

Promoting solution-processed CdTe nanocrystal solar cells by rationally controlled copper doping

Qichuan Huang ^a, Songwei Liu ^a, Chenbo Min ^a, Zheng Zhou ^a, Donghuan Qin ^{*a,c}, Dan Wang ^{a,c}, Wei Xu ^{a,c} and Lintao Hou ^{*b}

^a School of Materials Science and Engineering, South China University of Technology, Guangzhou, 510640, China;

^b Siyuan Laboratory, Guangzhou Key Laboratory of Vacuum Coating Technologies and New Energy Materials, Guangdong Provincial Key Laboratory of Optical Fiber Sensing and Communications, Department of Physics, Jinan University, Guangzhou 510632, China

^c Institute of Polymer Optoelectronic Materials & Devices, State Key Laboratory of Luminescent Materials & Devices, South China University of Technology, Guangzhou 510640, China

* Correspondence: qindh@scut.edu.cn (D.Q.); thlt@jnu.edu.cn (L.H.); Tel.: +86-020-8711-4346 (D.Q.); +86-020-8522-4386 (L.H.)

† These authors contributed equally to this work.

Table S1. The calculated HOMO and LUMO of the doped and undoped Cd₃₃Te₃₃ nanocrystals.

Configurations	HOMO (eV)	LUMO (eV)	HOMO-LUMO gap (eV)
Cd ₃₃ Te ₃₃	-5.21	-3.55	1.67
Cu to Cd	-5.20	-3.54	1.66
Cd ₃₂ CuTe ₃₃	-5.11	-3.51	1.59

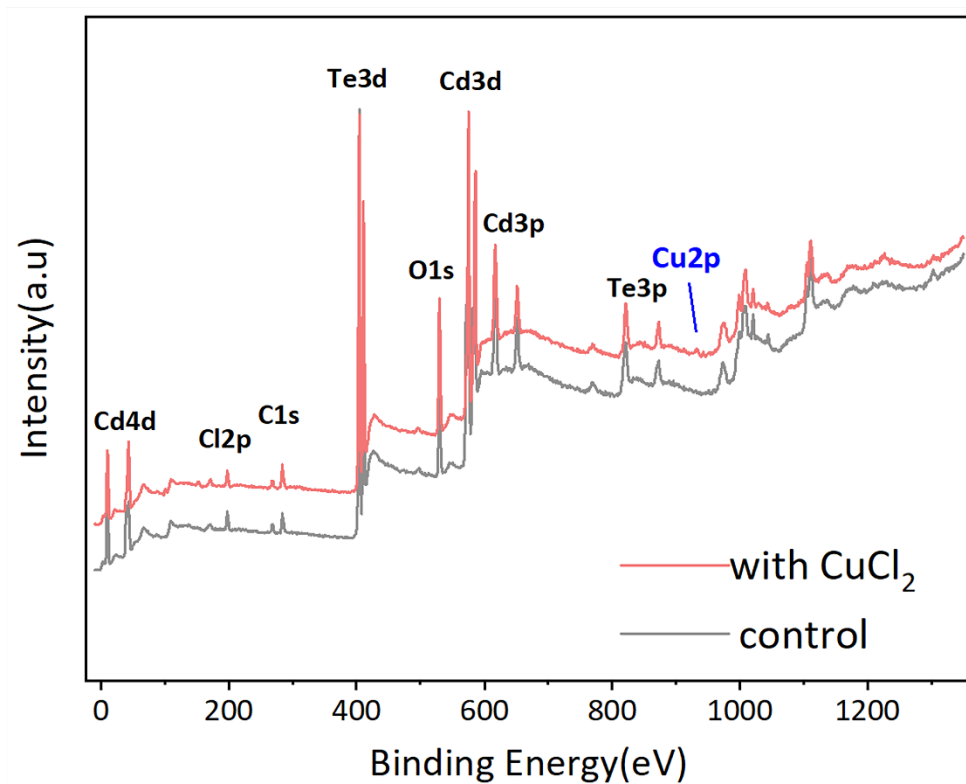


Figure S1. XPS full-scan spectra of CdTe NCs thin film w/ and w/o CuCl₂ doping.

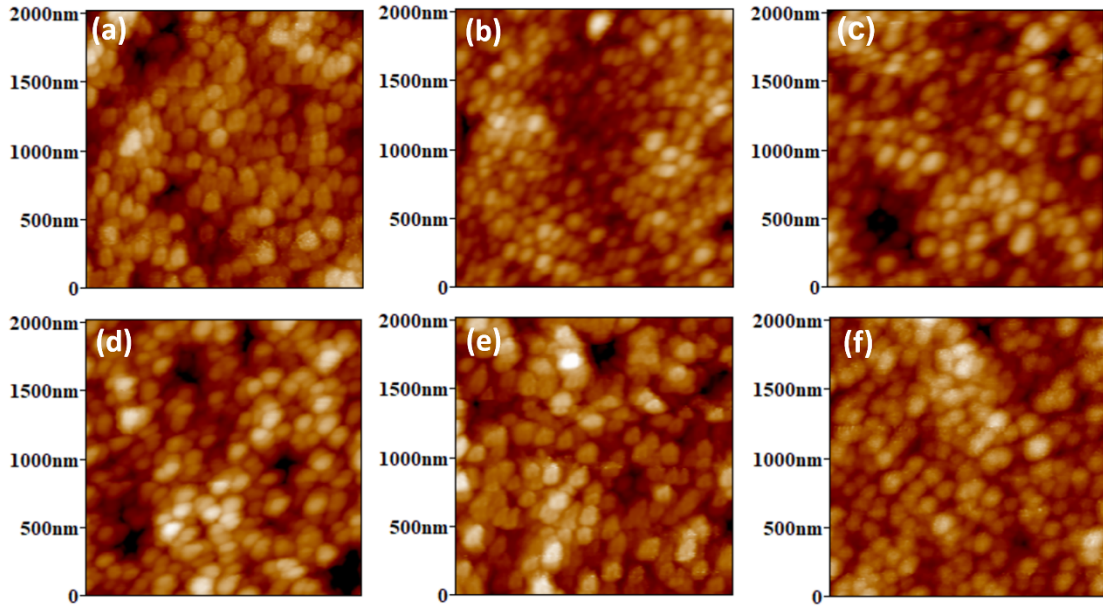


Figure S2. AFM images of CdTe with multiple copper salt doping at different concentration (a) $3\mu\text{g/mL}$ CuBr_2 ; (b) $6\mu\text{g/mL}$ CuBr_2 ; (c) $9\mu\text{g/mL}$ CuBr_2 ; (d) $12\mu\text{g/mL}$ CuBr_2 ; (e) $5\mu\text{g/mL}$ CuSO_4 ; (f) $6\mu\text{g/mL}$ $\text{Cu}(\text{NO}_3)_2$

Table S2. Summarized device performance with copper salt doping at different concentration

Copper salt	concentration	PCE (%)	JSC (mA cm^{-2})	FF (%)	VOC (V)
Control	$0\mu\text{g/mL}$	5.05	19.12	52.82	0.50
CuCl_2	$2\mu\text{g/mL}$	5.88	22.06	45.94	0.58
	$4\mu\text{g/mL}$	6.30	20.20	53.74	0.58
	$6\mu\text{g/mL}$	6.06	22.80	46.65	0.57
	$8\mu\text{g/mL}$	5.58	20.16	51.21	0.54
	$10\mu\text{g/mL}$	4.91	16.53	57.18	0.52
	1mg/mL	3.89	15.47	47.47	0.53
CuBr_2	$3\mu\text{g/mL}$	5.56	20.80	51.47	0.52
	$6\mu\text{g/mL}$	6.13	21.34	49.49	0.58
	$9\mu\text{g/mL}$	5.55	15.40	59.07	0.61
	$12\mu\text{g/mL}$	5.17	17.93	52.43	0.55
CuSO_4	$5\mu\text{g/mL}$	5.63	20.46	50.96	0.54
$\text{Cu}(\text{NO}_3)_2$	$6\mu\text{g/mL}$	5.85	17.85	54.62	0.60

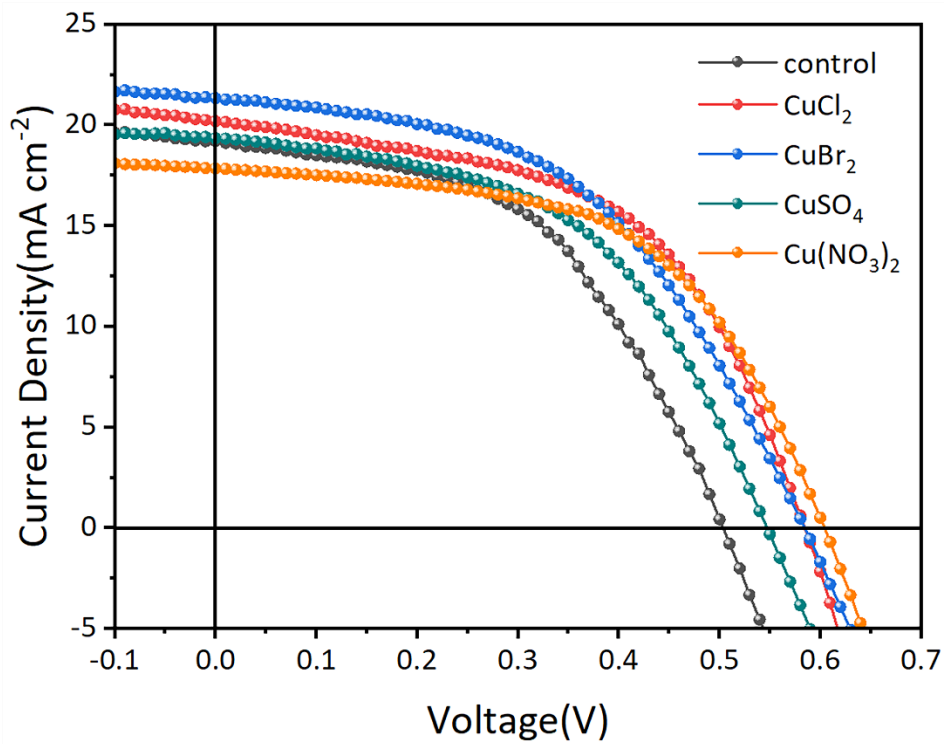


Figure S3. *J-V* characteristics of CdTe NCs solar cells with different copper salt doping

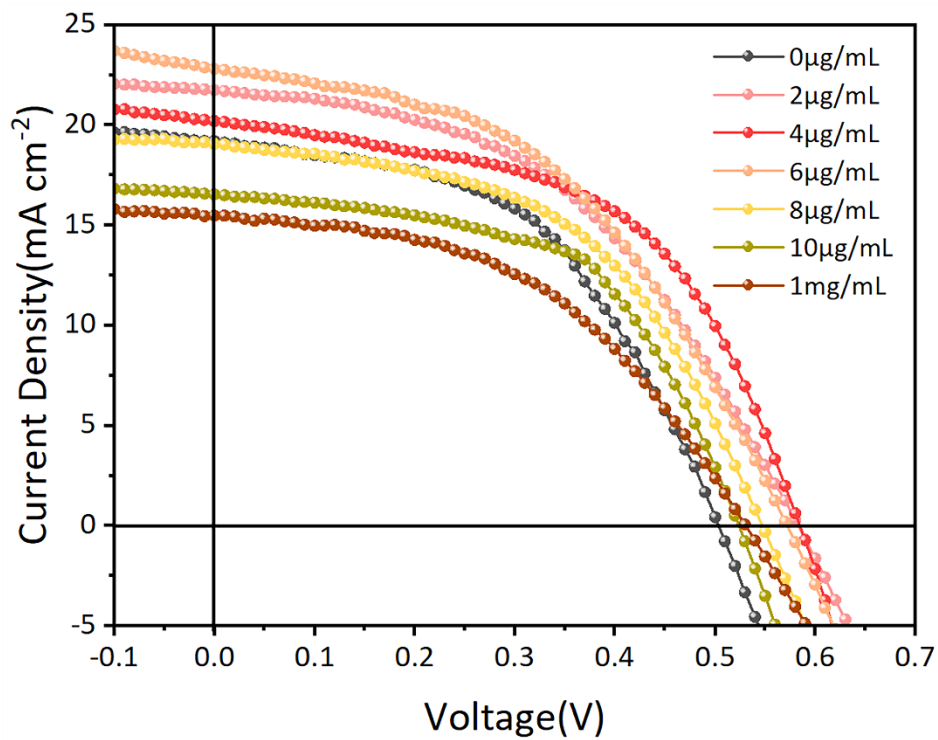


Figure S4. *J-V* characteristics of CdTe NCs solar cells with CuCl_2 doping at different concentration.

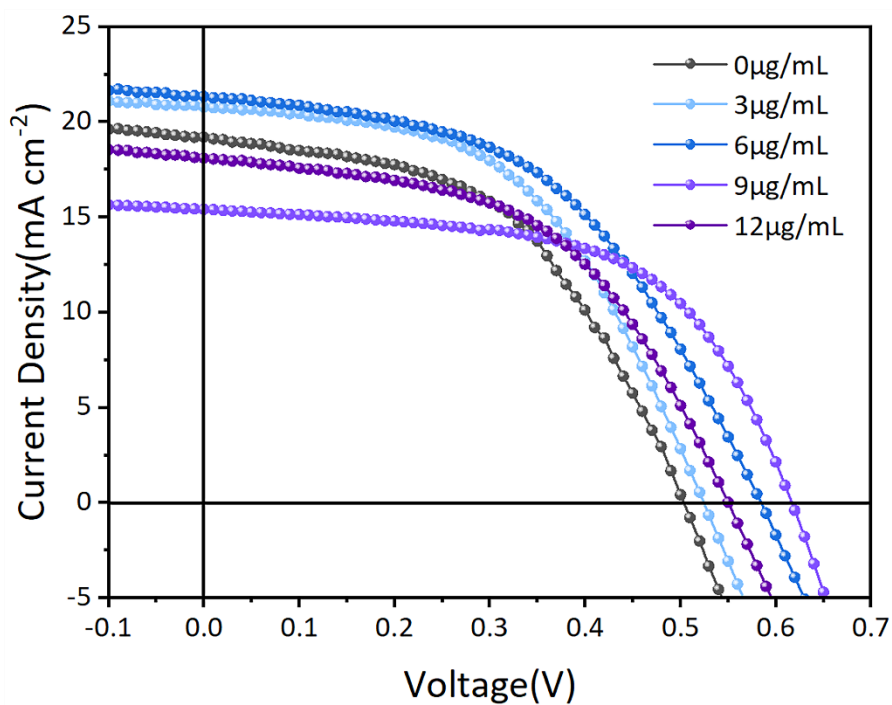


Figure S5. J - V characteristics of CdTe NCs solar cells with CuBr_2 doping at different concentration.

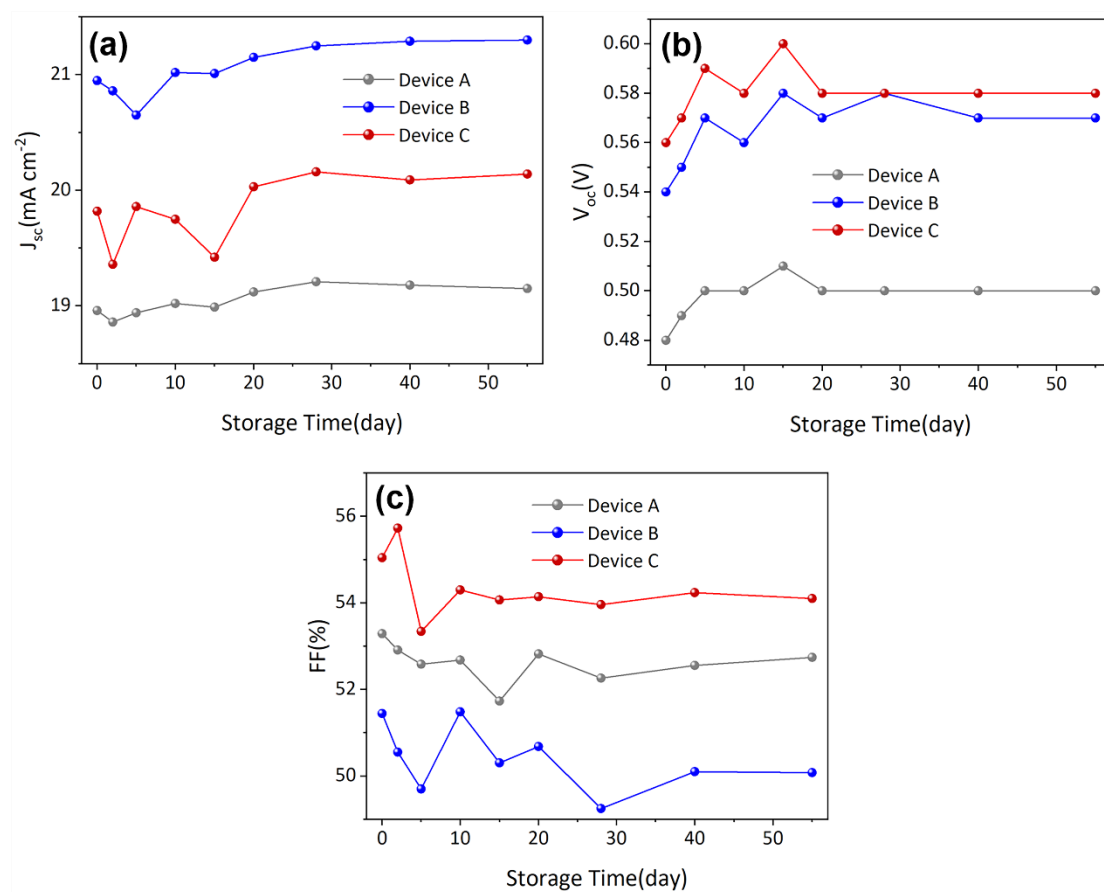


Figure S6. Stability of a) J_{sc} , b) V_{oc} and c) FF of CdTe NCs solar cells (Device A: control; Device B: with CuBr_2 doping; Device C: with CuCl_2 doping).

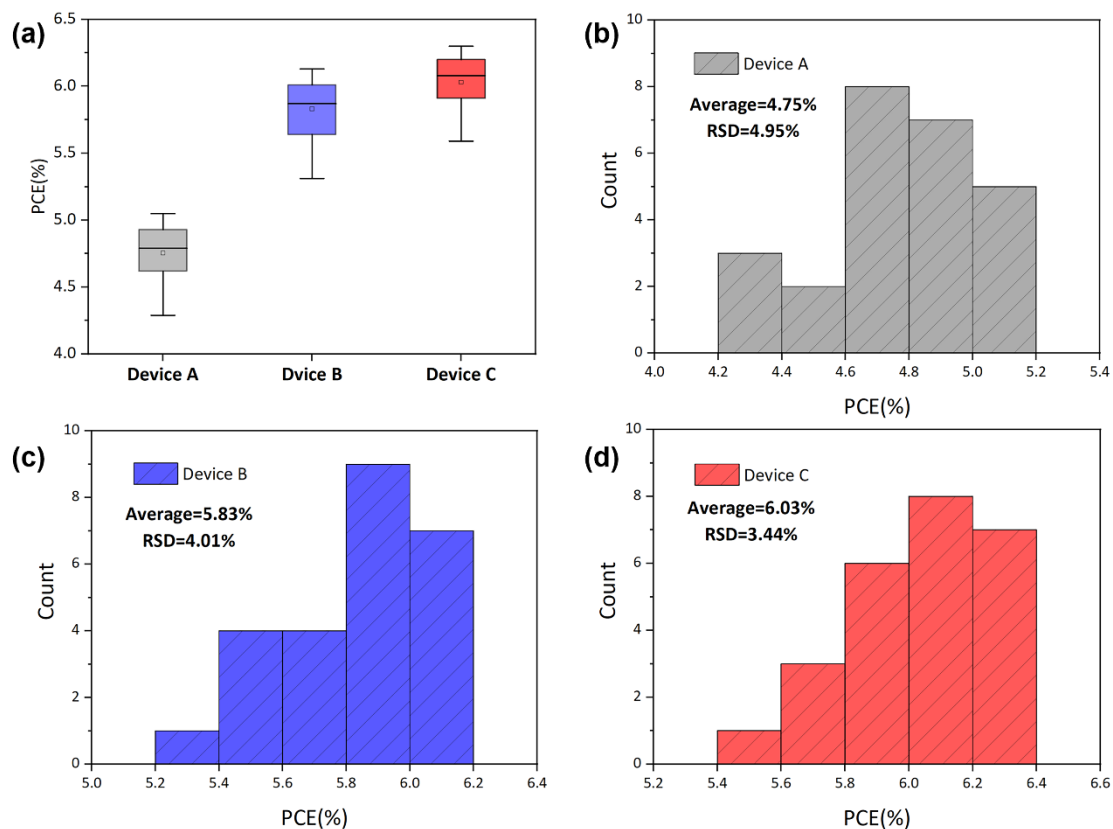


Figure S7. Statistical characterization: (a) Box diagram of repeatable device PCE; (b)~(d) PCE of distribution histogram of CdTe NCs solar cells (Device A: control; Device B: with CuBr₂ doping; Device C: with CuCl₂ doping; count of each device is 25).