

Efficient Perovskite Solar Cells Via Surface Passivation by a Multifunctional Small Organic Ionic Compound

Xin Wu^{1#}, Lu Zhang^{1#}, Zhuo Xu^{1#}, Selina Olthof³, Xiaodong Ren^{1*} Yucheng Liu¹,
Dong Yang⁴, Fei Gao^{1*} and Shengzhong (Frank) Liu^{1,2*}

¹Key Laboratory of Applied Surface and Colloid Chemistry, Ministry of Education; Shaanxi Key Laboratory for Advanced Energy Devices; Shaanxi Engineering Lab for Advanced Energy Technology, School of Materials Science and Engineering, Shaanxi Normal University, Xi'an 710119, China

²Dalian National Laboratory for Clean Energy; iChEM, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning, China; University of the Chinese Academy of Sciences, Beijing 100039, China

³Department Chemie, Universität zu Köln Luxemburgerstr. 116, 50939, Köln

⁴Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania 16802, United States

[#]These authors contributed equally to this work.

*Corresponding authors: rxd0313@snnu.edu.cn; feigao@snnu.edu.cn;
szliu@dicp.ac.cn

Keywords: perovskite solar cell, surface passivation, 1-Ethylpyridinium chloride, multifunctional, small organic ionic compound.

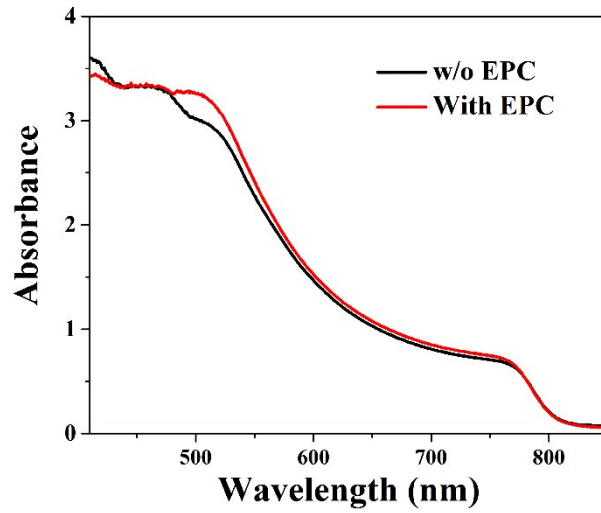


Figure S1. Absorption spectra of the perovskite film with and without EPC passivation.

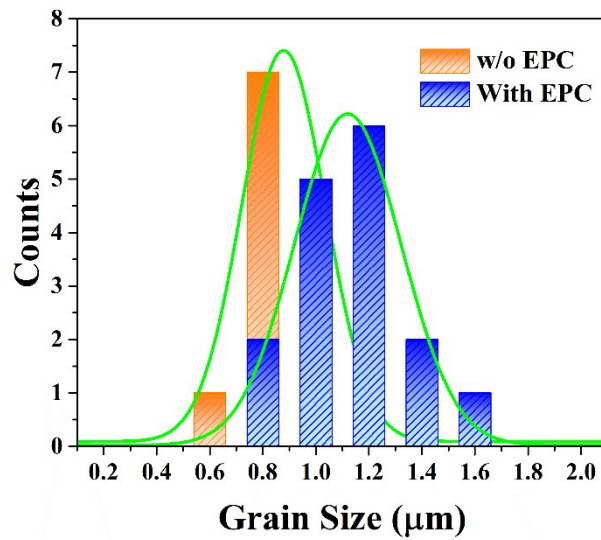


Figure S2. The grain size distribution of the perovskite thin films with and without EPC passivation.

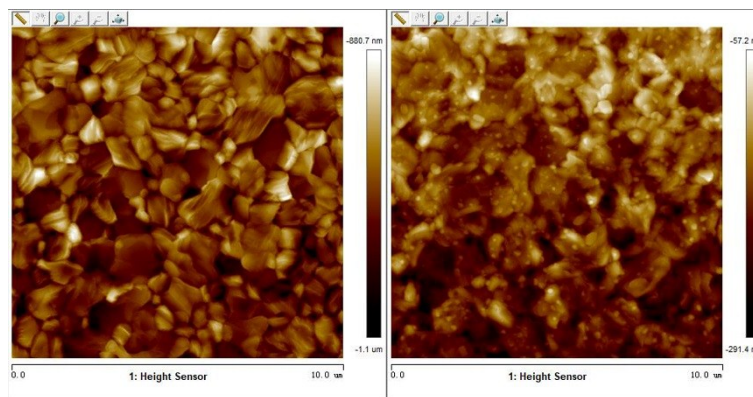


Figure S3. AFM topographical images of perovskite film without (a) and with (b) EPC passivation.

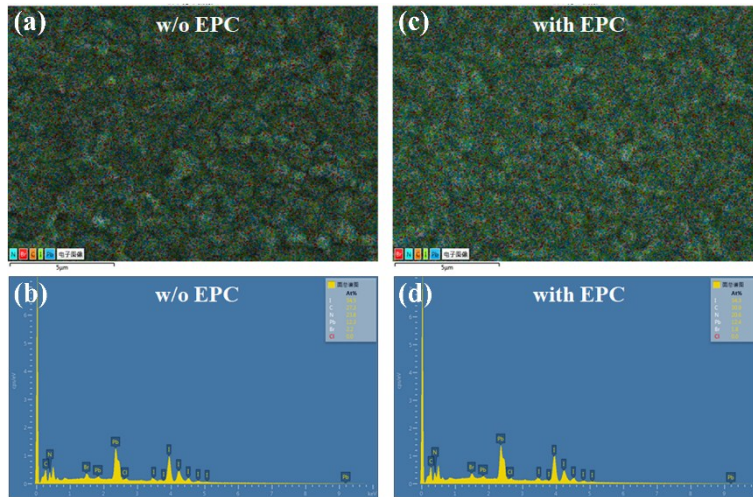


Figure S4. EDX mapping of I, C, N, Pb, and Br in perovskite film with and without EPC passivation.

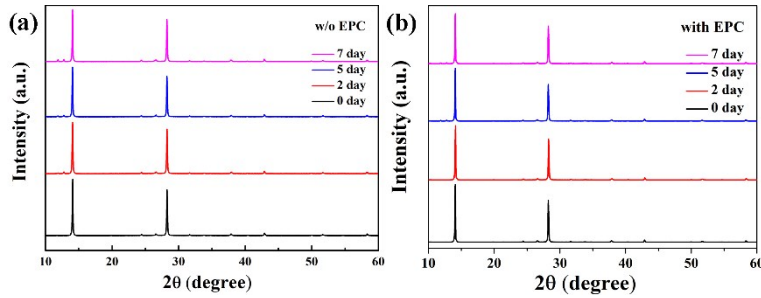


Figure S5. XRD pattern of the perovskite film without (a) and with (b) EPC passivation aging in ambient air condition (30~40 RH%).

Table S1. Fitting parameters of TRPL spectroscopy of the perovskite film without and with EPC passivation.

Sample	τ_{ave} (ns)	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)
w/o EPC	126.9	31.46	9.06	129.21	90.94
with EPC	314.8	10.39	0.38	314.84	99.62

Table S2. Fitting parameters of TRPL spectroscopy of the perovskite/spiro-OMeTAD film without and with EPC passivation.

Sample	τ_{ave} (ns)	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)
w/o EPC	58.08	3.73	12.61	58.58	87.39
with EPC	45.16	1.63	16.28	45.46	83.72

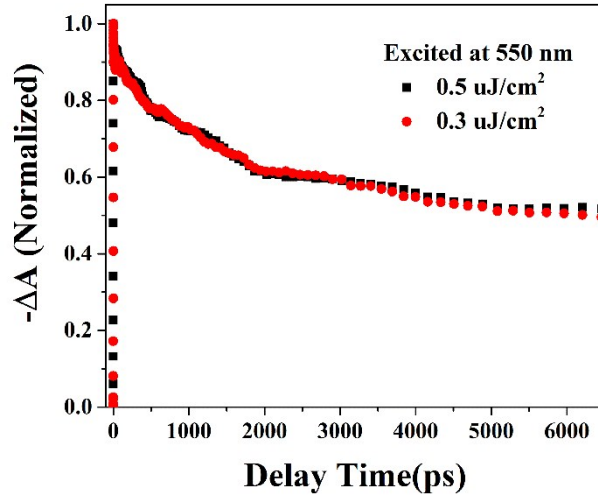


Figure S6. The relaxation dynamics as function of the pump fluence.

Table S3. Fitting parameters of TA spectroscopy of the perovskite/spiro-OMeTAD film without and with EPC passivation.

Sample	τ_1 (ps)	A_1 (%)	τ_2 (ns)	A_2 (%)
w/o EPC	54.56	31.63	1.19	68.37
with EPC	54.39	32.52	1.20	67.48

Table S4. Photovoltaic parameters in forward and reverse scans of the champion PSCs with and without EPC concentration.

		J_{sc} (mA cm ⁻²)	V_{oc} (V)	PCE (%)	FF	R_s (Ω)	R_{sh} (k Ω)	HI
w/o EPC	Reverse	24.28	1.044	19.52	0.769	46.3	31.84	0.079
	Forward	24.06	1.035	17.26	0.693	75.94	19.17	
with EPC	Reverse	25.02	1.053	21.19	0.805	47.71	75.76	0.023
	Forward	24.87	1.049	20.28	0.777	51.29	46.31	

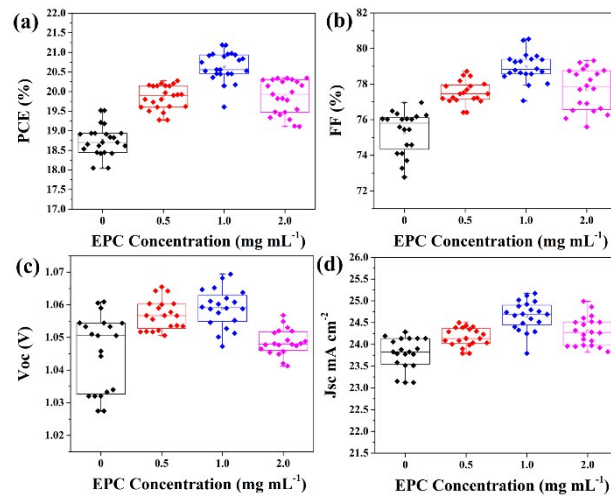


Figure S7. EPC concentration dependence of photovoltaic parameters: (a) open-circuit

voltage (V_{OC}); (b) short-circuit current density (J_{SC}); (c) PCE; (d) fill factor (FF). Results are shown with statistical distributions based on observations from 15 cells for each group.

Table S5. Photovoltaic parameters of the PSCs fabricated with different EPC concentration.

EPC concentration (mg mL ⁻¹)		J_{sc} (mA cm ⁻²)	V_{oc} (V)	PCE (%)	FF
0	Max	24.28	1.044	19.52	0.753
	Averag e	23.79 ± 0.35	1.045 ± 0.01	18.75 ± 0.37	0.769 ± 0.012
0.5	Max	24.40	1.059	20.27	0.785
	Averag e	24.16 ± 0.21	1.057 ± 0.004	19.80 ± 0.30	0.775 ± 0.006
1.0	Max	25.02	1.053	21.19	0.805
	Averag e	24.65 ± 0.33	1.059 ± 0.005	20.64 ± 0.36	0.789 ± 0.008
2.0	Max	24.86	1.046	20.34	0.782
	Averag e	24.30 ± 0.32	1.048 ± 0.004	19.86 ± 0.42	0.777 ± 0.010

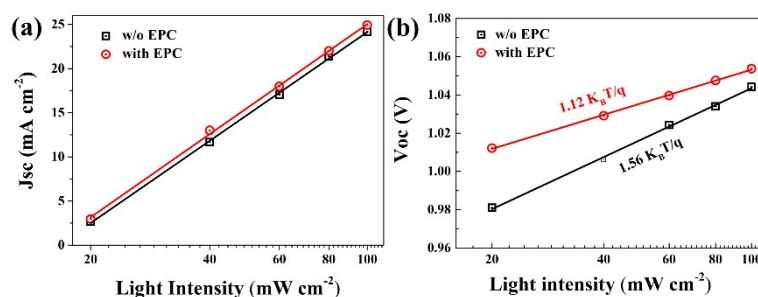


Figure S8 (a) J_{SC} vs. light intensity and (b) V_{OC} vs. light intensity with and without EPC passivation.