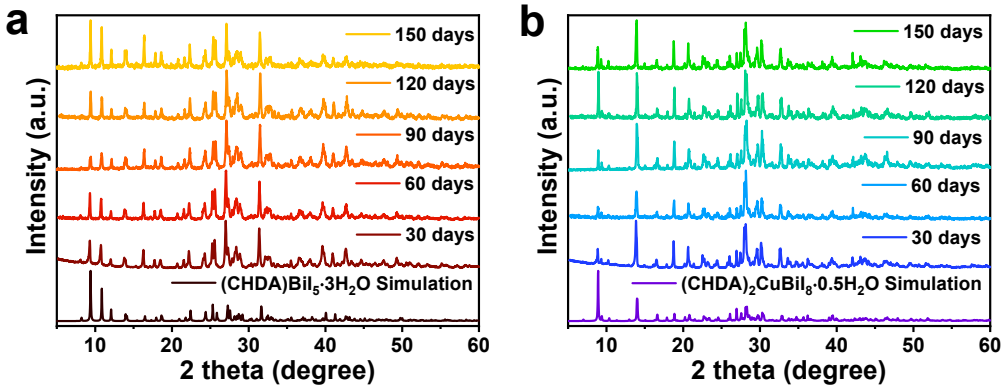

Fig. S8 XRD stability tests of a) $(CHDA)BiI_5 \cdot 3H_2O$ and b) $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$ powders, stored in ambient air at a humidity of ~70%RH.

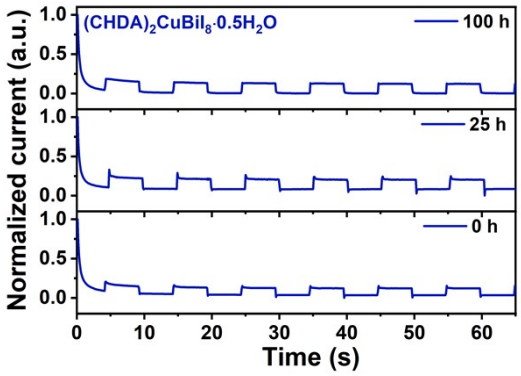

Fig. S9 Photoresponse of the unencapsulated $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$ SC device was measured for 100 h of exposure time in ambient air with humidity at ~70% RH.

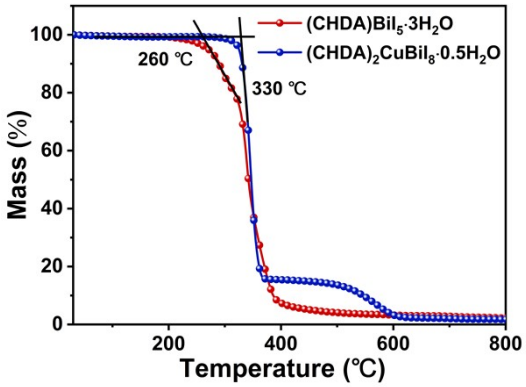

Fig. S10 TGA curves of $(CHDA)BiI_5 \cdot 3H_2O$ and $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$.

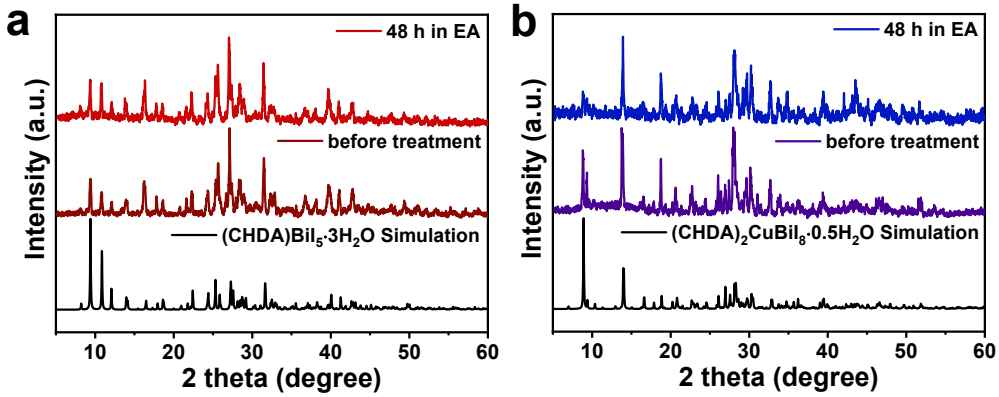

Fig. S11 a, b) the corresponding XRD patterns of two perovskite powders before and after soaking in EA.

Table S1. Concentration table of each raw materials in the synthesis process.

Product	CHDA	BiI_3	CuI
$(CHDA)BiI_5 \cdot 3H_2O$	0.06 mol L^{-1}	0.06 mol L^{-1}	--
$(CHDA)_2CuBiI_8 \cdot 0.5H_2O$	0.18 mol L^{-1}	0.06 mol L^{-1}	0.12 mol L^{-1}

Table S2. Crystallographic data of the $(CHDA)BiI_5 \cdot 3H_2O$ and $(CHDA)_2CuBiI_8 \cdot 0.5H_2O$.

Empirical formula	$C_6H_{16}N_2BiI_5 \cdot 3H_2O$	$(C_6H_{16}N_2)_2CuBiI_8 \cdot 0.5H_2O$
Formula weight (g/mol)	1013.73	1529.14
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	11.5808(8)	17.062(6)
b/Å	12.5195(8)	19.825(7)
c/Å	15.3418(9)	18.808(7)
α/°	90	90
β/°	111.928(3)	90.297(5)
γ/°	90	90
Volume/Å^3	2063.4(2)	6362(4)
Z	4	8
ρ_{calc} (g/cm^3)	3.263	3.193
Goodness-of-fit on F^2	1.056	1.026

References

1 H. N. Al-Shareef, D. Dimos, M. V. Raymond, R.W. Schwartz, C. H. Mueller, *J. Electroceram.* **1997**, *1*, 145-153.

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3 H. Liu, J. Zhu, D. Xiao, X. Gong, J. Liang, X. Li, X. Zhu, *Appl. Phys. Lett*. **2007**, *91*, 182907.