Australian National University

High Open-Circuit Voltage Perovskite Solar Cells: Role of Surface Passivation

--Jun Peng

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Background

- The quality of perovskite bulk is good.

  (PL quantum efficiency: high; PCE >23%; FF > 0.8)

- V_{oc} still well bellow the theoretical value.

  (Theoretical V_{oc}~1.35 V for ~1.6 eV perovskite)

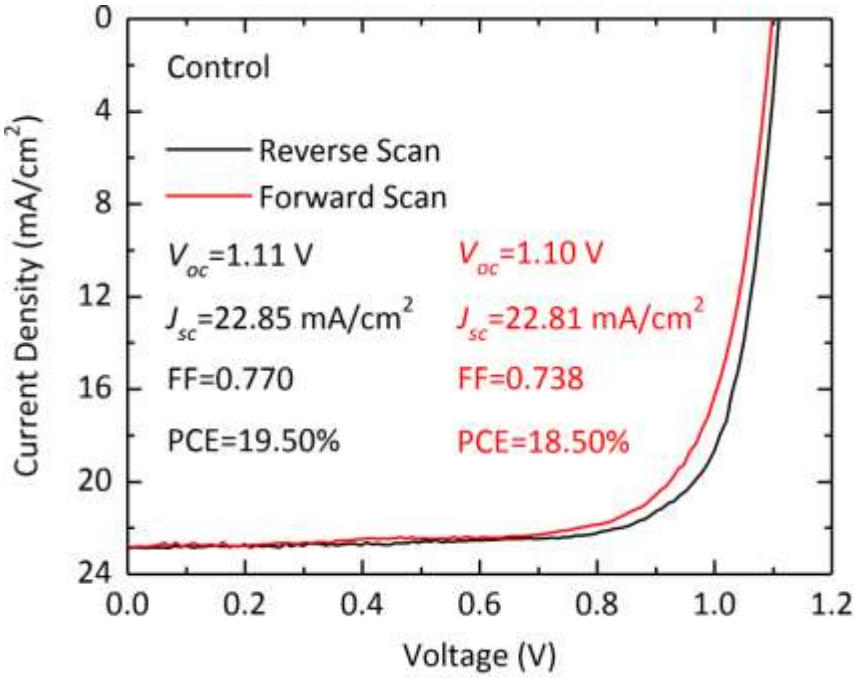
- *J-V* Hysteresis.

- Defect-induced interfacial recombination.

  (Defects: under-coordinated Pb (Pb^{2+}), halide vacancies, ions)

T. Miyasaka *et al*., *JACS*. **2009**, 131, 6050; W. Tress, *Adv. Energy Mater*. **2017**, 7, 1602358;
S. D. Stranks, *ACS Energy Lett.* **2017**, 2, 1515; M. Grätzel *et al*., *Science*, **2016**, 354, 206;
H. J. Snaith *et al*., *Science*, **2013**, 342, 341; P. Schulz, *ACS Energy Lett.* **2018**, 3, 1287;

Background



Low V_{oc} ~ 1.11 V.

J-V Hysteresis behaviour.

Slow response in V_{oc} and J_{sc}.

Reason:
Defect-induced recombination at the interface between perovskite and transport layers.

FTO/c-TiO_x/m-TiO_2/Perovskite/Spiro-OMeTAD/Au

'Perovskite' represents $Cs_{0.07}Rb_{0.03}FA_{0.765}MA_{0.135}PbI_{2.55}Br_{0.45}$ (E_g~1.62 eV).

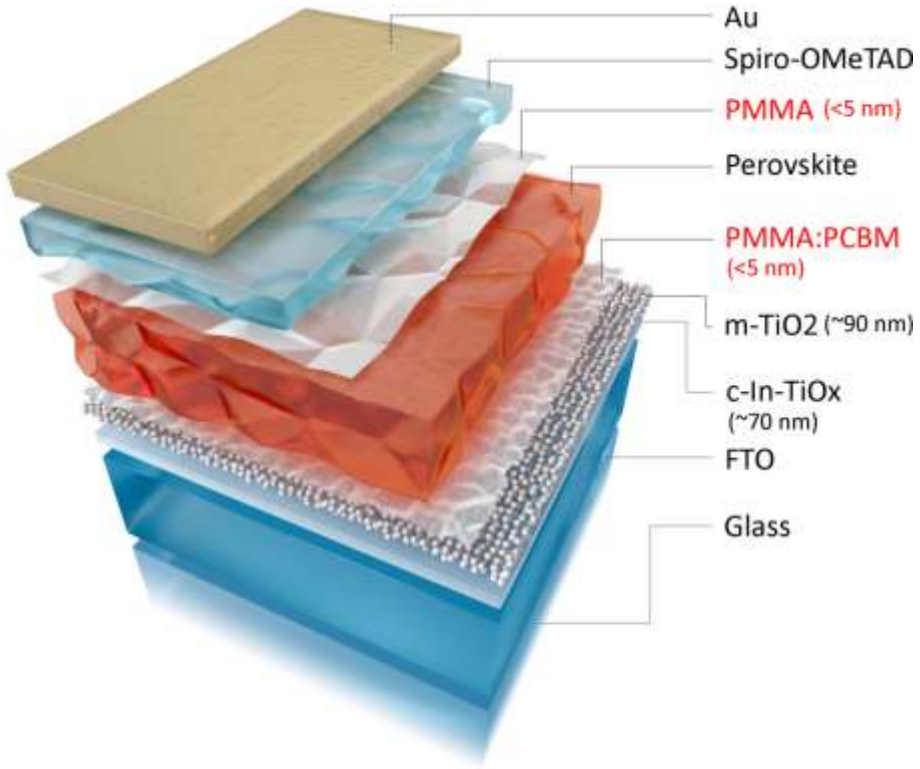
Background

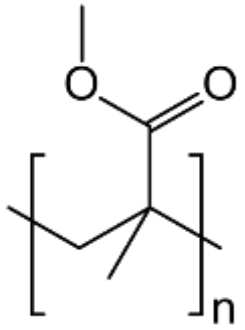
Passivation Materials:

- PCBM, C_{60} and other fullerene-based materials.
- PCDTBT, PVP, PMMA, Al_2O_3.
- Thiophen, Pyridine, Cl-TiO_2.
- Others.

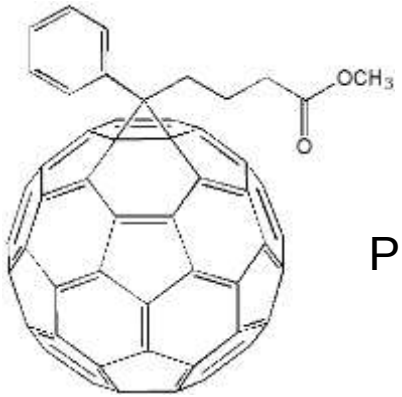
J. Huang *et al*., *Nat. Commun*. **2014**, 5, 5784; A. Petrozza *et al.*, *Energy Environ.Sci.* **2015**, *8*, 2365; M. Grätzel *et al.*, *Nat. Energy* **2016**, *1*, 16142; Y. Yang *et al*., *Sci. Adv.* **2017**, *3*, e1700106; H. J. Snaith *et al.*, *ACS Nano* **2014**, *8*, 9815; E. H. Sargent *et al*., *Science* **2017**, *355*, 722;

Surface Passivation





PMMA

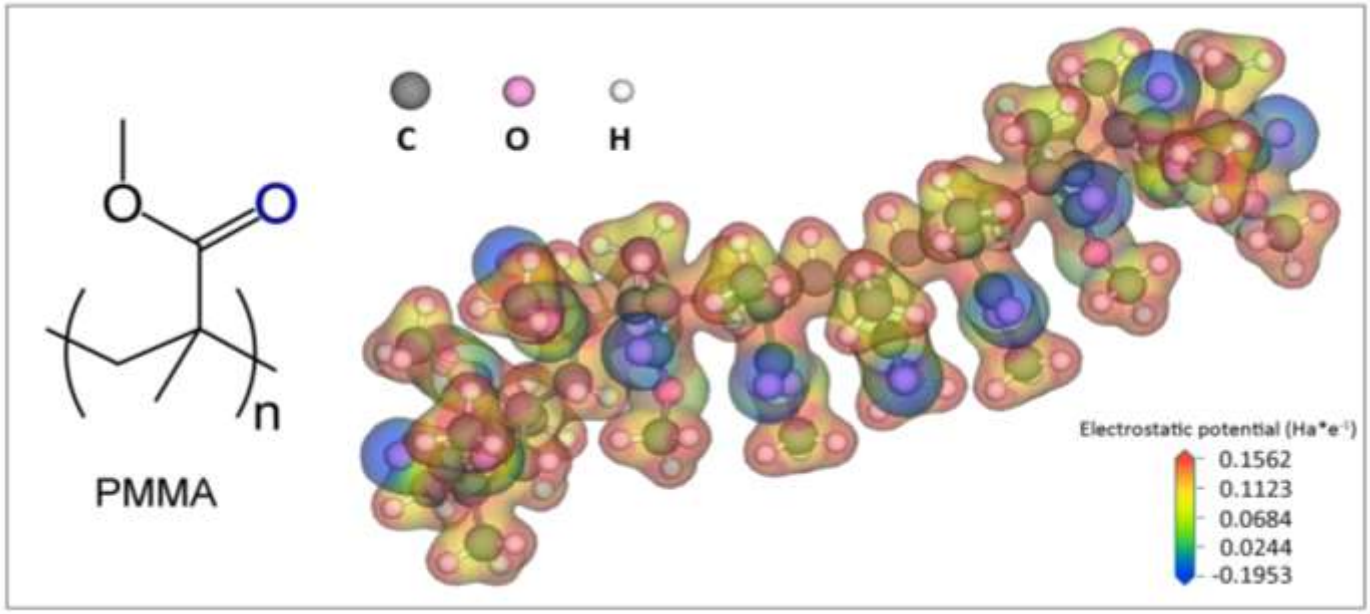


PCBM

Jun Peng *et al. Adv. Energy Mater.* **2017**, *7,* 1601768.
Jun Peng *et al. Energy Environ. Sci.* **2017**, *10*, 1792.
Jun Peng *et al. Adv. Energy Mater.* **2018**, *8*, 1801208.

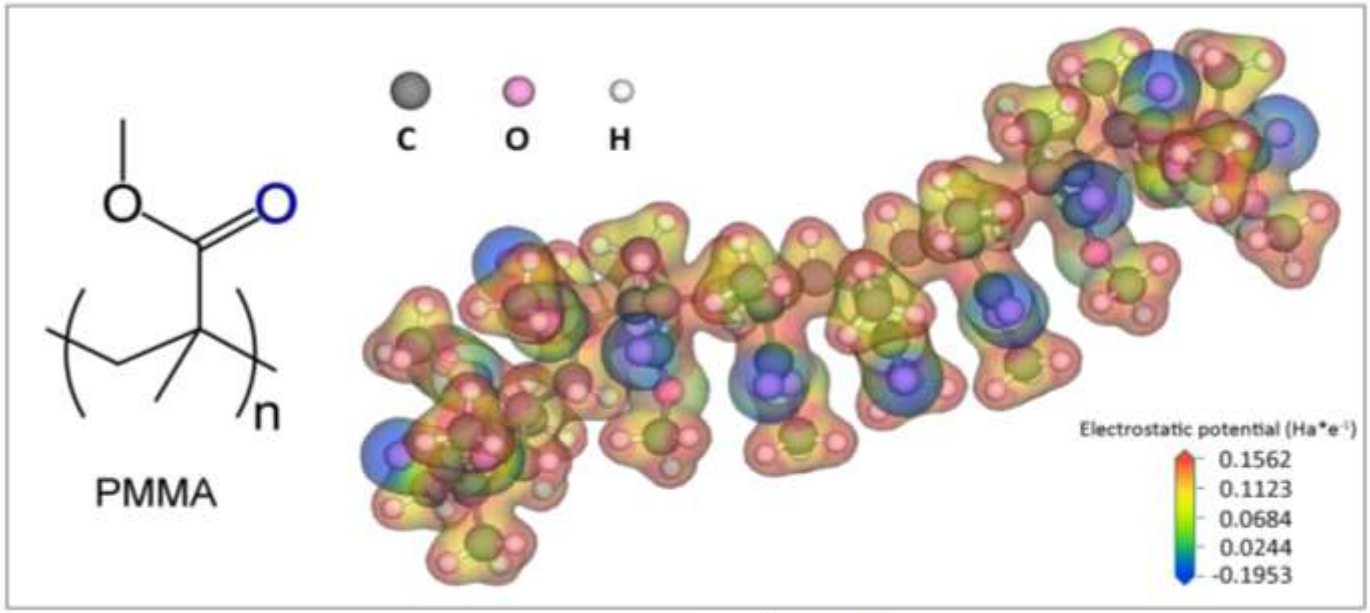
Role of carbonyl group in PMMA

DFT

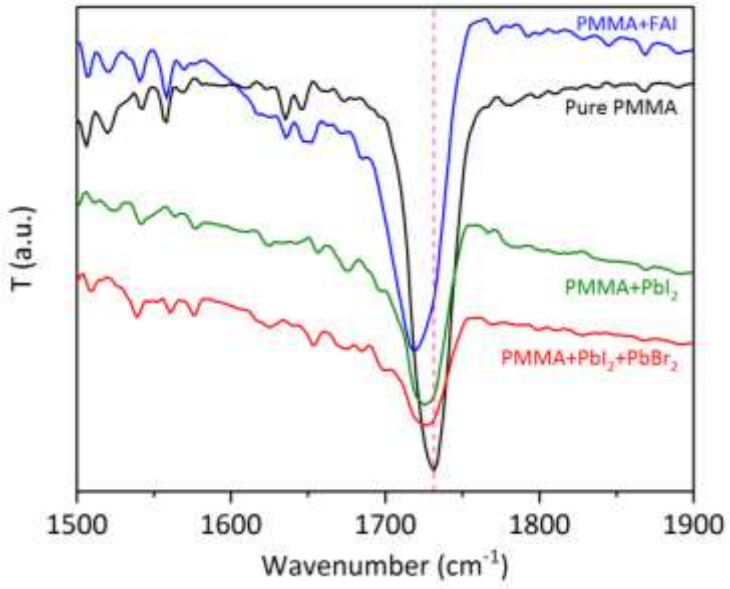


Role of carbonyl group in PMMA

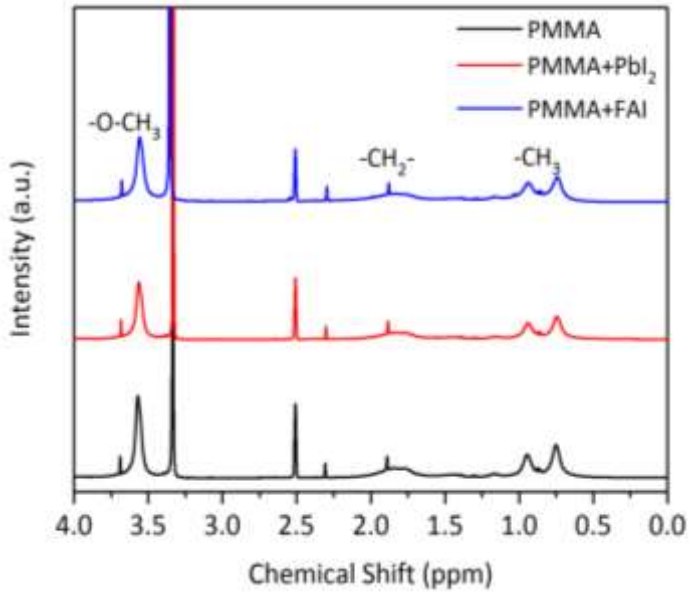
DFT



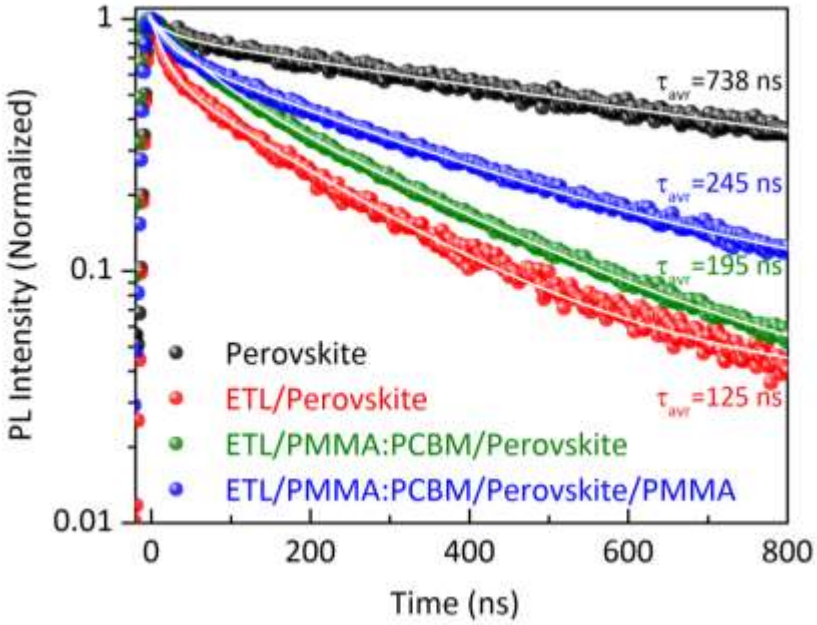
FTIR

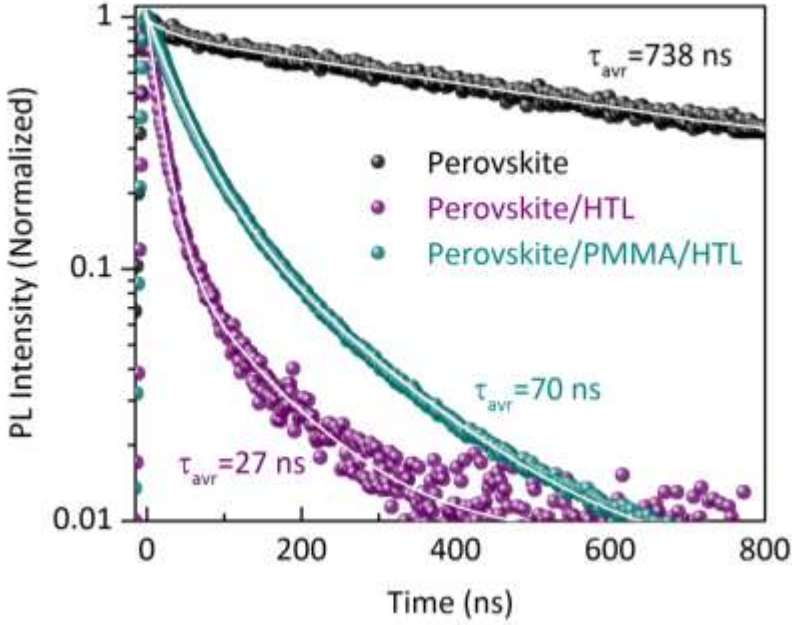


NMR



Transient PL Measurements

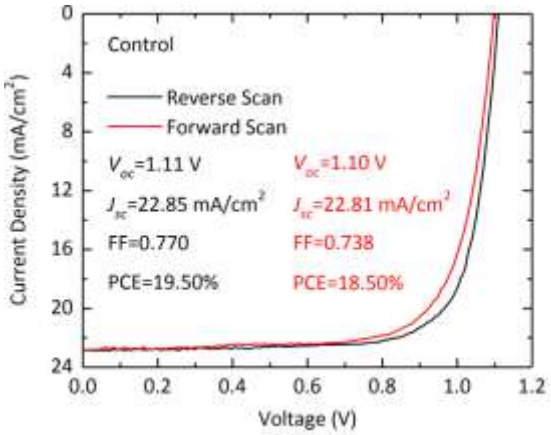


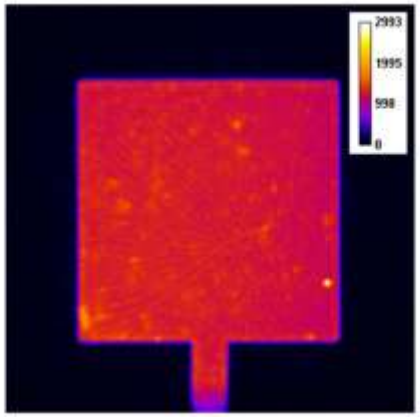


PMMA can effectively mitigate the defect-induced recombination at the interface between perovskite and transport layers.

'Perovskite' represents $Cs_{0.07}Rb_{0.03}FA_{0.765}MA_{0.135}PbI_{2.55}Br_{0.45}$.

Performance *vs* PL Imaging

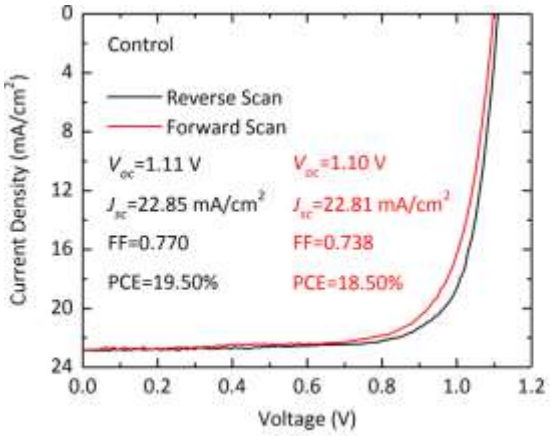


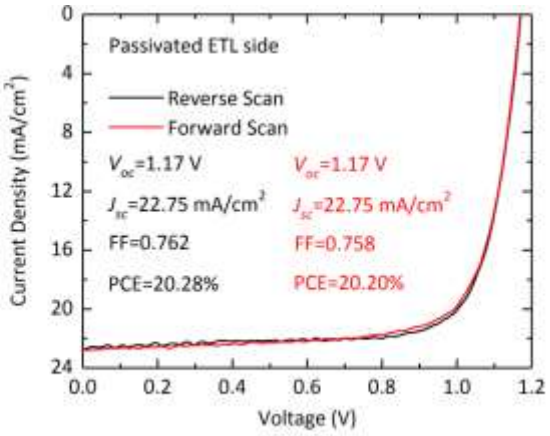


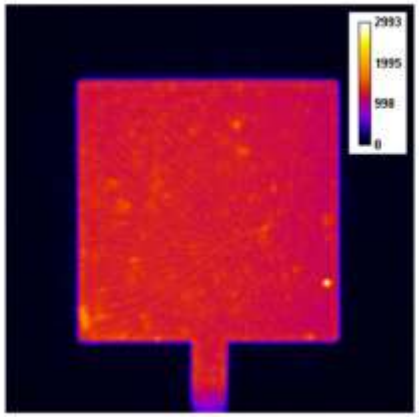
State-steady PL imaging: complete cells @ open-circuit.

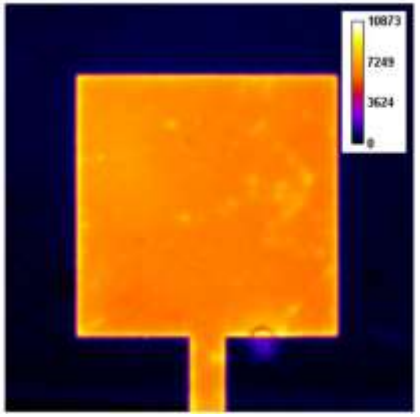
(Light Source: Royal blue LED; Intensity: 100 mW/cm^2)

Performance *vs* PL Imaging









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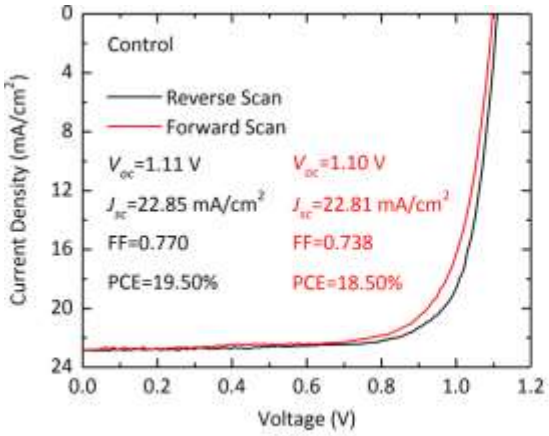
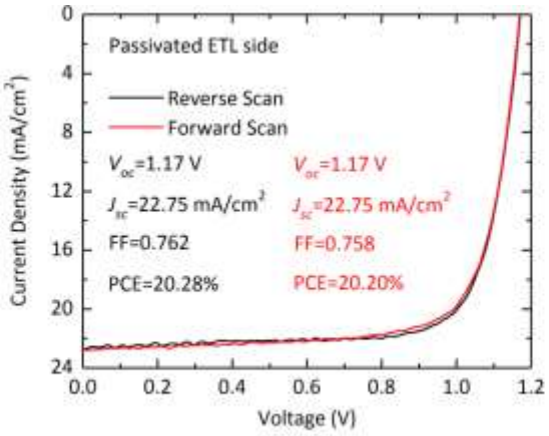
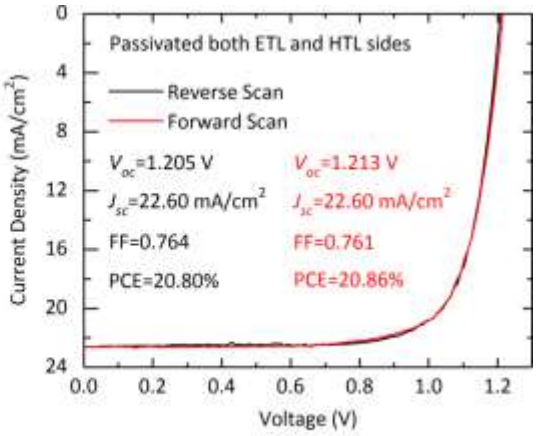
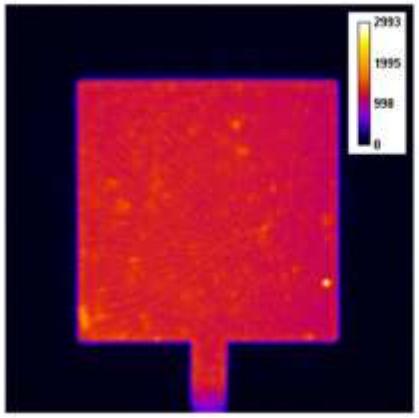
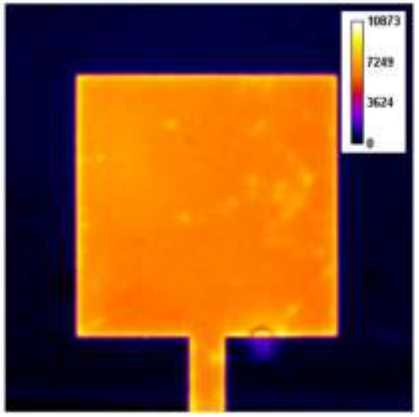
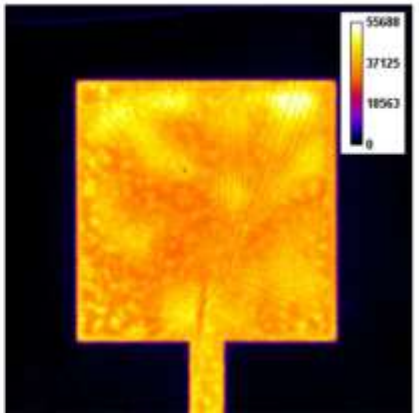








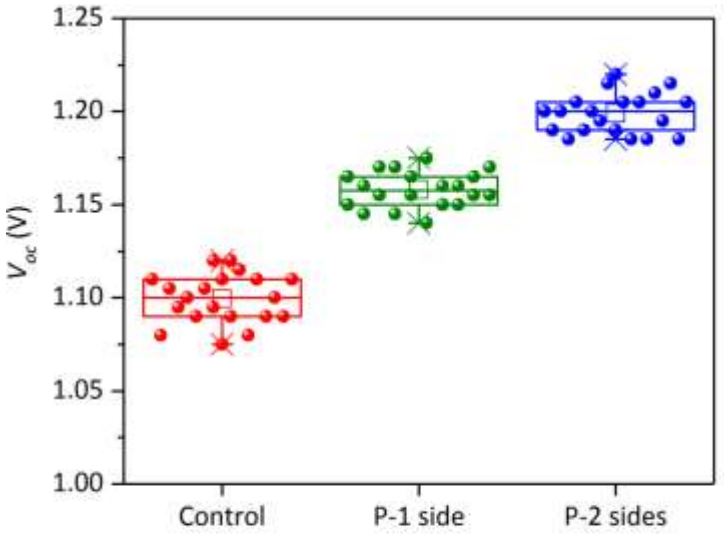


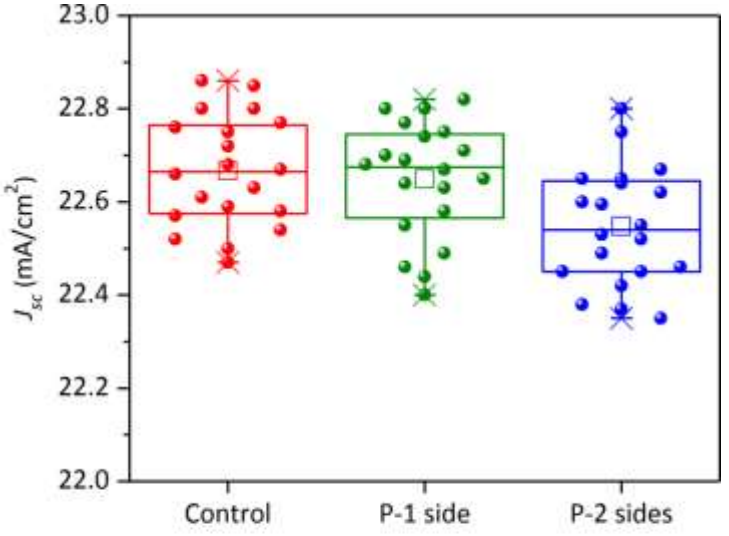


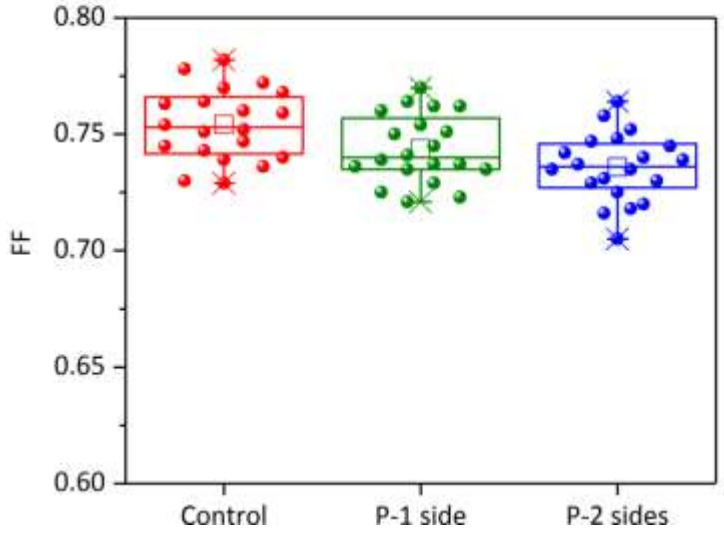
State-steady PL imaging: complete cells @ open-circuit.

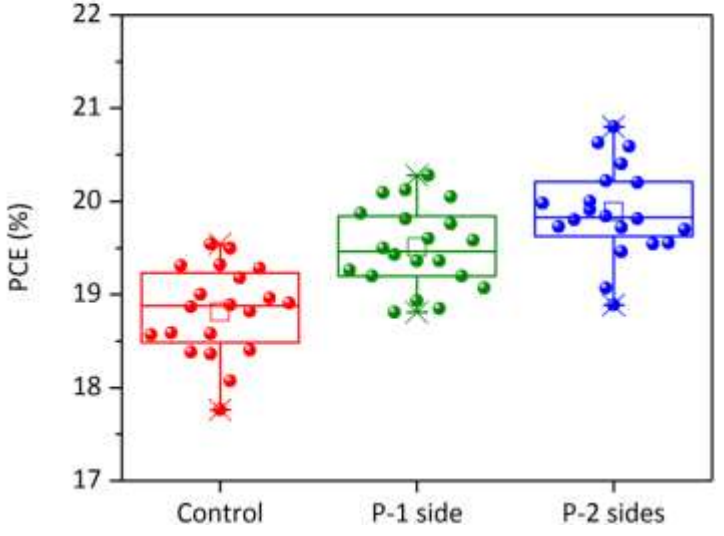
(Light Source: Royal blue LED; Intensity: 100 mW/cm^2)

Performance vs Surface Passivation

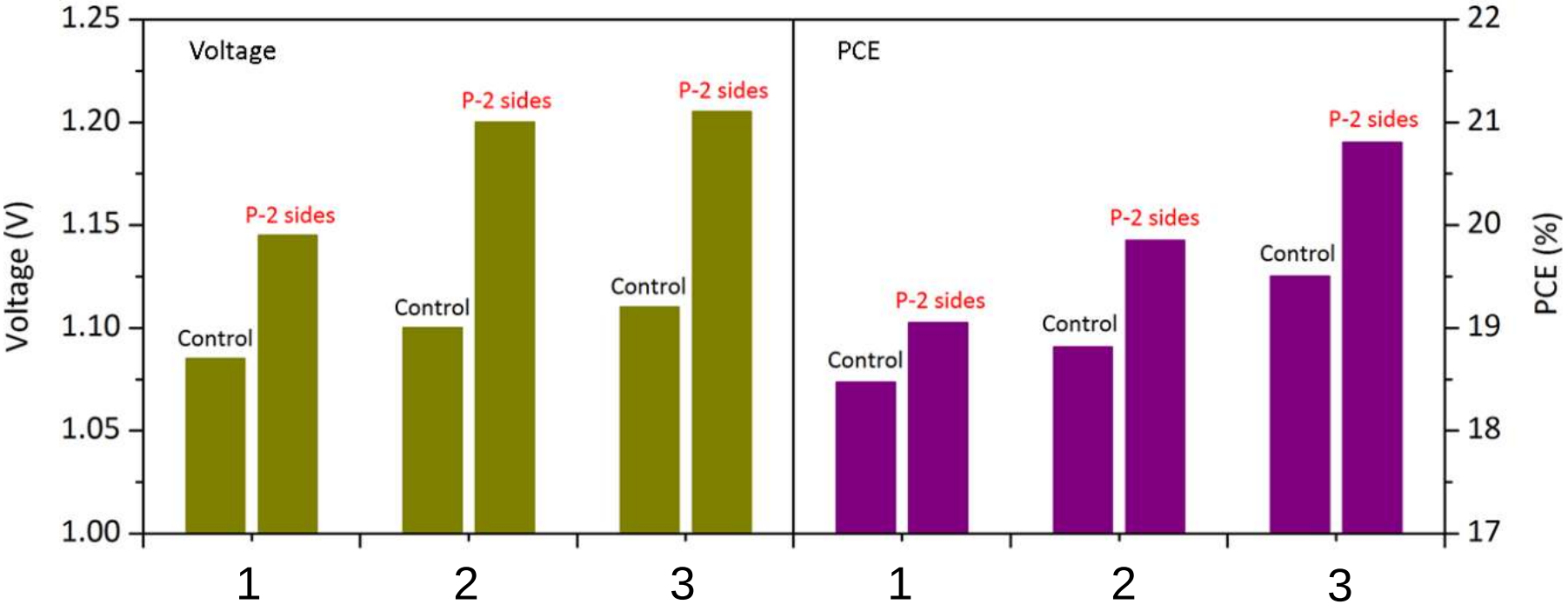








Universality: Double-side Passivation



1. $MAPbI_3$: 1.085 V => 1.145 V;
2. $FA_{0.85}MA_{0.15}PbI_{2.55}Br_{0.45}$: 1.10 V => 1.20 V;
3. $Cs_{0.07}Rb_{0.03}FA_{0.765}MA_{0.135}PbI_{2.55}Br_{0.45}$: 1.11 V => 1.205 V.

Suitable for different transport layers (e.g. SnO_2, CuSCN et al.).

Summary

- Revealed the passivation mechanism of PMMA.

  Carbonyl group (*C*=*O*) can effectively passivate the under-coordinated Pb atoms (Pb^{2+}) the dominant defects within perovskite.

- Significantly reduced the defect-induced recombination at the interface between perovskite and transport layers.

- Boosted the V_{oc} up to 1.22 V for 1.62 eV bandgap perovskite.

- Demonstrated the universality of PMMA passivation.

- Development of new conductive polymers with *C*=*O* groups could further increase performance.

Acknowledgement

Thanks to:

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A/Prof. Juntao Li (School of Physics, Sun Yat-sen University)

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Supported by:

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Australian Renewable Energy Agency

Australian Nanotechnology Network

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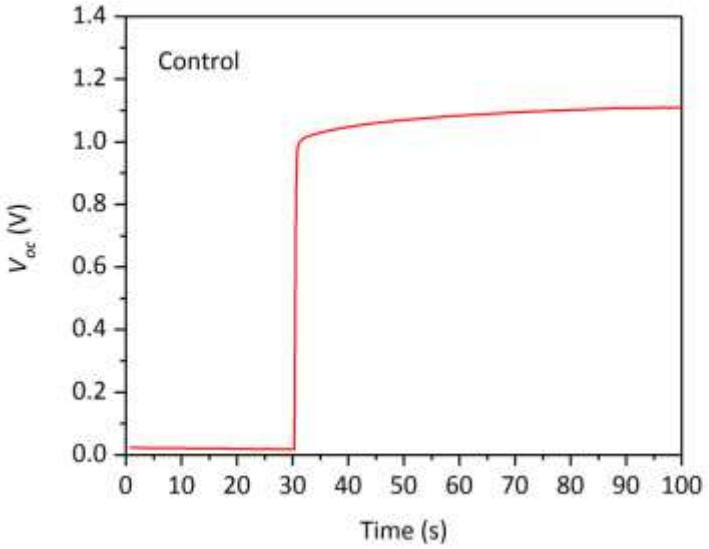
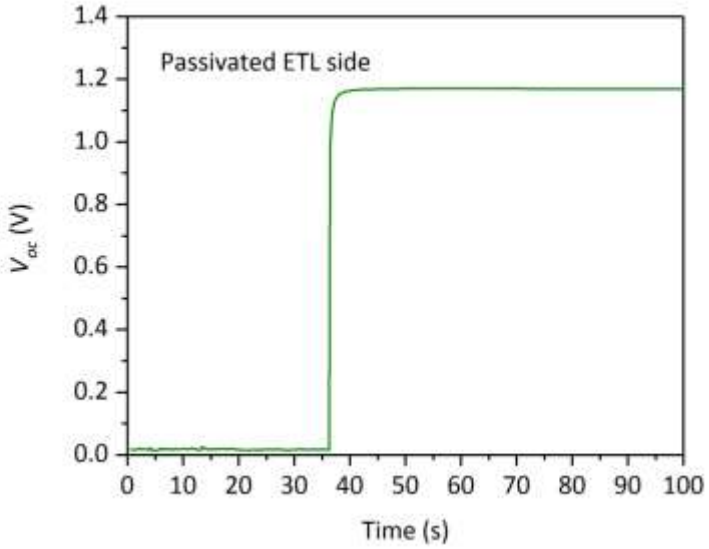
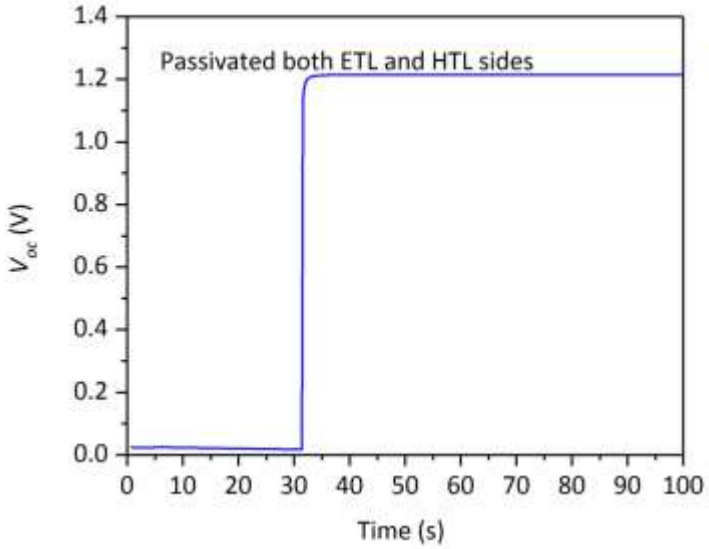
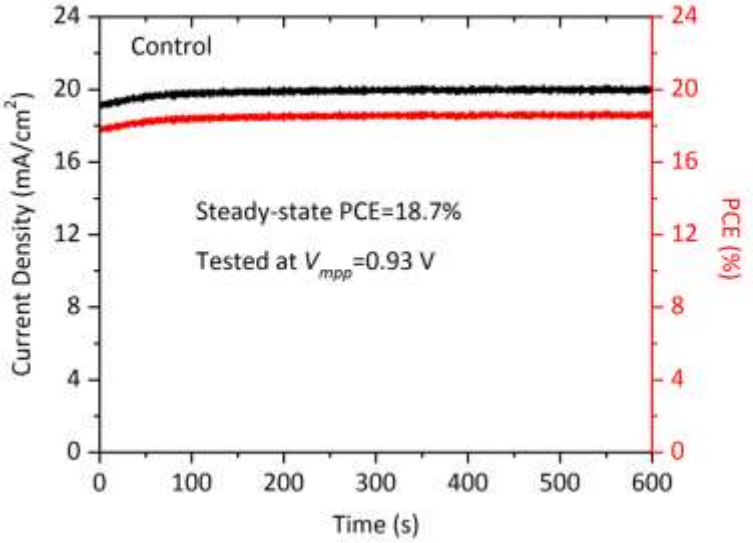
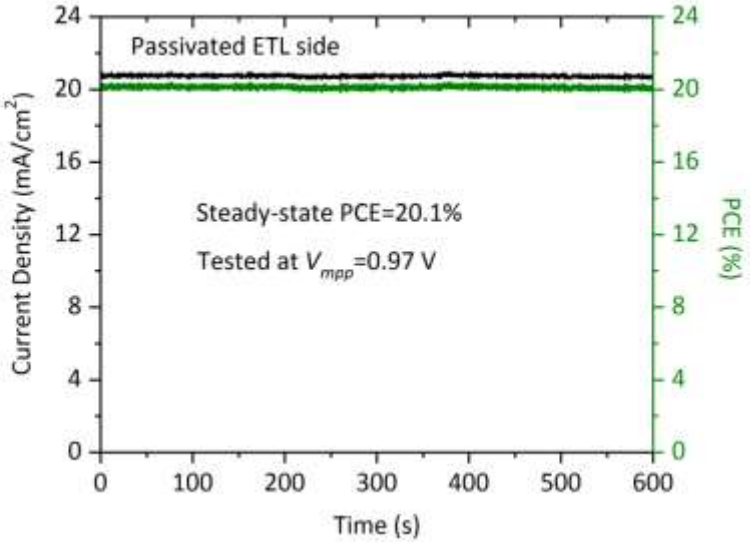
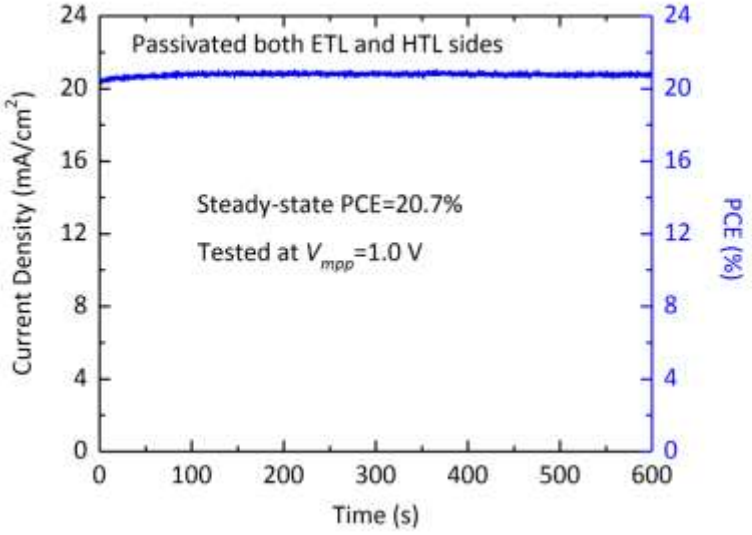

Control
V_{oc} (V)
Time (s)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0 10 20 30 40 50 60 70 80 90 100

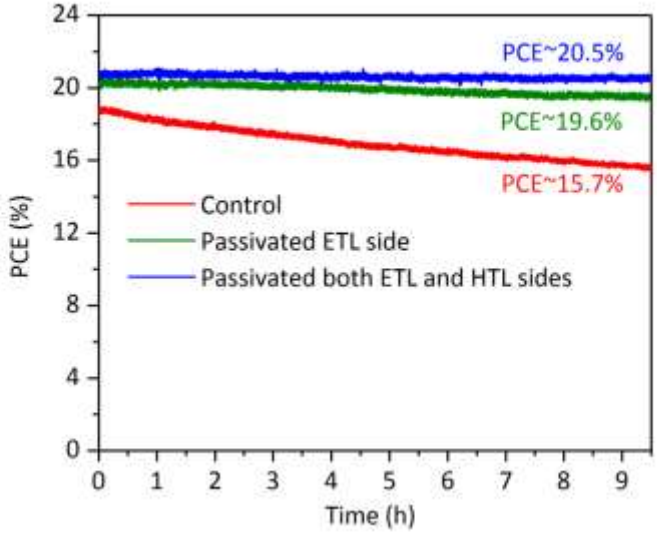

Passivated ETL side
V_{oc} (V)
Time (s)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0 10 20 30 40 50 60 70 80 90 100

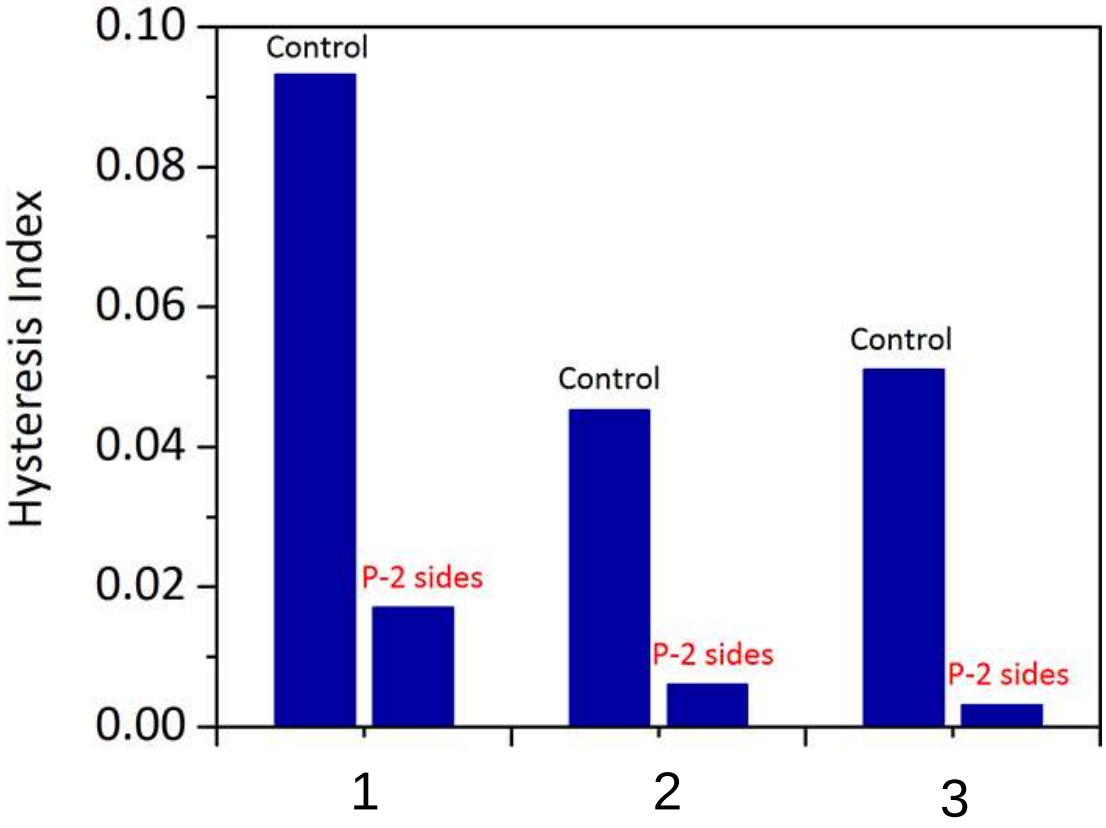

Passivated both ETL and HTL sides
V_{oc} (V)
Time (s)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0 10 20 30 40 50 60 70 80 90 100


Control
Steady-state PCE=18.7%
Tested at V_{mpp}=0.93 V
Current Density (mA/cm^2)
PCE (%)
Time (s)

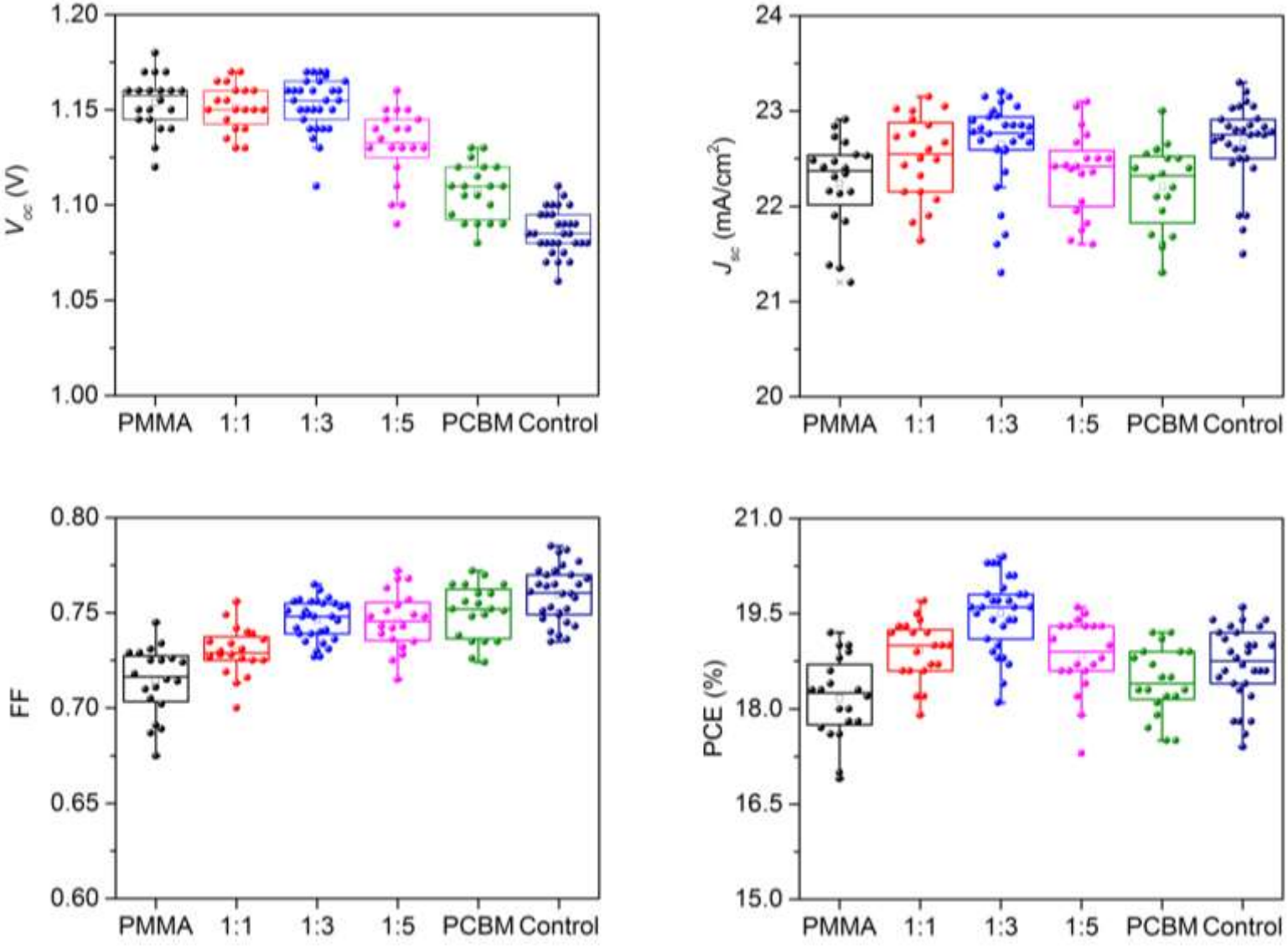

Passivated ETL side
Steady-state PCE=20.1%
Tested at V_{mpp}=0.97 V
Current Density (mA/cm^2)
PCE (%)
Time (s)


Passivated both ETL and HTL sides
Steady-state PCE=20.7%
Tested at V_{mpp}=1.0 V
Current Density (mA/cm^2)
PCE (%)
Time (s)


PCE~20.5%
PCE~19.6%
PCE~15.7%
Control
Passivated ETL side
Passivated both ETL and HTL sides
PCE (%)
Time (h)



Hysteresis index is defined as: $|(PCE_{reverse} - PCE_{forward})|/ PCE_{reverse}$.



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