

## Supporting Information

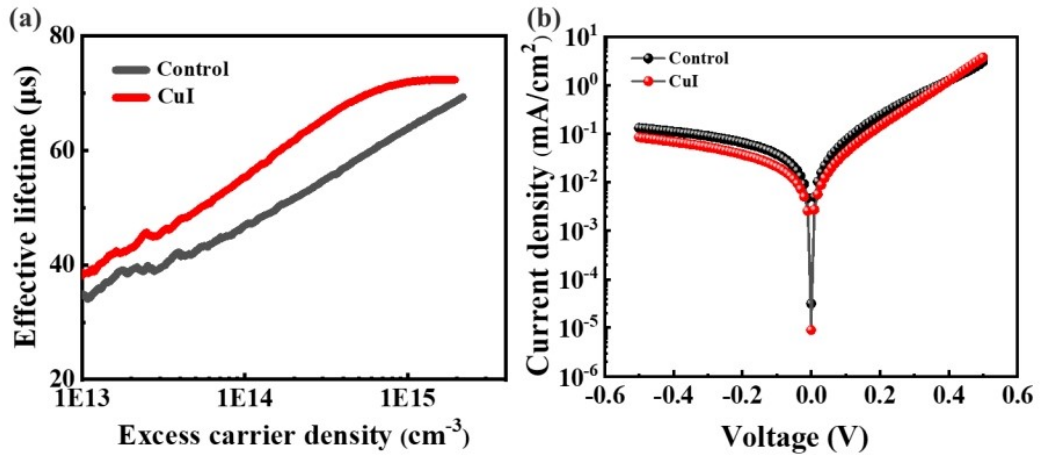
### **Solution-Processed Copper (I) Iodide via Co-Doping for Enhanced Hole Selective Contacts in P-Type Crystalline Silicon Solar Cells**

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Lingbo Xu<sup>1</sup>, Ping Lin<sup>1</sup>, Can Cui<sup>1\*</sup>, Xuegong Yu<sup>2</sup>, Peng Wang<sup>1\*</sup>

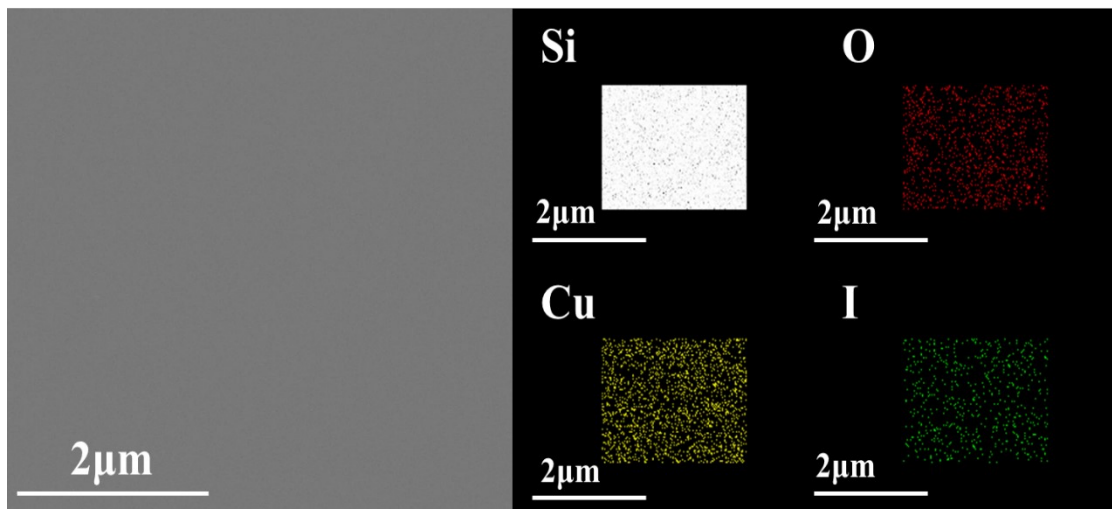
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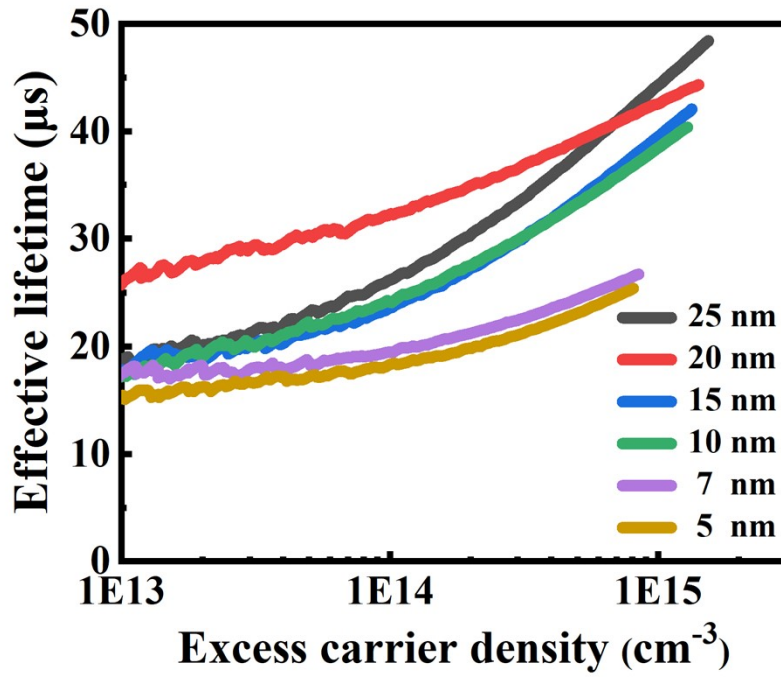
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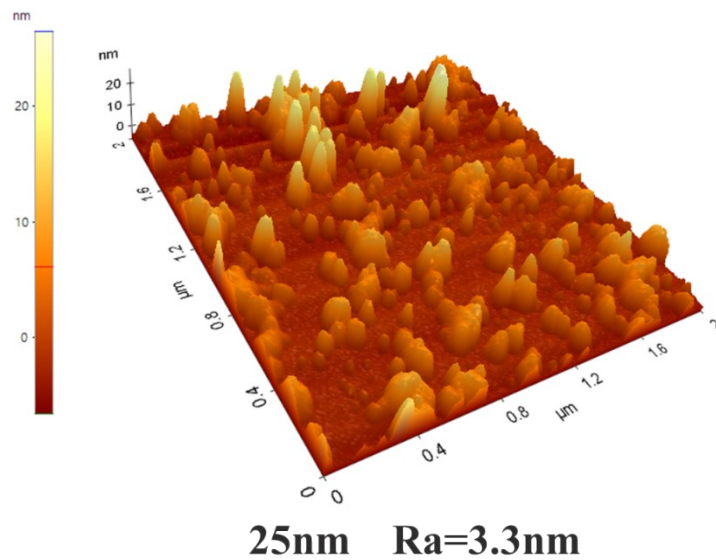
**Figure S1.** (a) Effective carrier lifetime of p-Si wafers without (the control) and with CuI films. (b) Dark J-V curves of the control and CuI/p-Si heterojunction solar cell devices.



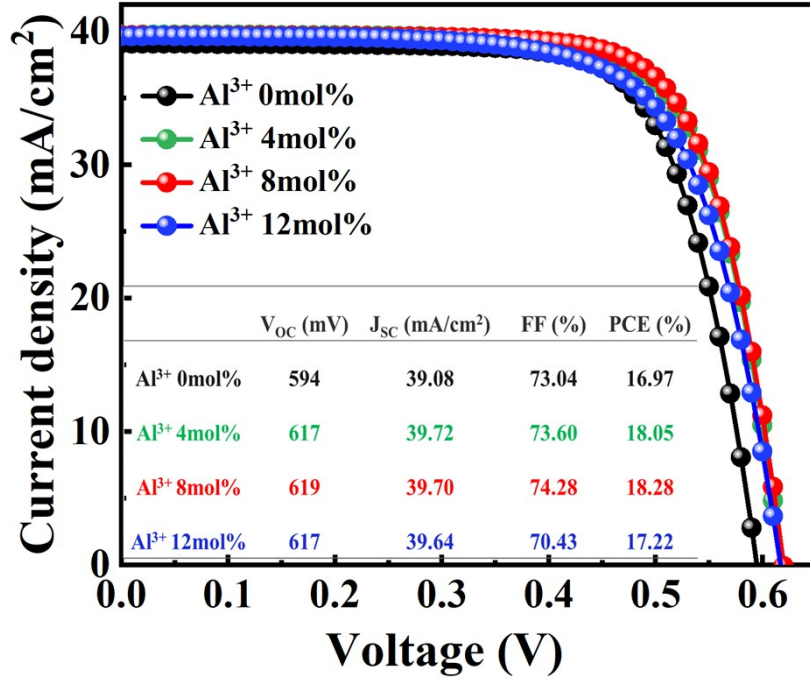
**Figure S2.** SEM image and element distribution of  $\text{I}_2:\text{CuI}$  film.



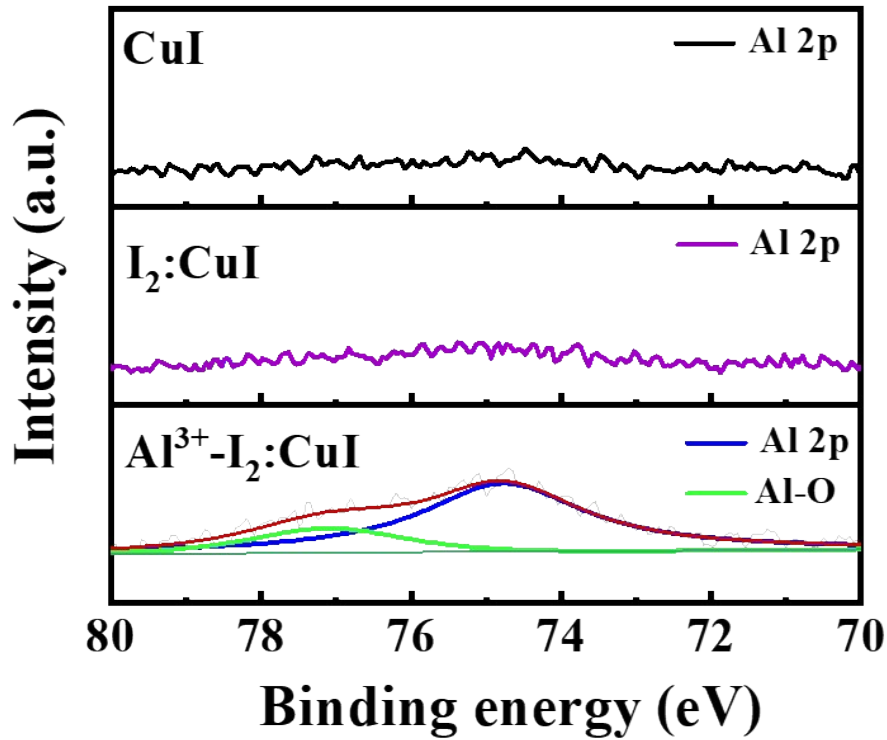
**Figure S3.** Effective carrier lifetime of p-Si wafers coated by I<sub>2</sub>:CuI films with different thickness.



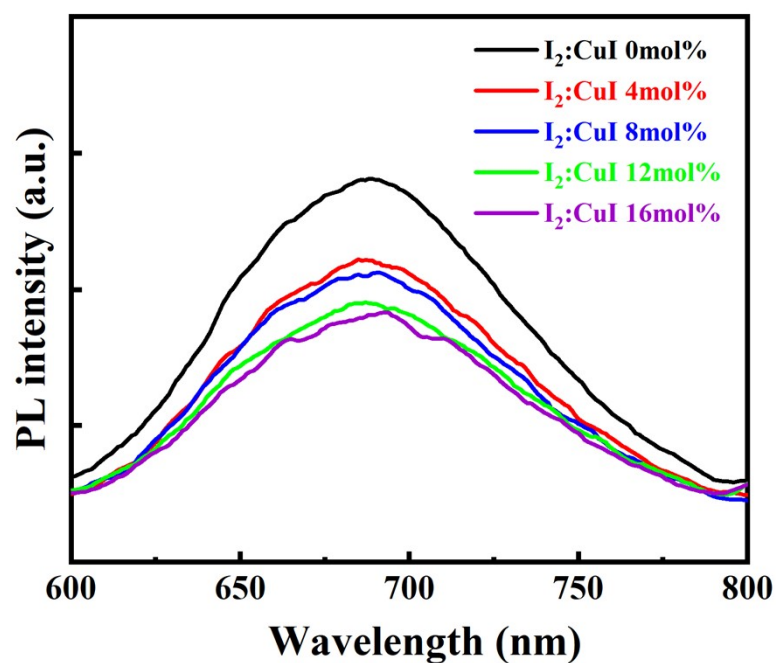
**Figure S4.** AFM image of I<sub>2</sub>:CuI film with the thickness of 25 nm.



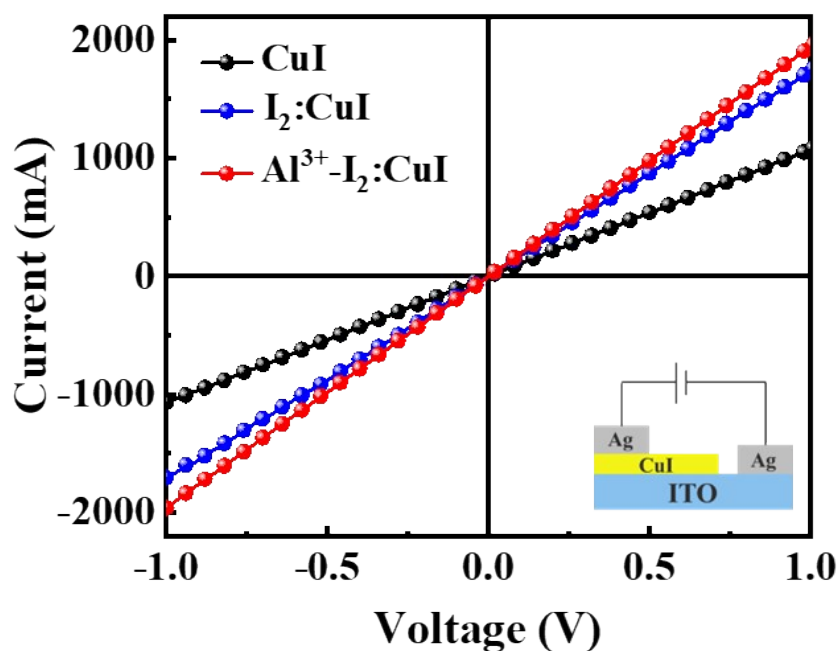
**Figure S5.** Illuminated J-V curves of  $Al^{3+}$ - $I_2$ :CuI/p-Si heterojunction solar cell devices with different  $Al^{3+}$  doping concentrations.



**Figure S6.** Al 2p XPS spectra of pristine CuI,  $I_2$ :CuI and  $Al^{3+}$ - $I_2$ :CuI films.

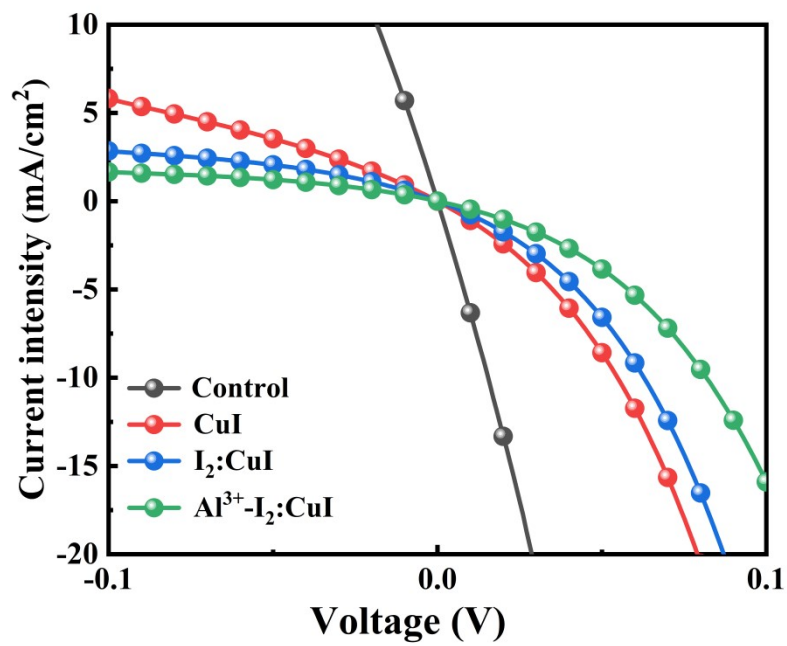


**Figure S7.** Steady-state PL spectra of CuI films with different I<sub>2</sub> doping concentrations.



**Figure S8.** The conductivity measurement of pristine CuI, I<sub>2</sub>:CuI and Al<sup>3+</sup>-I<sub>2</sub>:CuI films.

The inset shows the test structure.



**Figure S9.** Dark J-V curves of the carrier transport layers on n-Si substrates. The inset shows the contact structure.

**Table S1.** Photovoltaic parameters of I<sub>2</sub>:CuI/p-Si heterojunction solar cells with different I<sub>2</sub> doping concentrations.

I <sub>2</sub> :CuI	V <sub>OC</sub> (mV)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
0%	584	39.82	61.92	14.41
4%	576	39.76	68.40	15.68
8%	576	39.86	71.94	16.54
12%	569	39.71	70.63	15.96
16%	562	39.55	67.1	14.93

**Table S2.** Photovoltaic parameters of I<sub>2</sub>:CuI/p-Si heterojunction solar cells with different thickness of CuI films.

Thickness	V <sub>OC</sub> (mV)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
5 nm	546	39.73	70.17	15.23
7 nm	580	39.44	71.85	16.46
10 nm	594	39.60	73.77	17.37
15 nm	594	39.38	71.28	16.67
20 nm	591	39.52	67.50	15.77
25 nm	592	39.37	66.63	15.53

**Table S3.** Parameters of pristine CuI, I<sub>2</sub>:CuI and Al<sup>3+</sup>-I<sub>2</sub>:CuI films measured by Hall effect.

	Carrier concentration (cm <sup>-3</sup> )	Mobility (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	Conductivity (S cm <sup>-1</sup> )
CuI	2.52 × 10 <sup>18</sup>	52.9	21.33
I <sub>2</sub> :CuI	4.64 × 10 <sup>18</sup>	34.1	25.32
Al <sup>3+</sup> -I <sub>2</sub> :CuI	3.77 × 10 <sup>19</sup>	28.3	170.70

**Table S4.** Simulation parameters of the CuI/p-Si heterojunction solar cells at 300 K.

Parameters	p-Si	CuI <sup>1</sup>	I <sub>2</sub> :CuI	Al <sup>3+</sup> -I <sub>2</sub> :CuI
Thickness(cm)	1.75 × 10 <sup>-2</sup>	1 × 10 <sup>-6</sup>	1 × 10 <sup>-6</sup>	1 × 10 <sup>-6</sup>
Shallow uniform acceptor density (cm <sup>-3</sup> )	1 × 10 <sup>16</sup>	1 × 10 <sup>19</sup>	1.5 × 10 <sup>19</sup>	2.0 × 10 <sup>19</sup>
Dielectric constant	11.9	6.5	6.5	6.5
Electron affinity (eV)	4.05	2.35	2.35	2.35
Bandgap (eV)	1.124	2.9	2.97	2.93
CB effective density of states (cm <sup>-3</sup> )	2.843 × 10 <sup>19</sup>	2.2 × 10 <sup>18</sup>	2.2 × 10 <sup>18</sup>	2.2 × 10 <sup>18</sup>
VB effective density of states (cm <sup>-3</sup> )	2.682 × 10 <sup>19</sup>	1.8 × 10 <sup>18</sup>	1.8 × 10 <sup>18</sup>	1.8 × 10 <sup>18</sup>
Electron mobility (cm <sup>2</sup> /Vs)	1107	100	100	100
Hole mobility (cm <sup>2</sup> /Vs)	424.6	43.9	43.9	43.9

1 J. Hossain, M. Rahman, M. M. A. Moon, B. K. Mondal, M. F. Rahman and M. H. K.

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