

IPEROP·23
23rd - 24th January, 2023
KOBE · Japan

PEROVSKITE AND ORGANIC PHOTOVOLTAICS AND OPTOELECTRONICS

nanoGe

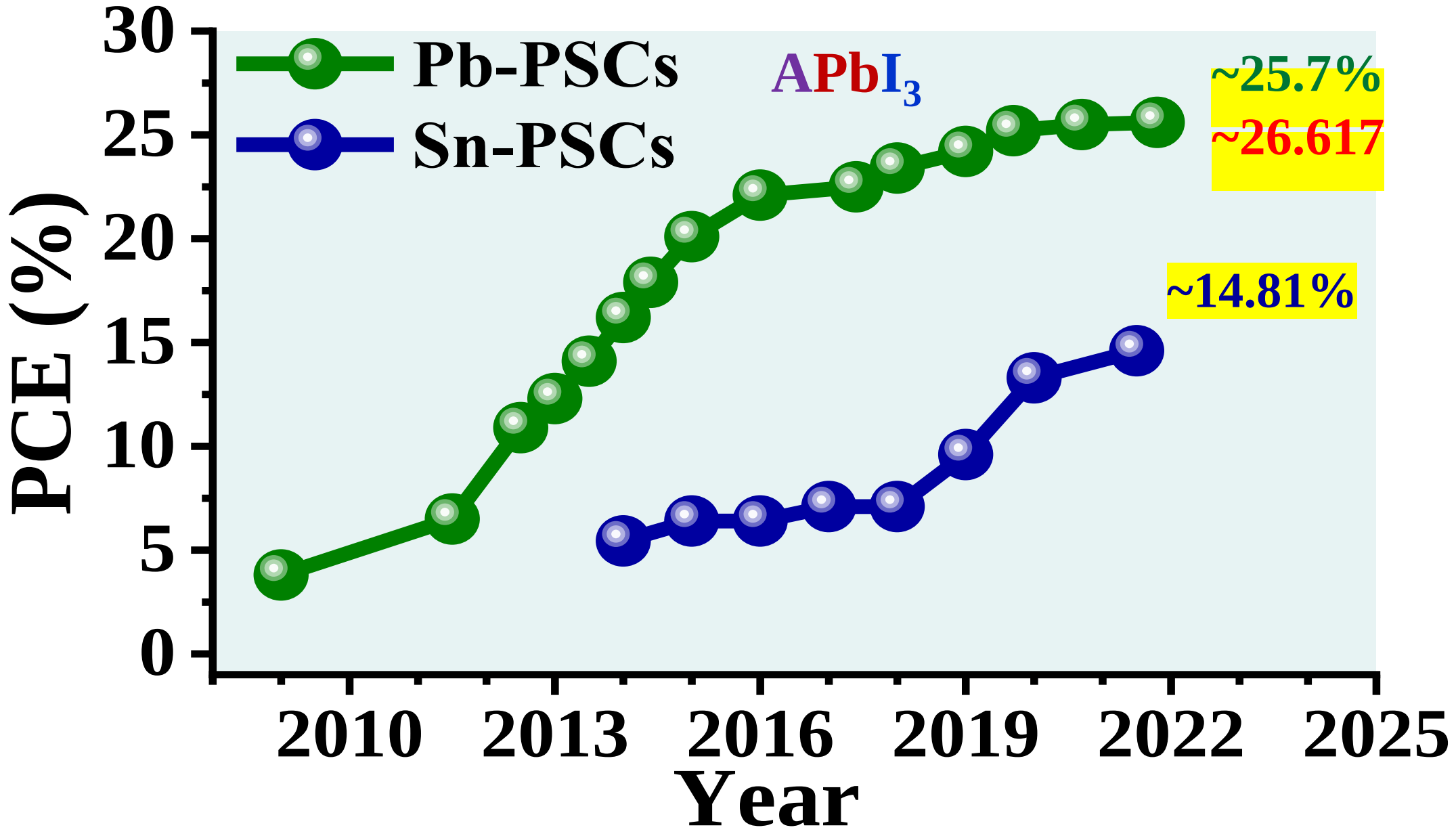
fundació Scito

Surface Passivation with Multifunctional Fluoroarene Molecule for High-Efficiency and Stable MA-Free Perovskite Solar Cells

Dhruba B. **Khadka**, Yasuhiro Shirai, Masatoshi Yanagida, Terumasa Tadano, Kenjiro **Miyano**

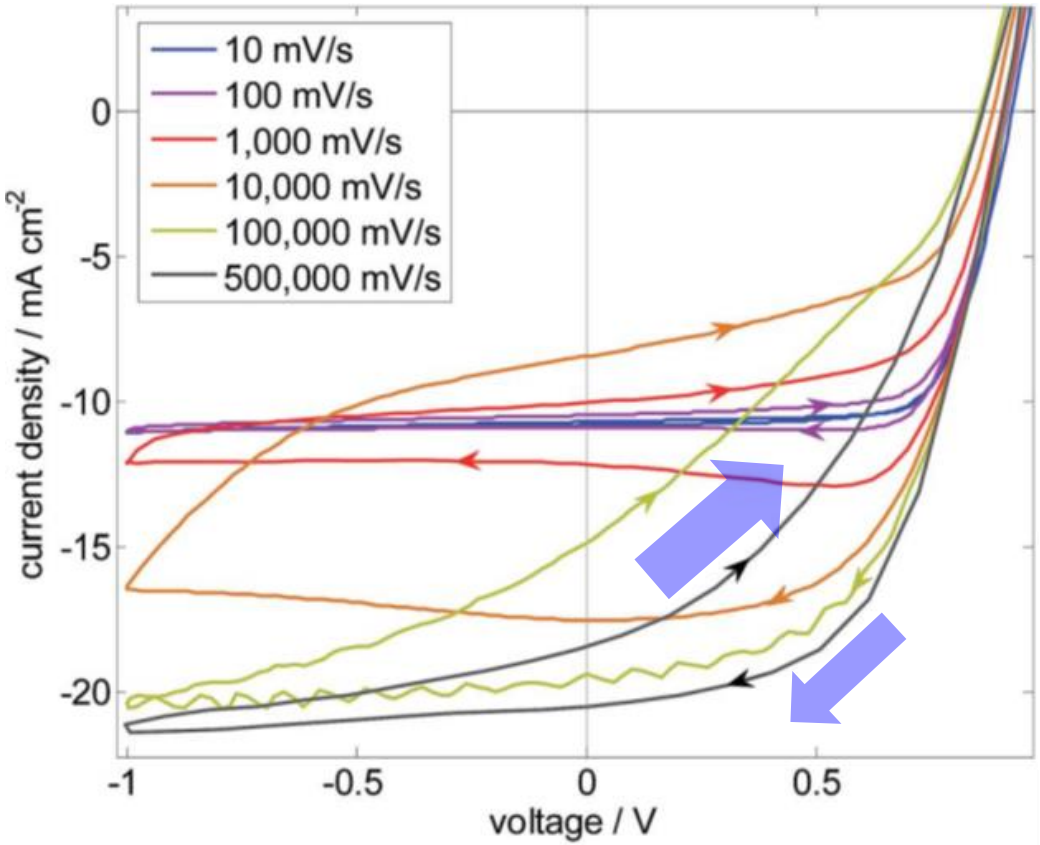
Photovoltaic Materials Group
Global Research Center for Environment and Energy based on Nanomaterials Science(GREEN)
National Institute for Materials Science (NIMS), Tsukuba, Japan

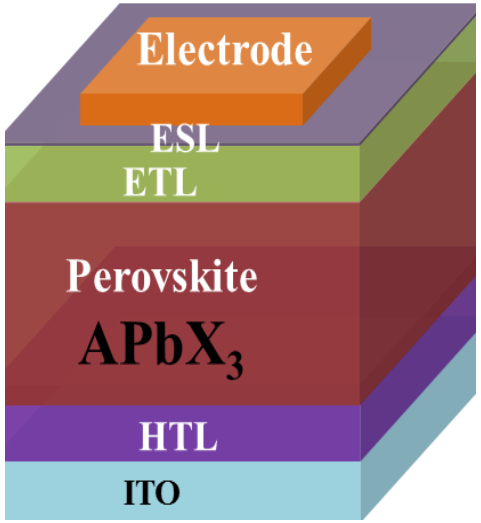
Halide Perovskite Solar Cells: Startling Progress



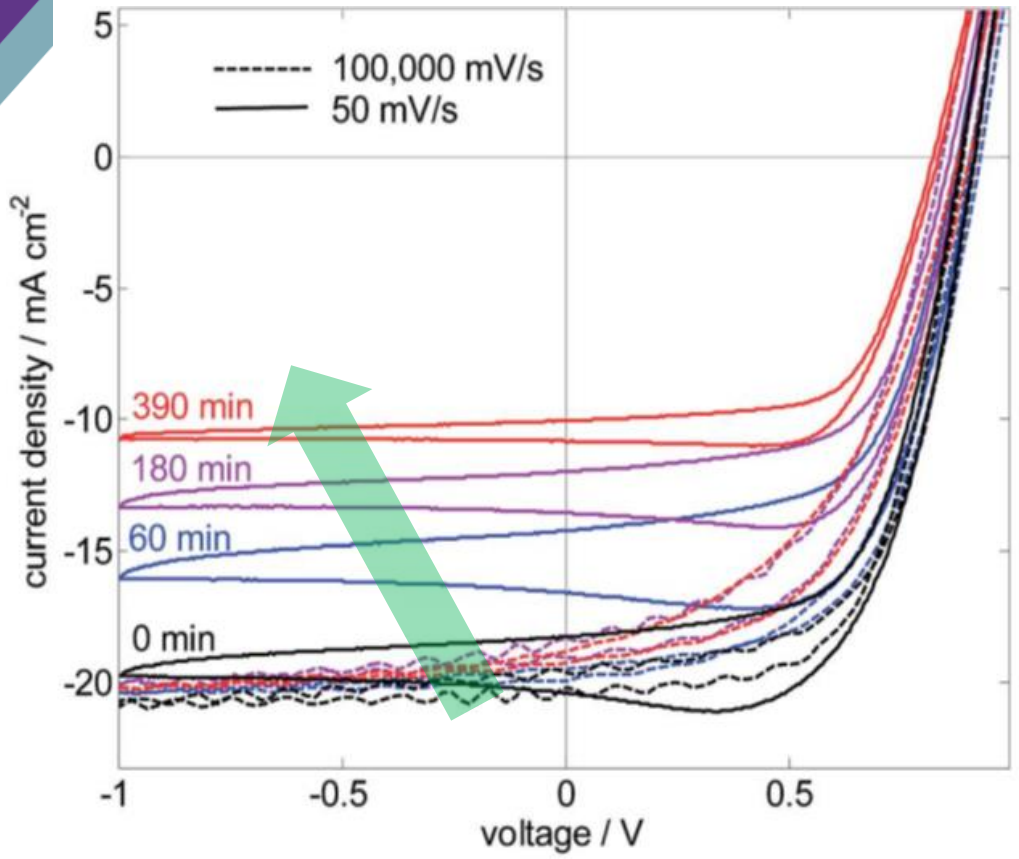
Perovskite Solar Cell: Limitation Issue

J-V hysteresis





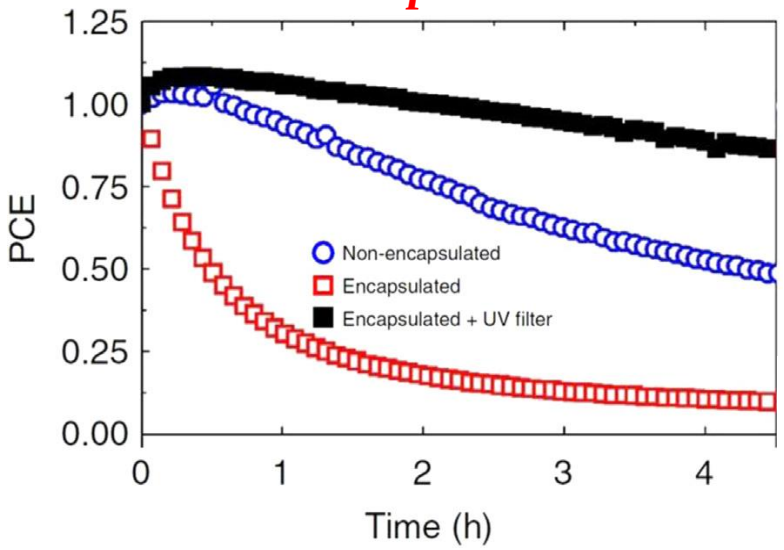
Device degradation

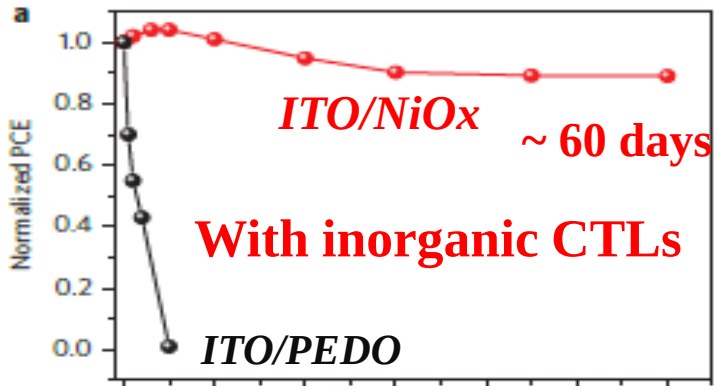


Energy Environ. Sci., 2015, 8, 995–1004

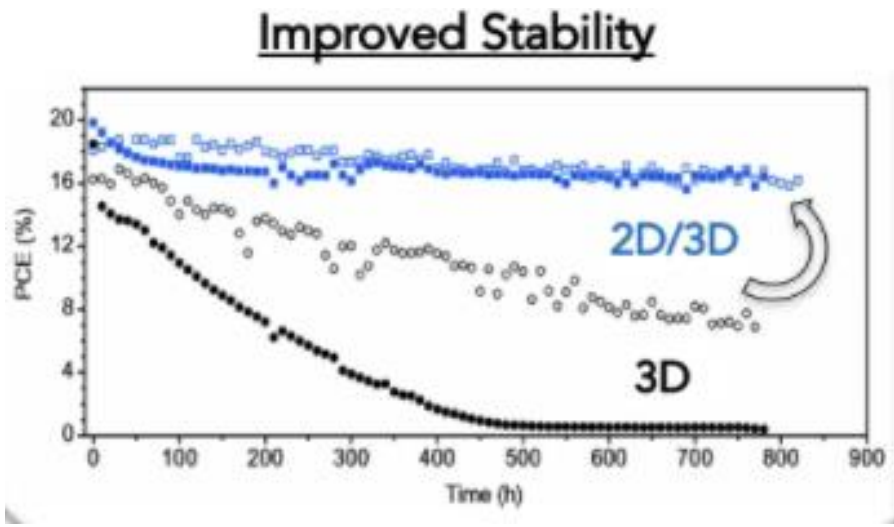
Device Stability Issue

Encapsulation

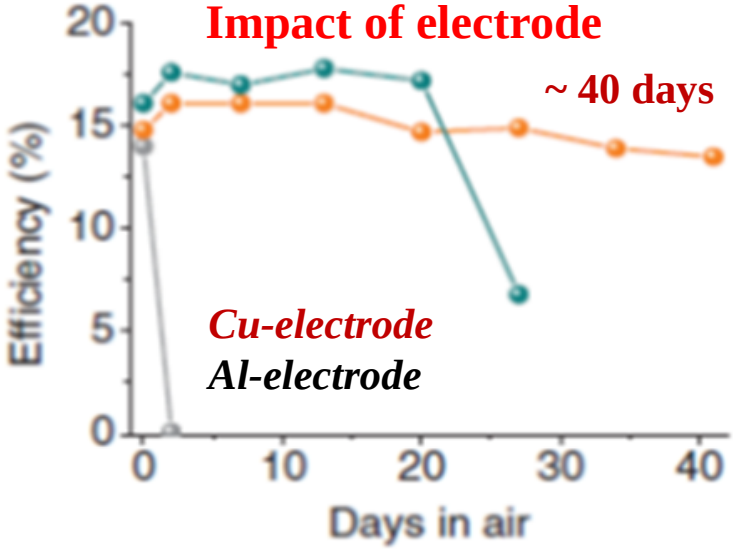


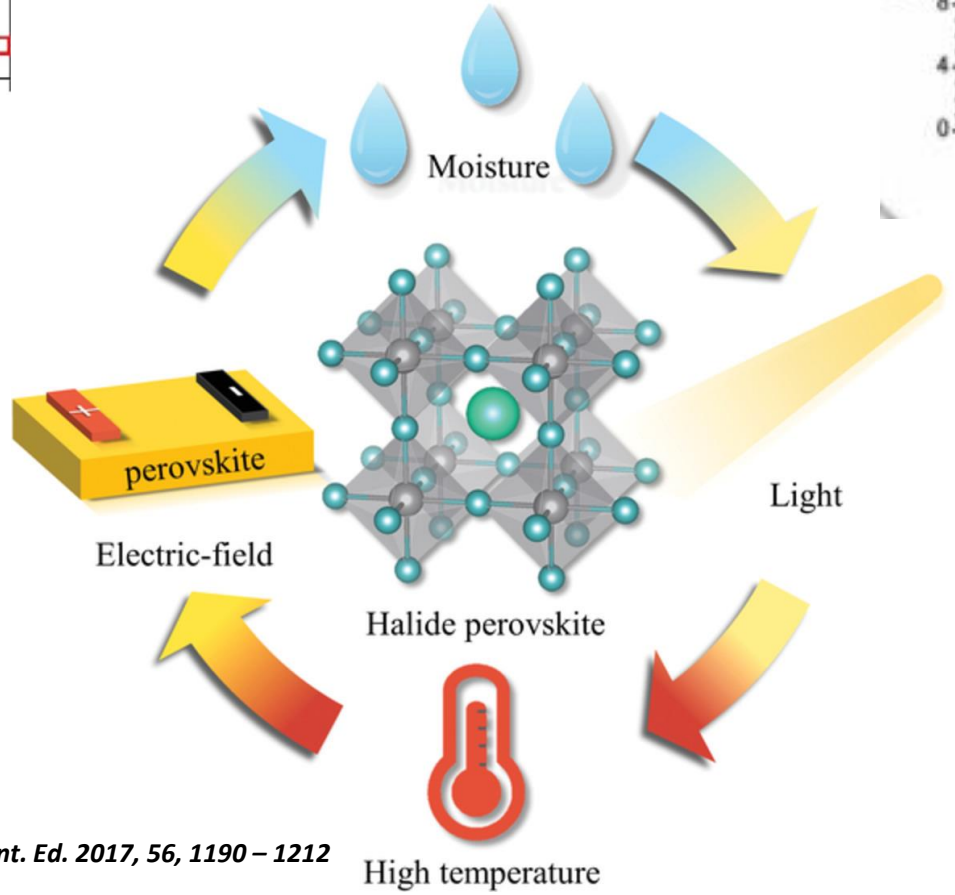


Standard: 85C/85%- RH; 1000 hours

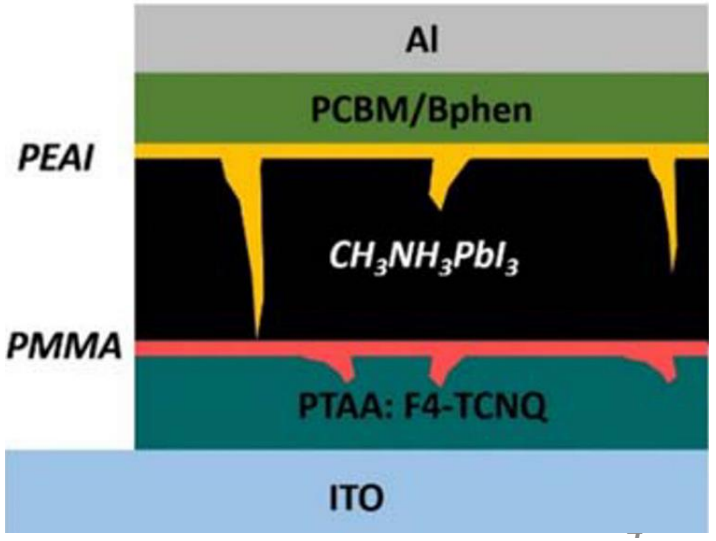


Impact of electrode





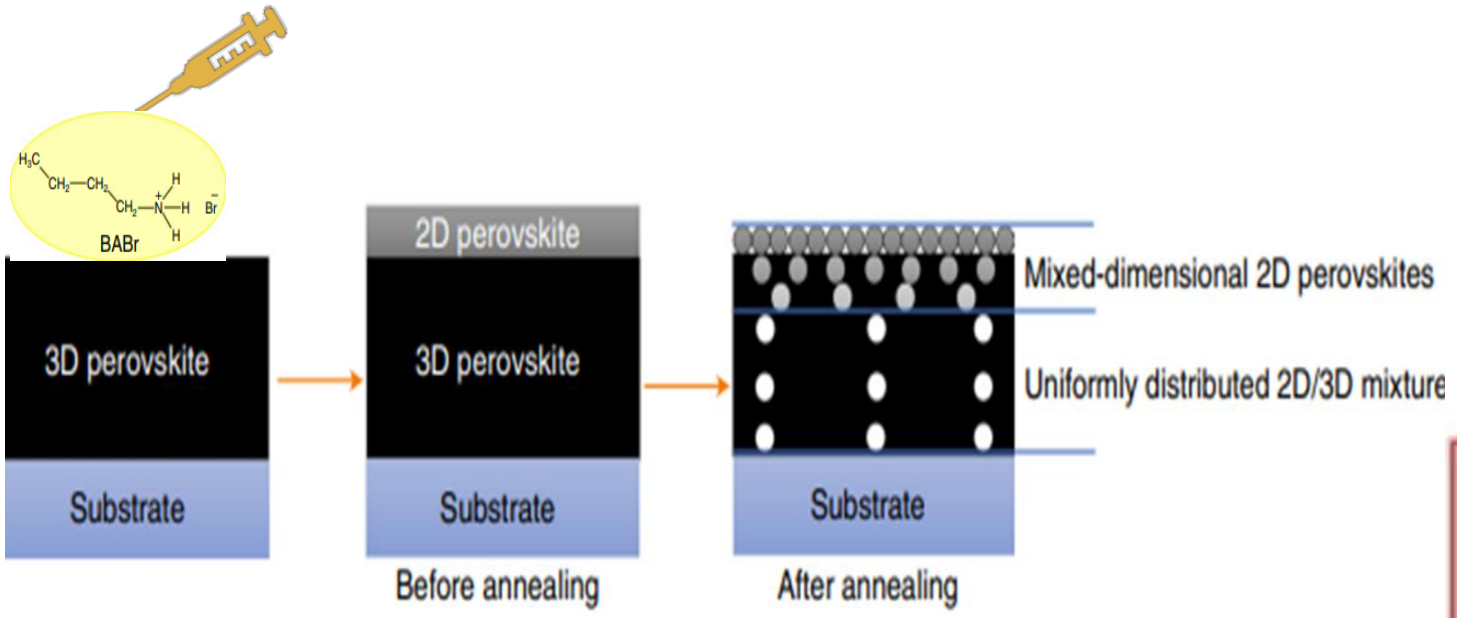
Interfacial passivation

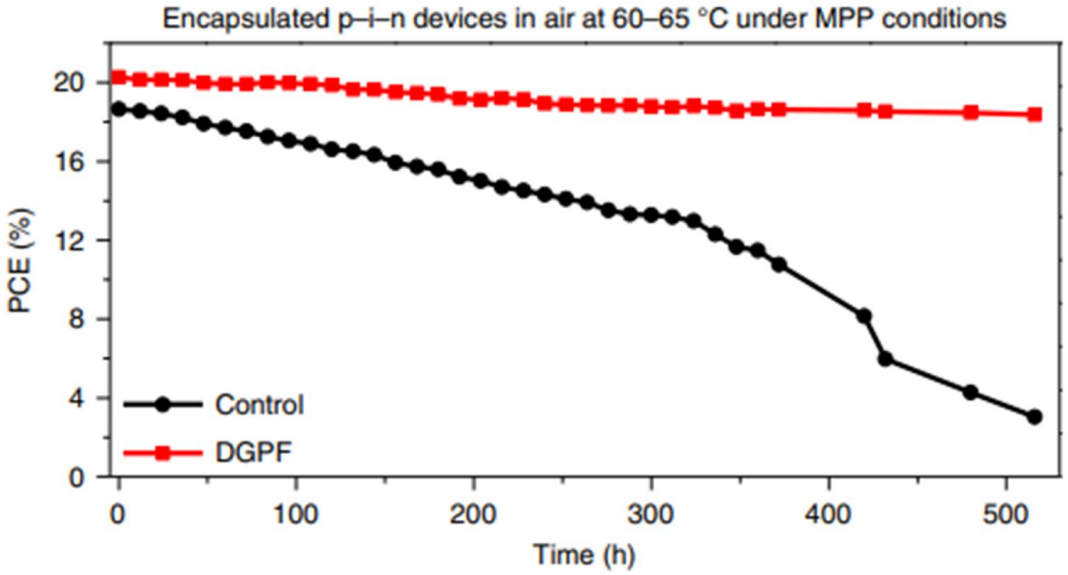


- *Adv. Energy Mater. 2016, 1600372;*
- *Nature NanoTech. 2016, 11,75-81 ;*

Angew. Chem. Int. Ed. 2017, 56, 1190 – 1212

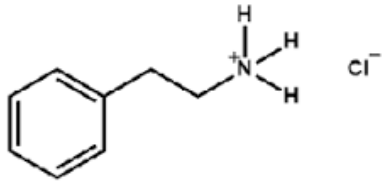
Perovskite Solar Cells: Reports- Surface Passivation

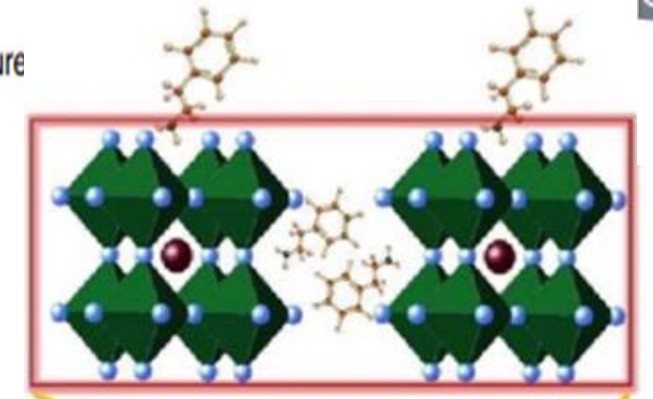


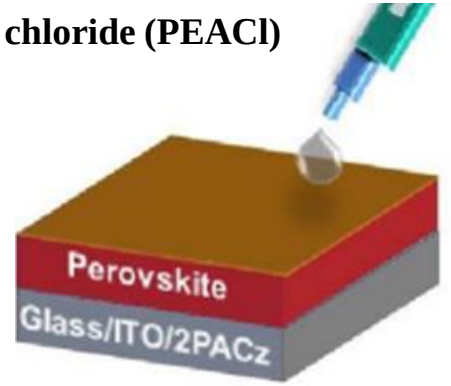


Gang Li and co-workers, *Nature Photonics*, 2021, 15, 681

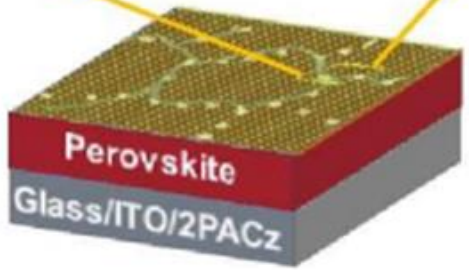
Phenethylammonium chloride (PEACl)



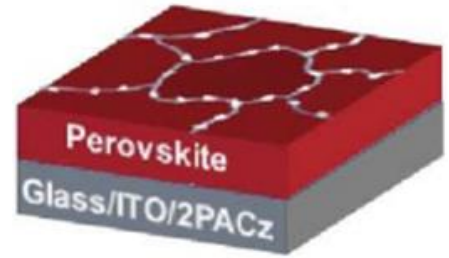




Surface Passivation (SP)



GBP&SP

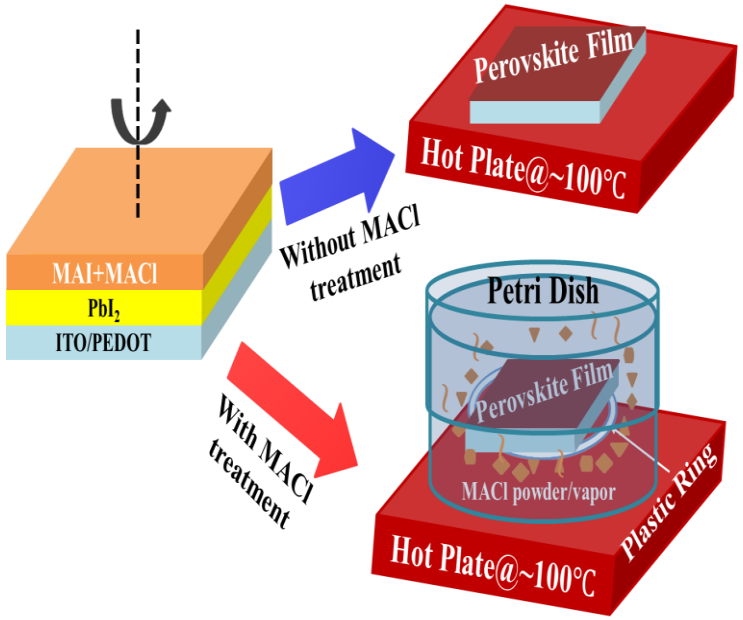


Grain Boundary Passivation (GBP)

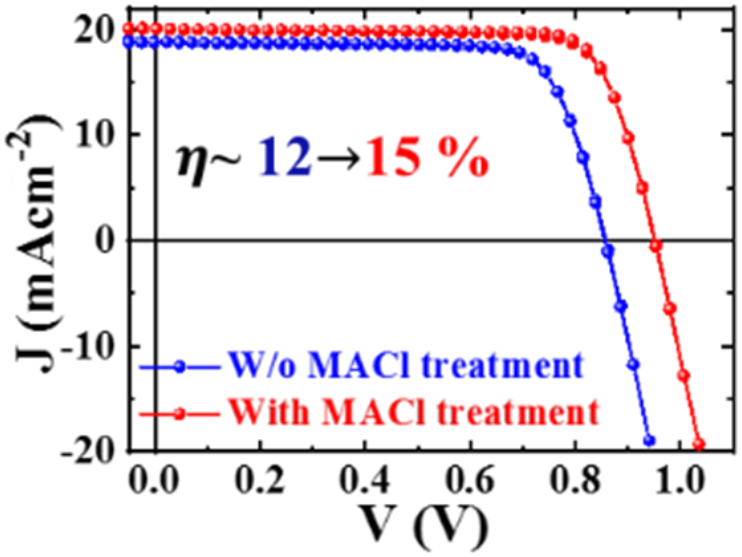
Ulrich W. Paetzold and co-workers, Energy Environ. Sci., 2021,14, 5875

1. Perovskite Solar Cells: Vapor Surface treatment

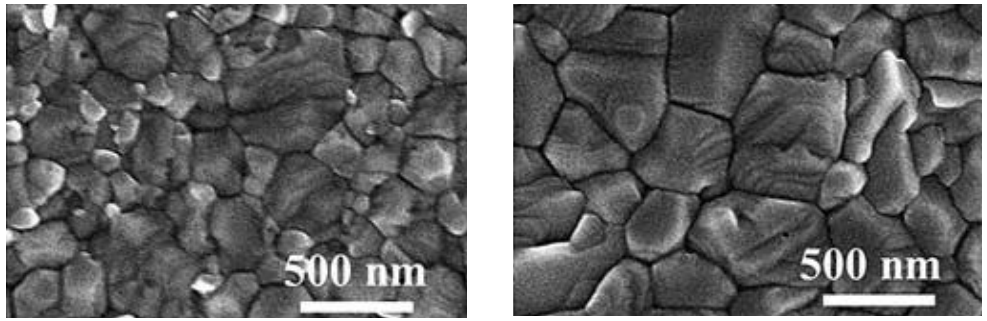
Film crystallization



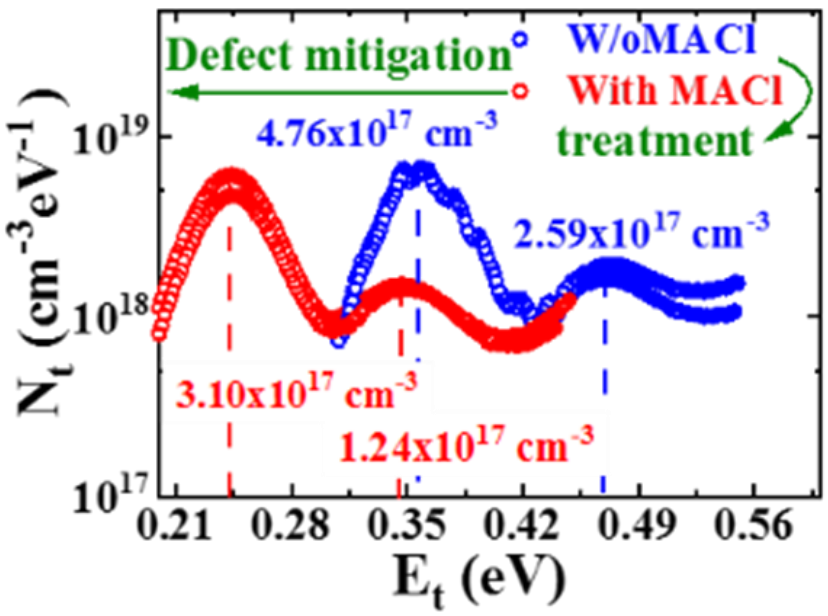
PCE- Improved



Control **MACl-treated**



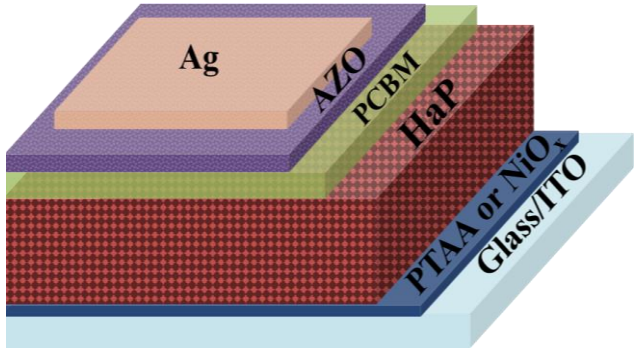
Defect passivation

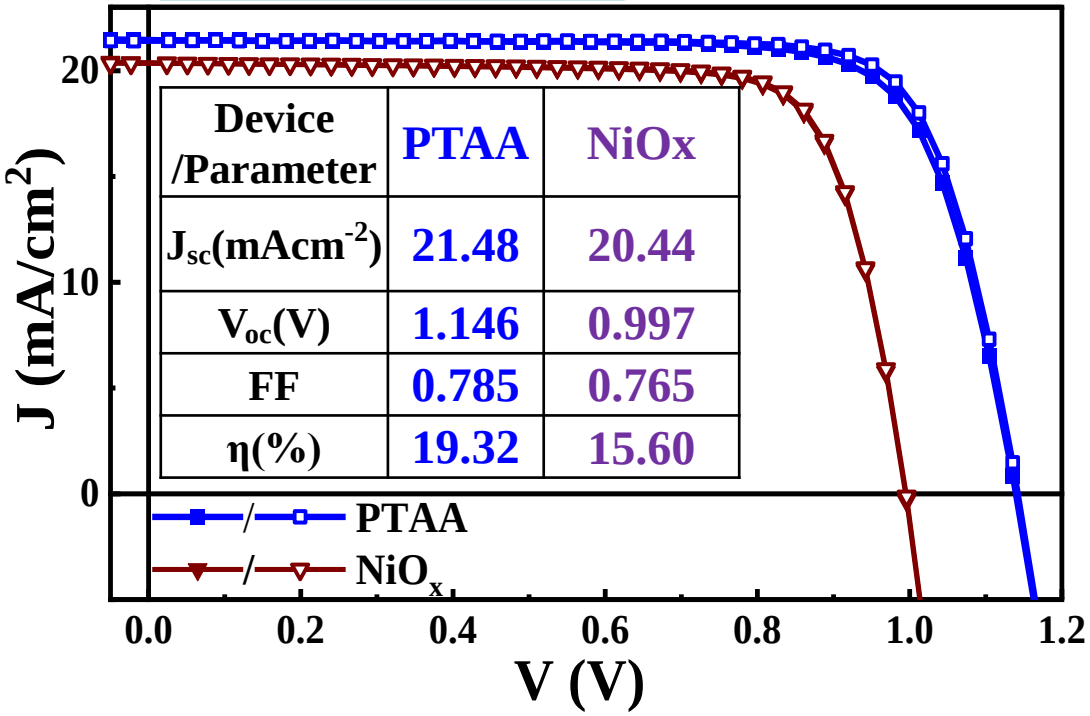


1. Morphology
2. Defect mitigation
3. Improve in optoelectronic quality

- *Khadka et al., Sustain. Energy Fuels, 2017, 1, 755*
- *Khadka et al., J. Mater. Chem. C, 2017, 5,8819*

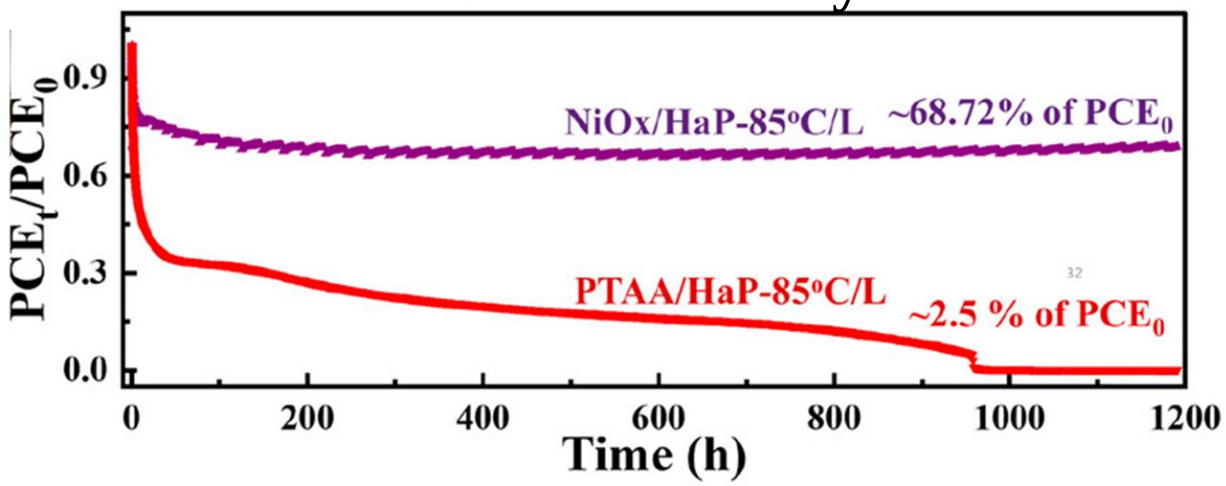
2. PSCs: Impact of carrier transport layer

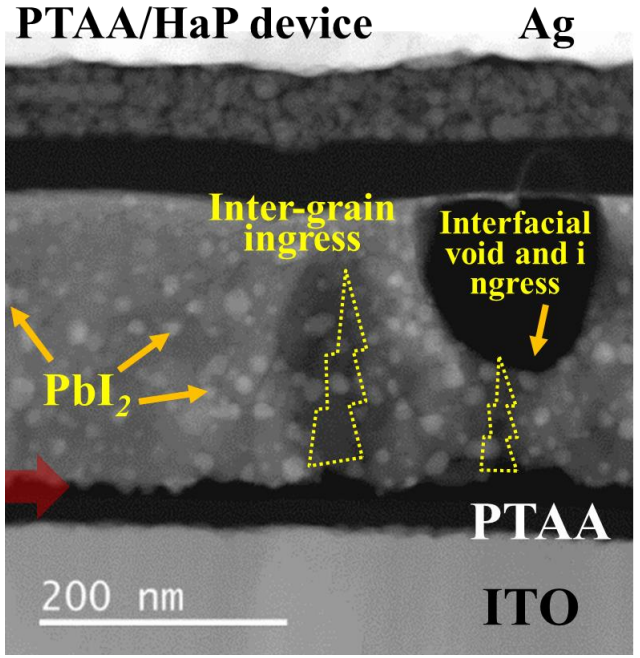


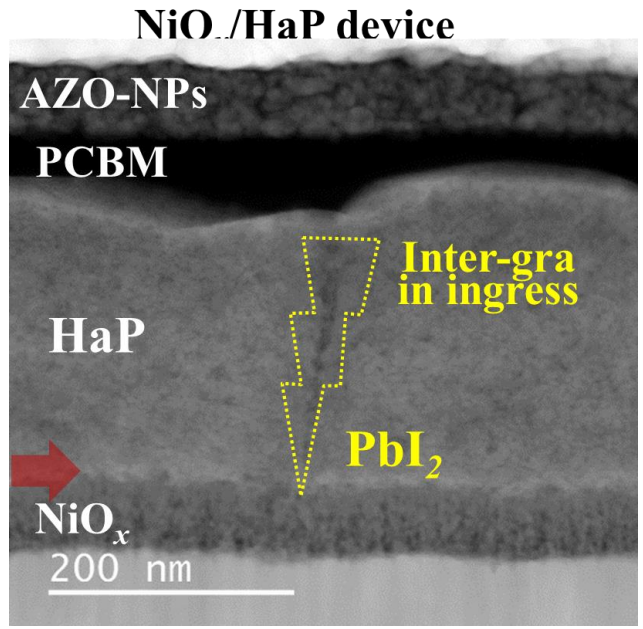


Device /Parameter	PTAA	NiOx
J_{sc}(mAcm^{-2})	21.48	20.44
V_{oc}(V)	1.146	0.997
FF	0.785	0.765
η(%)	19.32	15.60

Device stability

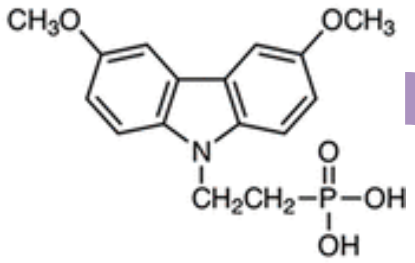




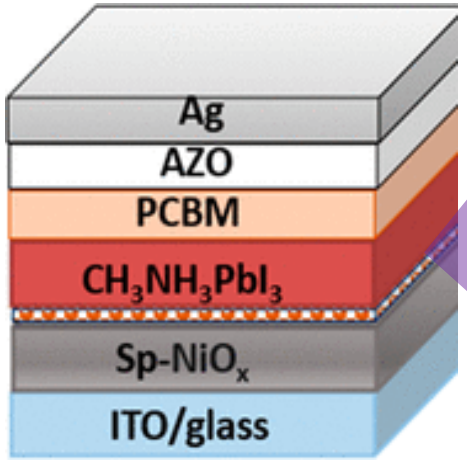


- Khadka et al. ACS Appl. Energy Mater. 2021, 4, 10, 11121
- Khadka et al. ACS Appl. Mater. Interfaces, 2018, 11, 7055
- Khadka et al, ACS Appl. Mater. Interfaces, 2018,10, 22074
- Khadka et al., J. Mater. Chem. C, 2018, 6, 162-170

3. PSCs: NiO_x-surface treatments



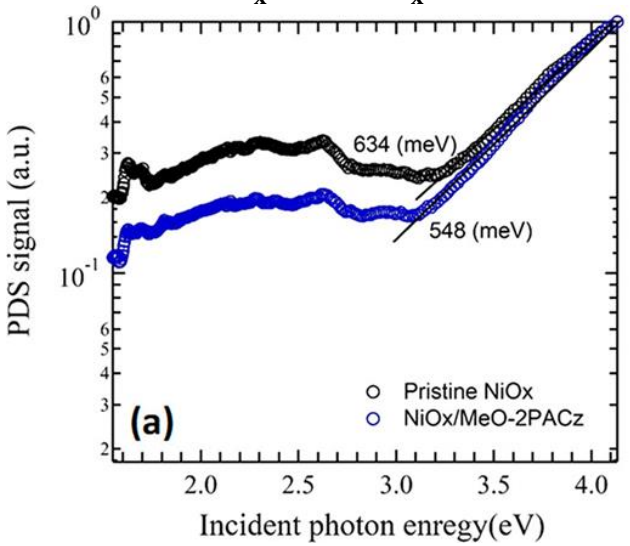
MeO-2PACz



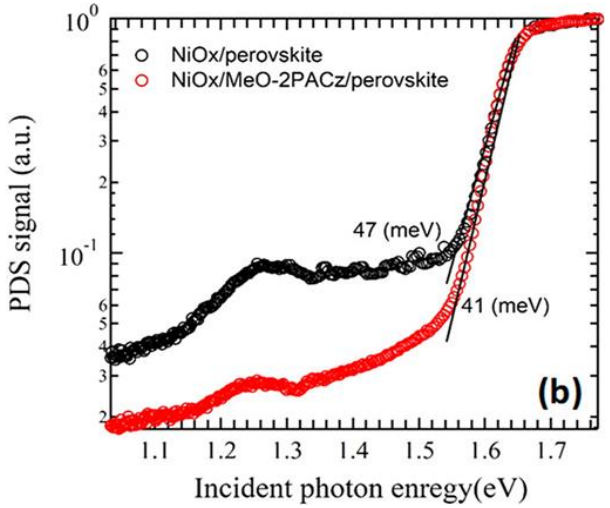
- *Miyano and co-workers, ACS Omega* **2022,** *7*, 12147.

Photothermal Deflection Spectroscopy

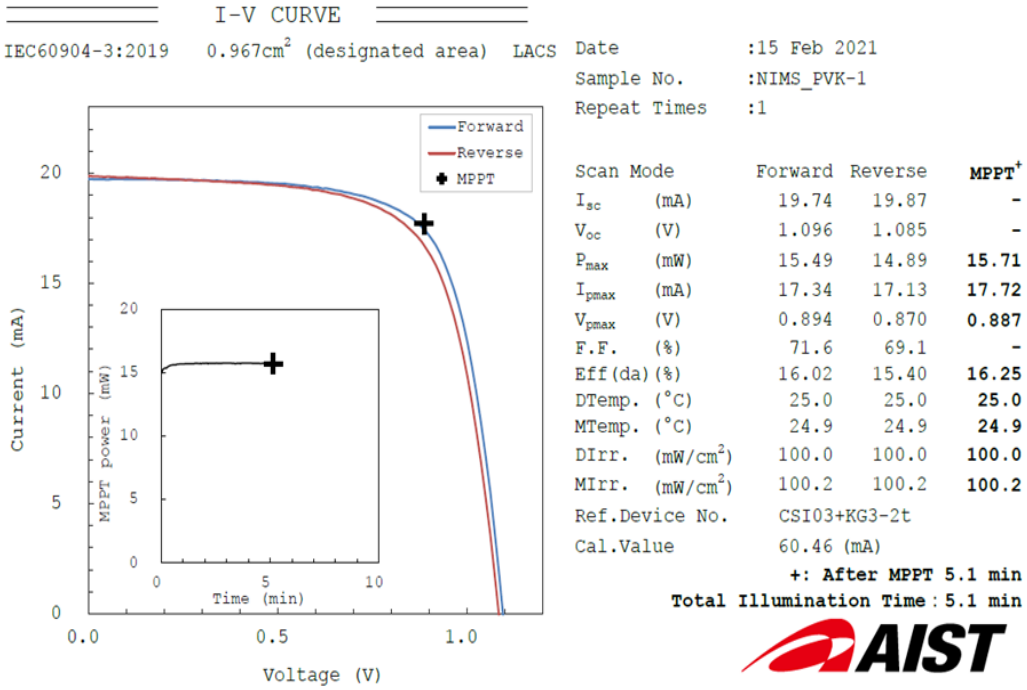
: NiO_x and NiO_x/MeO-2PACz



NiO_x band gap: 3.5~3.7 eV



- ✓ **PCE: 15.60 → 17.2%**
- ✓ **Certified PCE→16.3% @1 cm²**
- ✓ **MAPI device with ~ 270 nm**



Date :15 Feb 2021
Sample No. :NIMS_PVK-1
Repeat Times :1

Scan Mode		Forward	Reverse	MPPT+
I_{sc}	(mA)	19.74	19.87	-
V_{oc}	(V)	1.096	1.085	-
P_{max}	(mW)	15.49	14.89	**15.71**
I_{pmax}	(mA)	17.34	17.13	**17.72**
V_{pmax}	(V)	0.894	0.870	**0.887**
F.F.	(%)	71.6	69.1	-
Eff(da)	(%)	16.02	15.40	**16.25**
DTemp.	(°C)	25.0	25.0	**25.0**
MTemp.	(°C)	24.9	24.9	**24.9**
DIrr.	(mW/cm²)	100.0	100.0	**100.0**
MIrr.	(mW/cm²)	100.2	100.2	**100.2**
Ref.Device No.		CSI03+KG3-2t		
Cal.Value		60.46 (mA)		

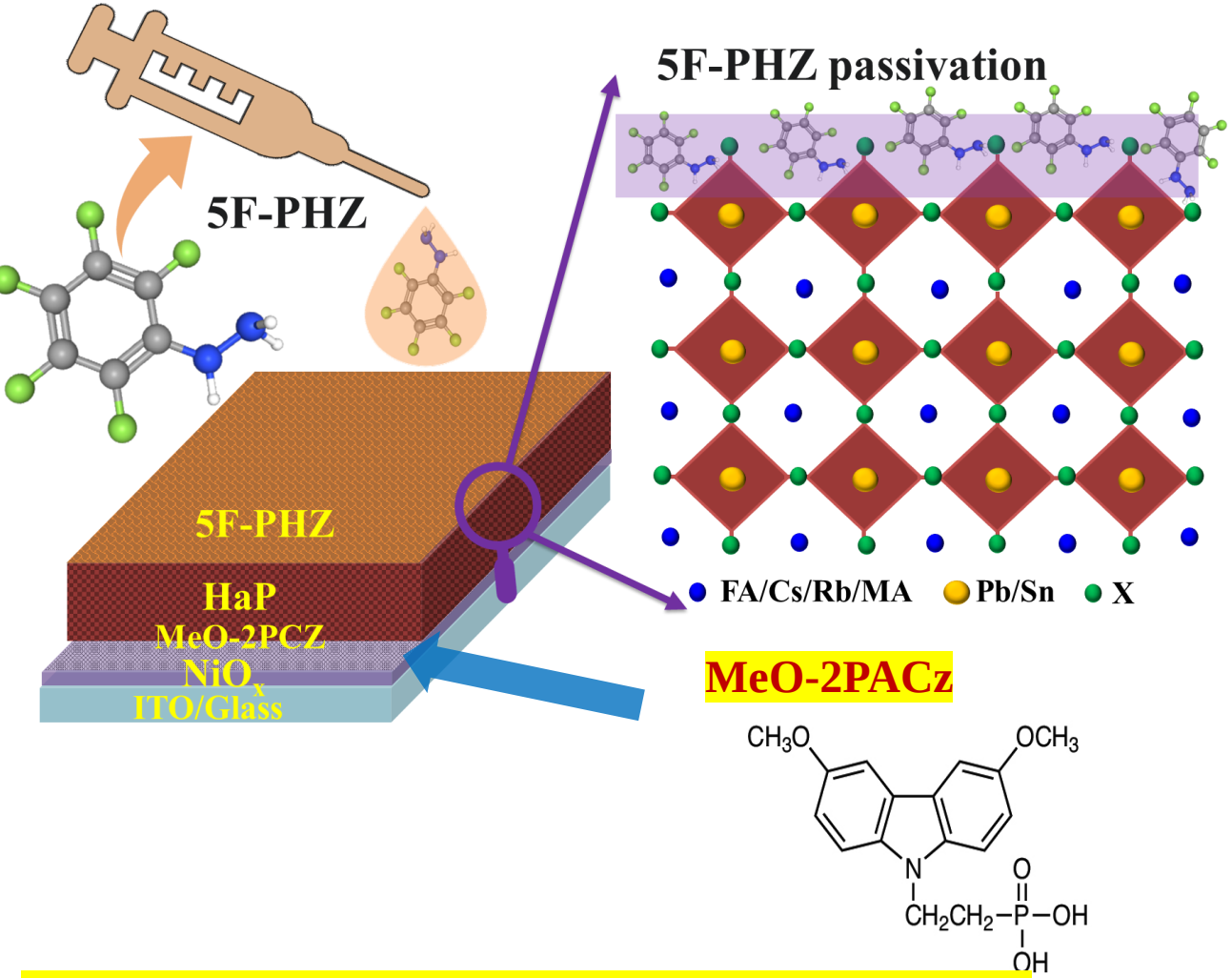
+: After MPPT 5.1 min
Total Illumination Time : 5.1 min

AIST

4. PSCs: Passivation on top and bottom of the perovskite layer

✓ Two-step → One-step method; ~270nm → ~500nm

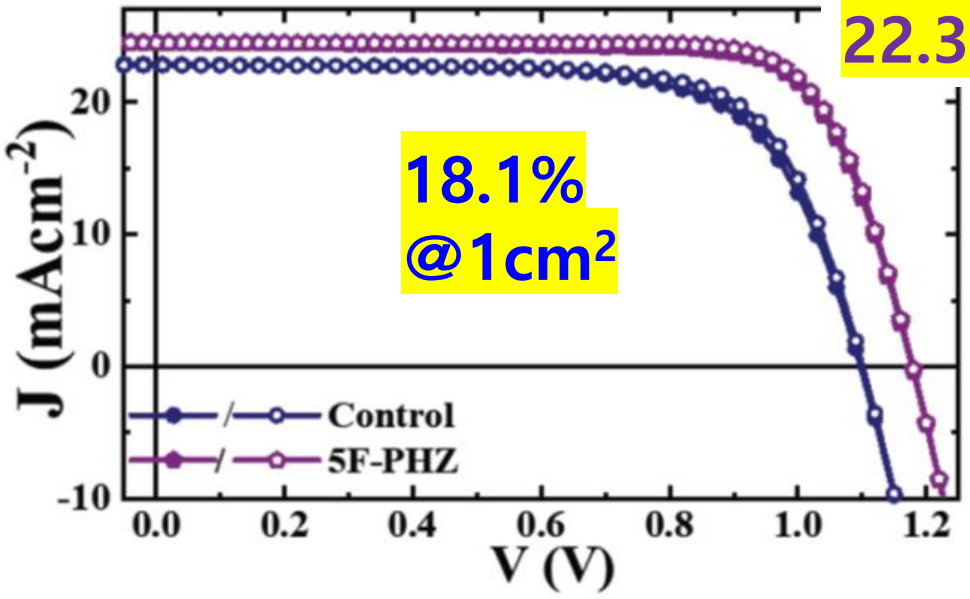
✓ $MAPbI_3$ → $FA_{0.84}Cs_{0.12}Rb_{0.04}PbI_3$



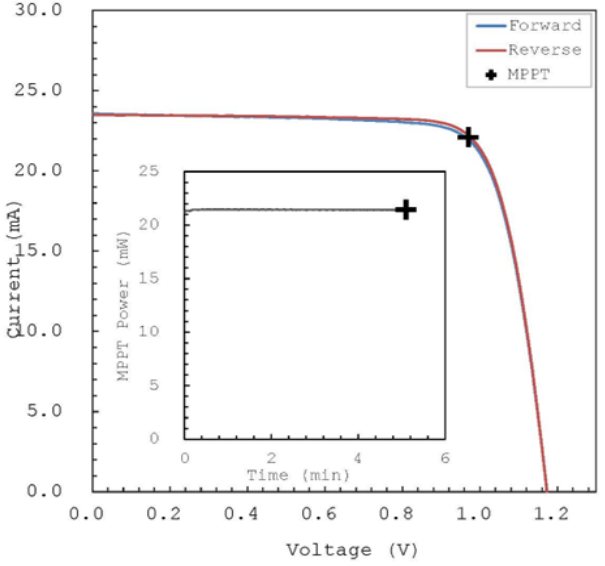
MeO-2PACz

22.3%

18.1%
@1cm²



IEC 60904-3:2019 1.026 cm² (designated area) LACS

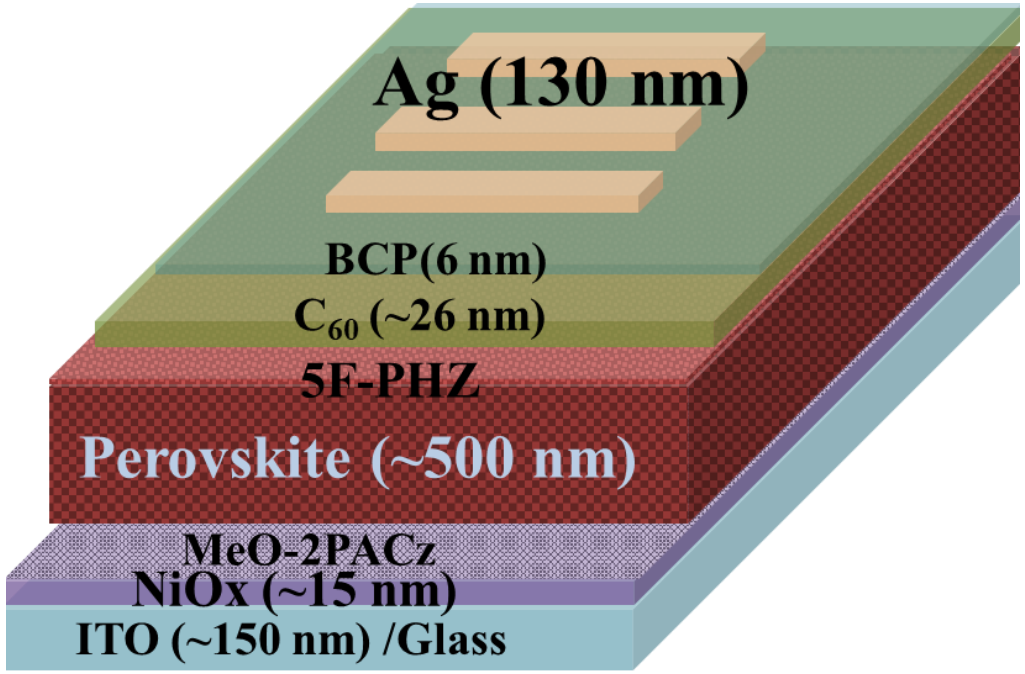


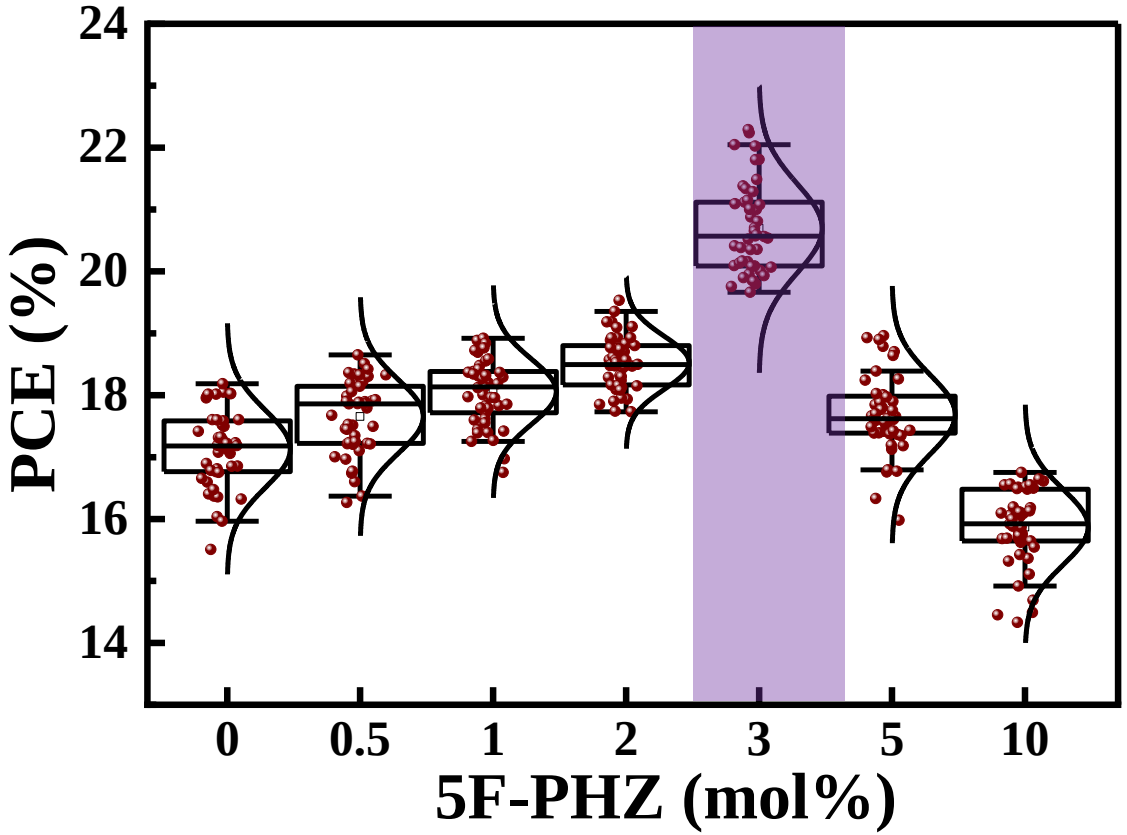
Date		:14 Feb 2022		
Sample No.		:NIMS_FAPVK-3		
Repeat Times		:1		
Scan Mode		Forward	Reverse	MPPT+
I_{sc}	(mA)	23.58	23.50	-
V_{oc}	(V)	1.173	1.173	-
P_{max}	(mW)	21.31	21.56	21.44
I_{pmax}	(mA)	21.89	22.17	22.11
V_{pmax}	(V)	0.973	0.973	0.970
F.F.	(%)	77.0	78.2	-
Eff(da)	(%)	20.77	21.01	20.90
DTemp.	(°C)	25.0	25.0	25.0
MTemp.	(°C)	25.2	25.2	25.2
Dirr.	(mW/cm²)	100.0	100.0	100.0
Mirr.	(mW/cm²)	99.6	99.6	99.6
Ref.Device No.		CSI03+KG3-2t		
Cal.Val.of Ref.		60.22 (mA at 100mW/cm²)		

+: After MPPT 5.1 min
Total Illumination Time : 5 min

Khadka et al. Adv. Energy Mater. 2022, 12, 2202029

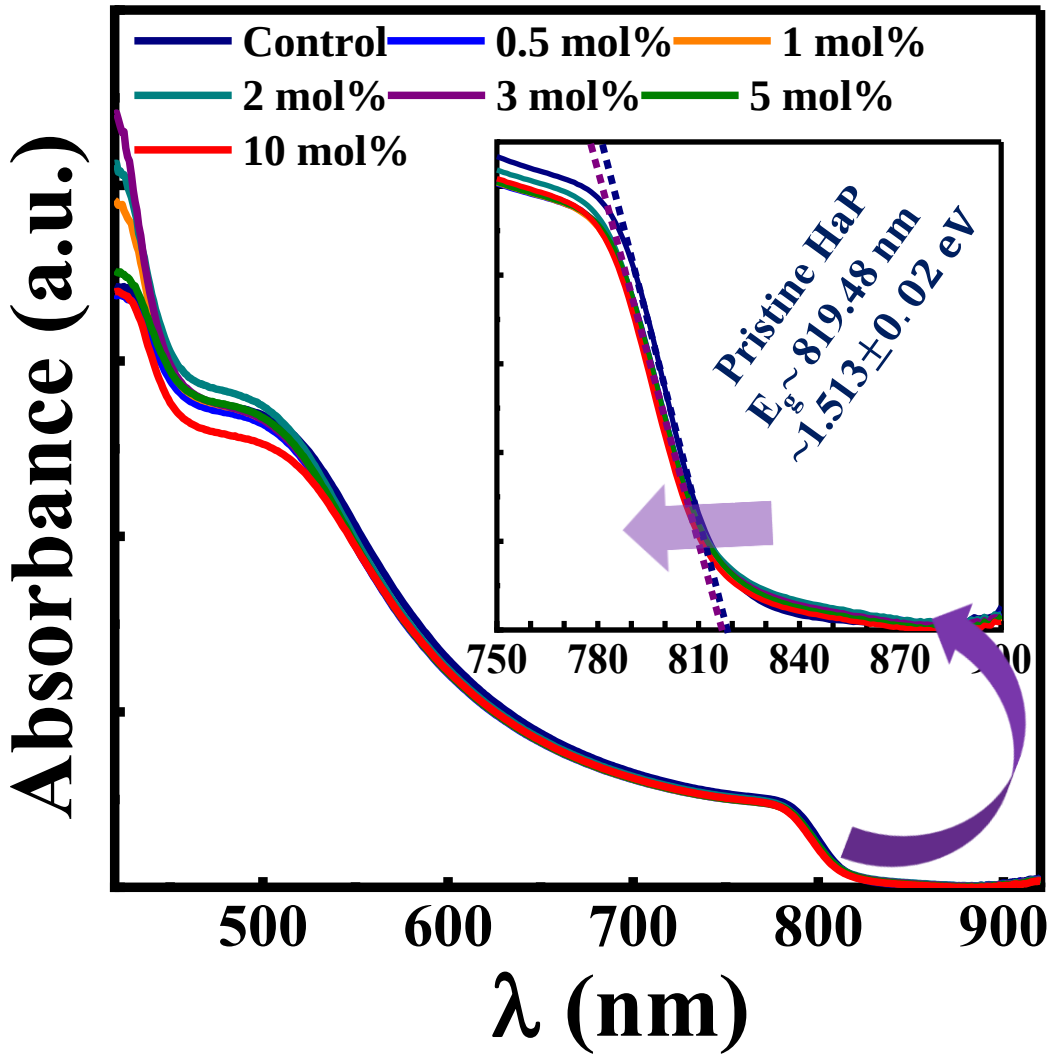
Pb-HaP: 5F-PHZ treated: Device trend

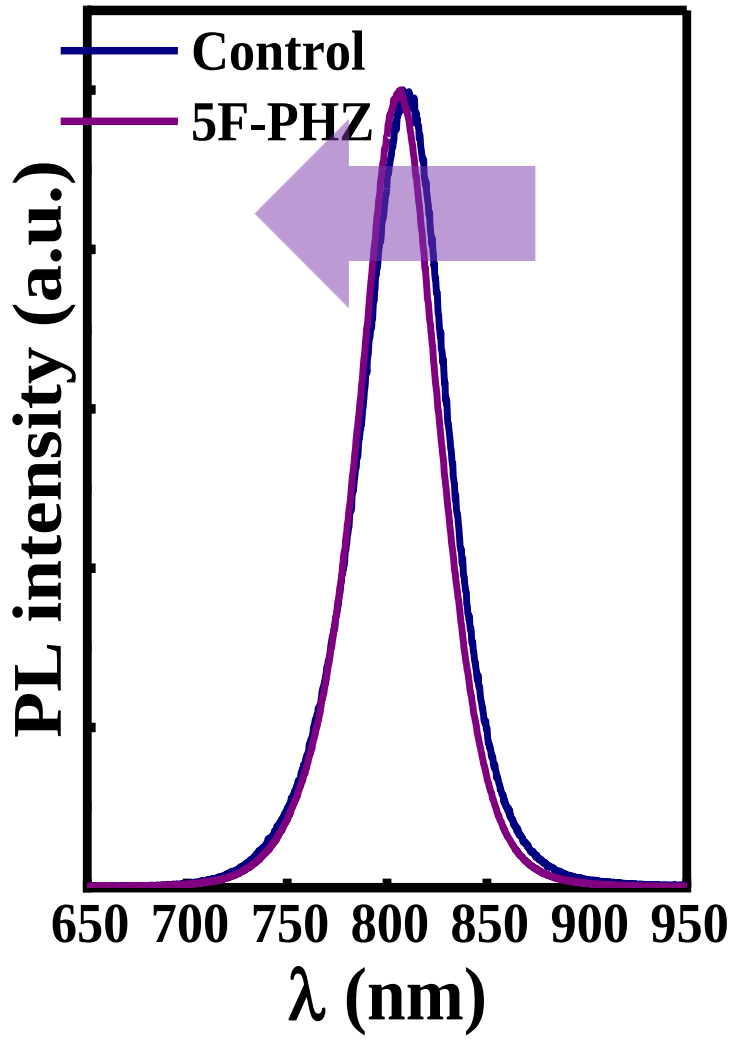




5F-PHZ treated: Opto-physical properties

✓ **Absorption spectra**



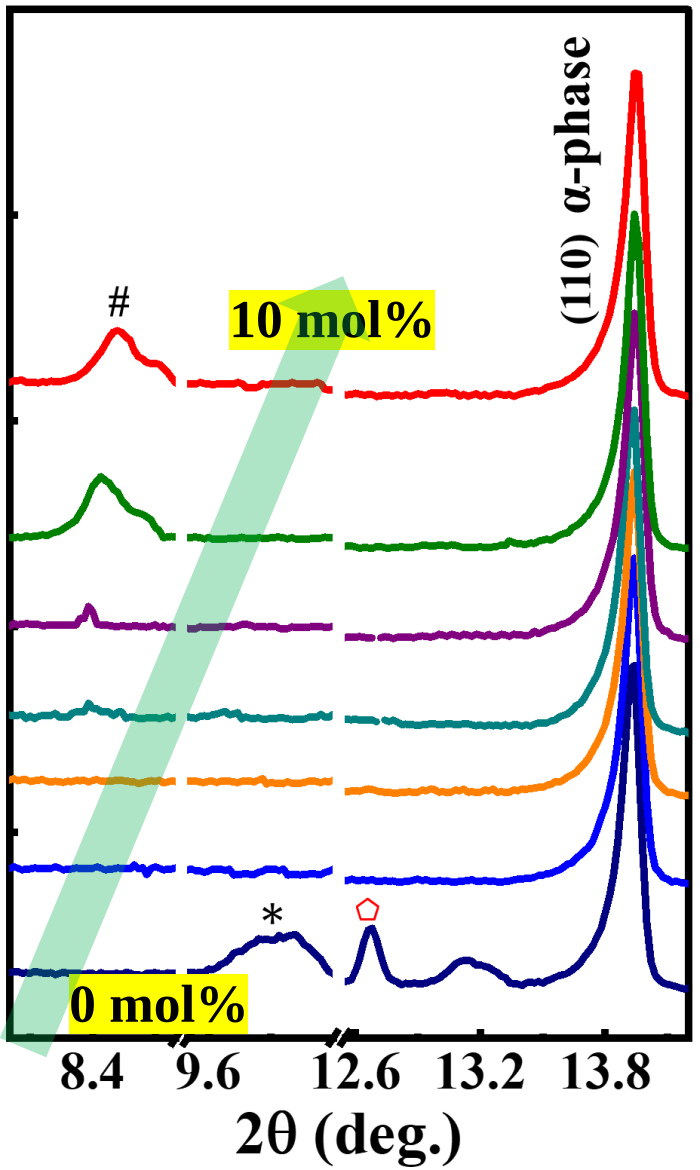


✓ **PL characteristics peak**

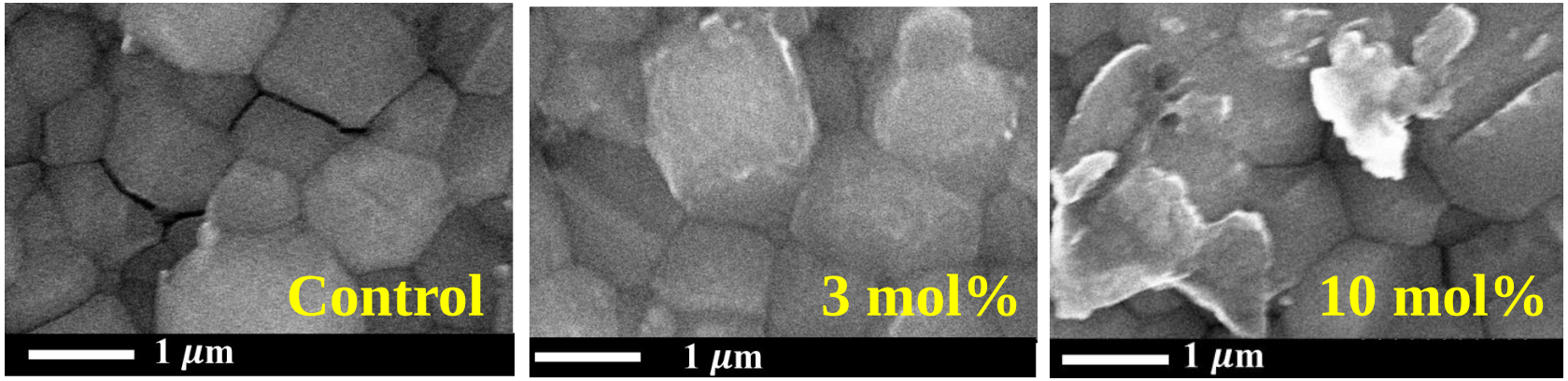
✓ **Blue shift with 5F-PHZ**

5F-PHZ treated: Effect on materials growth

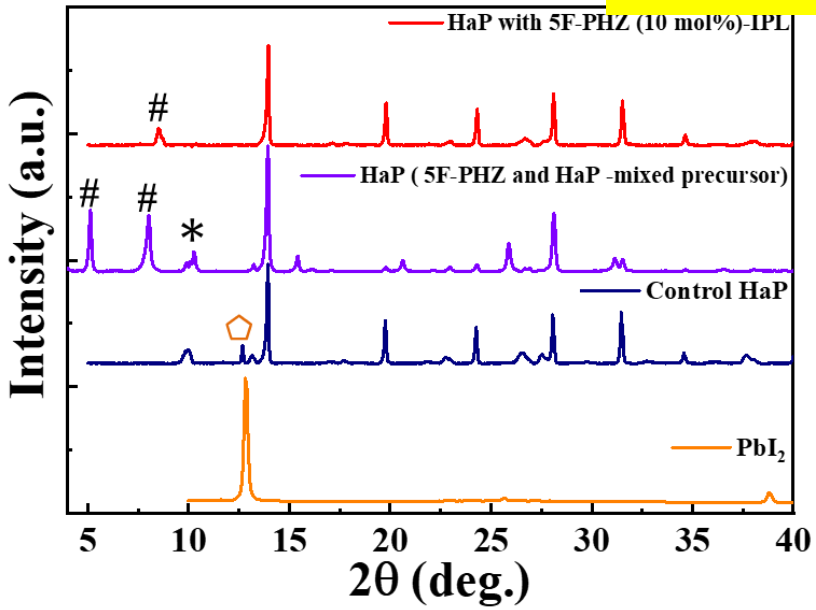
XRD results

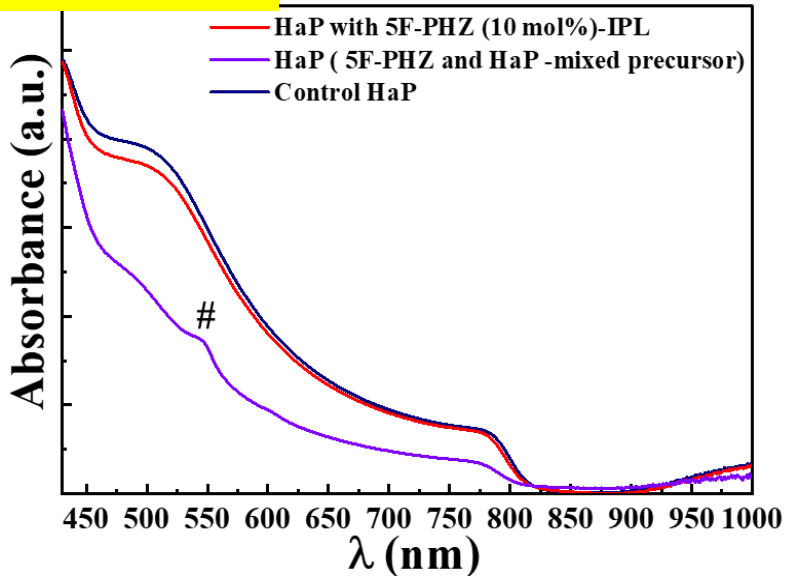


✓ **5F-PHZ additive: well coverage on the surface**

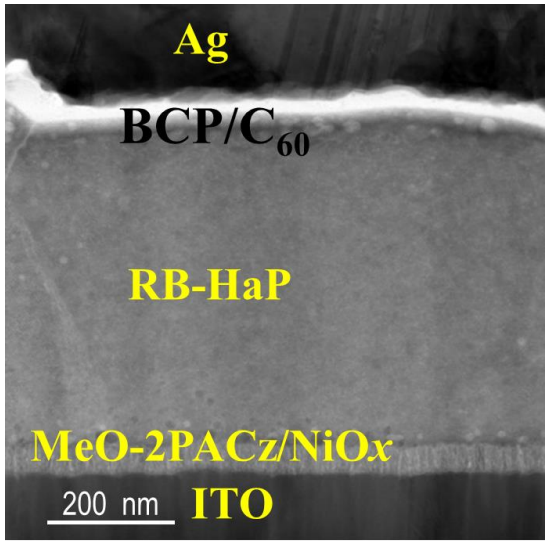


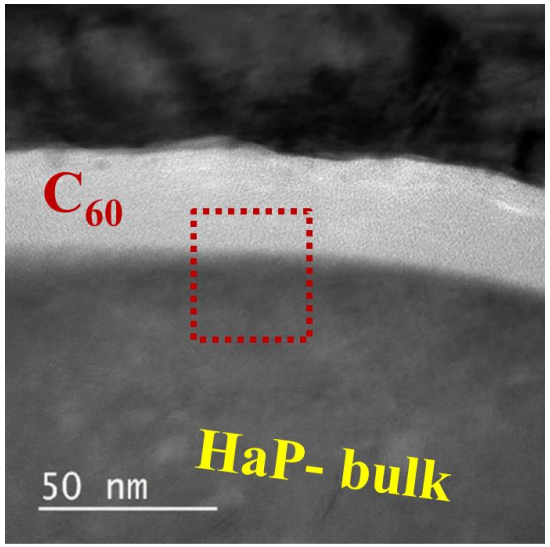
Mixed precursor

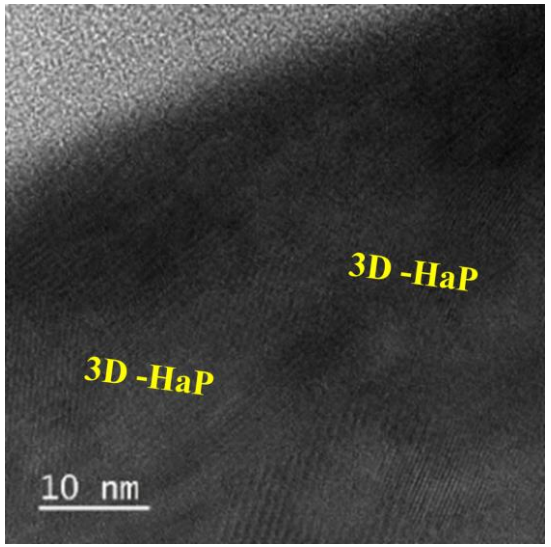


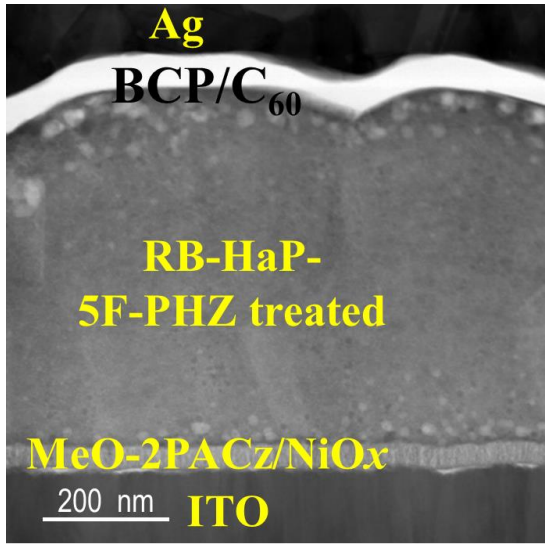


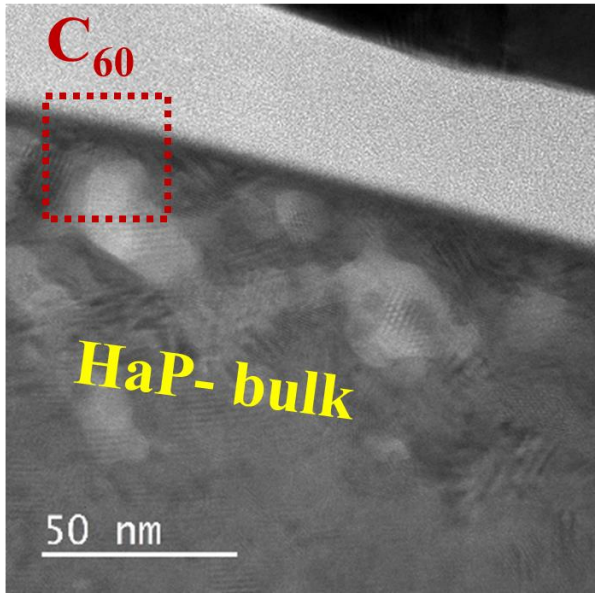
7. STEM images: Interface formation

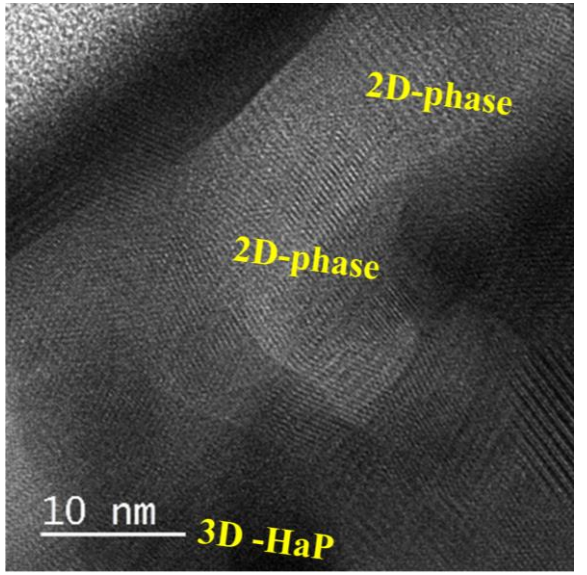




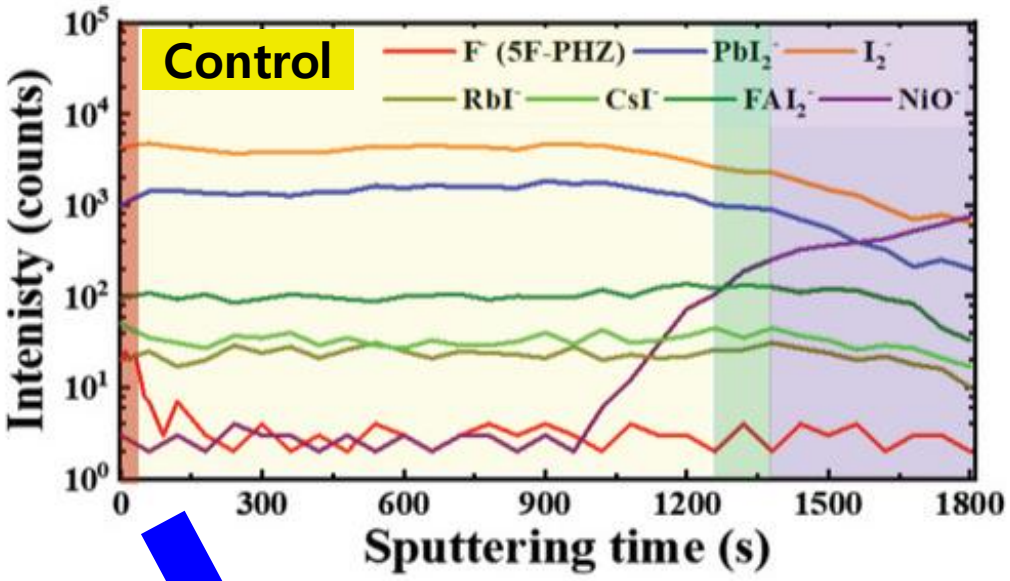


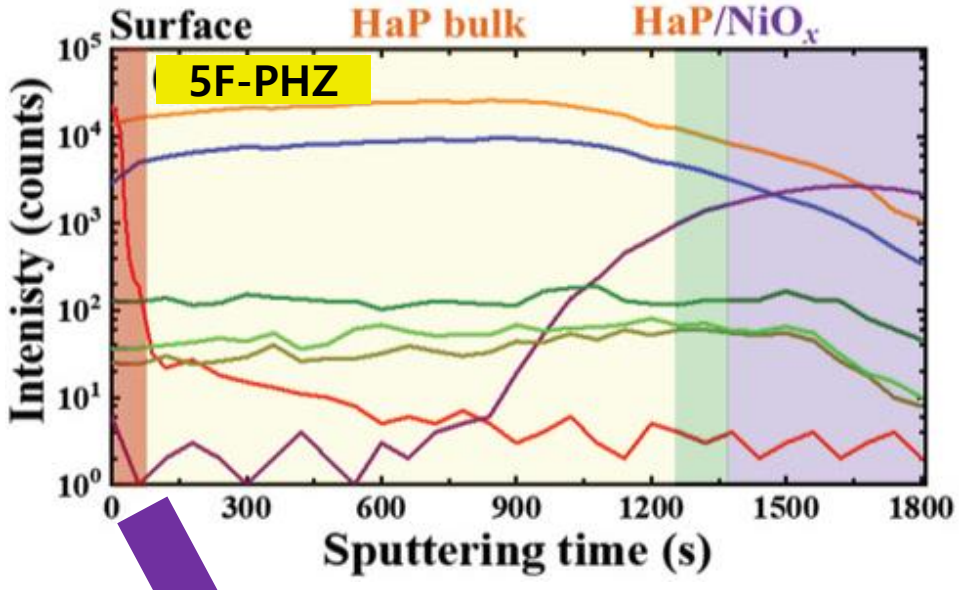


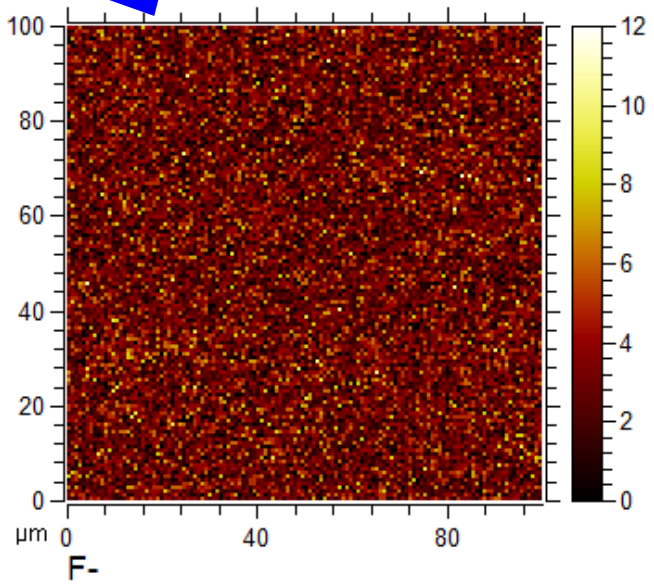




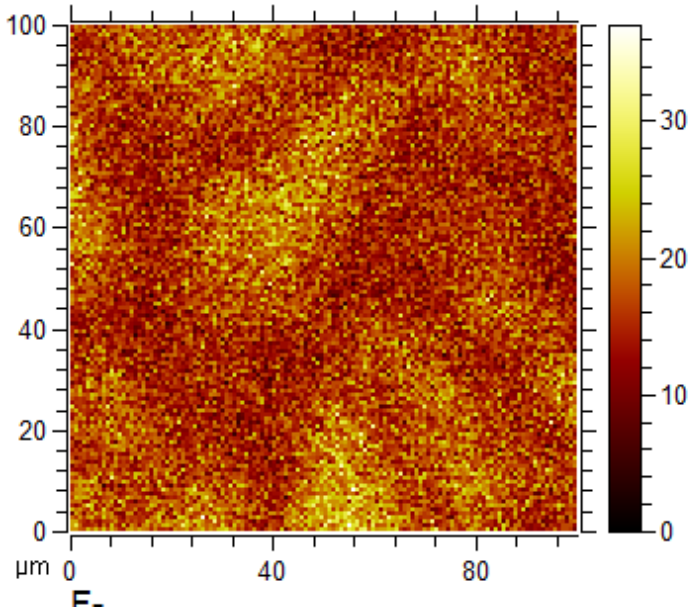
PSCs-5F-PHZ: ToF-SIMS spectra





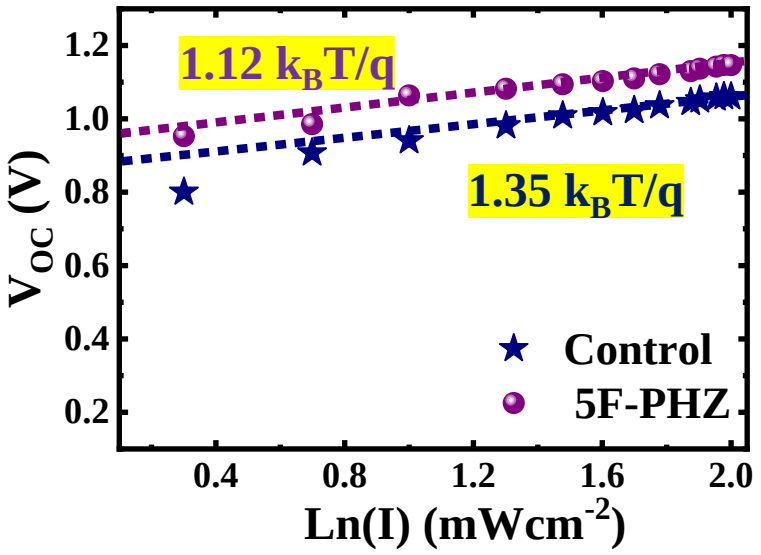


ToF-SIMS; 5F-PHZ
2D images



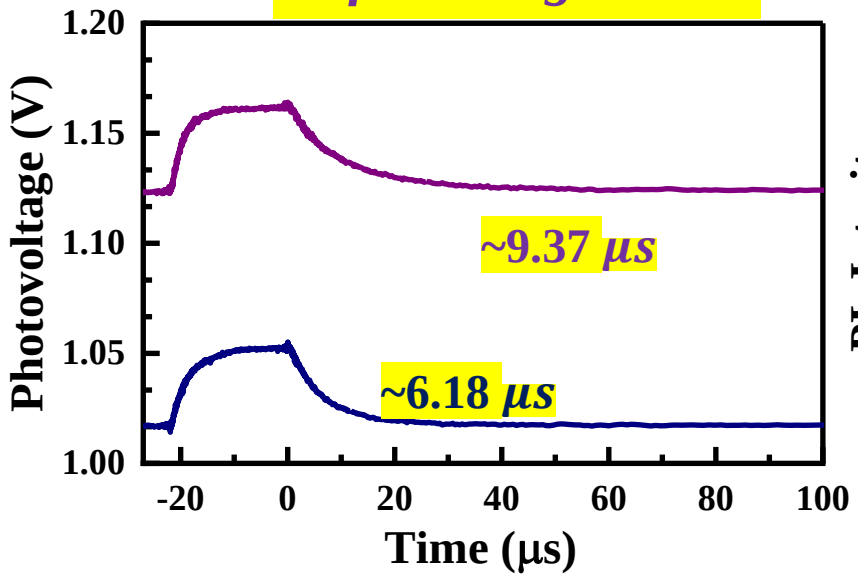
6. PSCs- NiO_x-surface treatments: PhotoPhysics

V_{OC}-I analysis



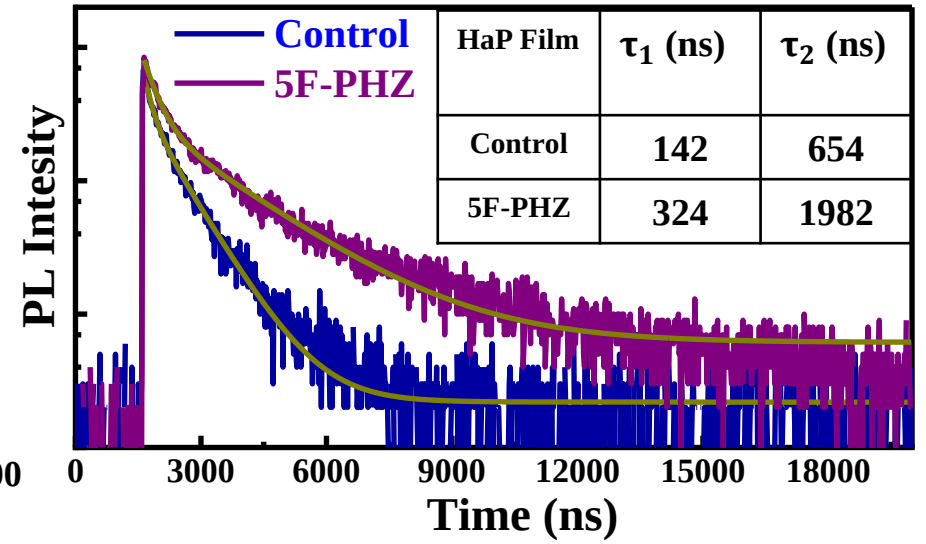
Transient Photovoltage response

Longer lifetime: defect mitigation



TRPL results

Longer carrier lifetime

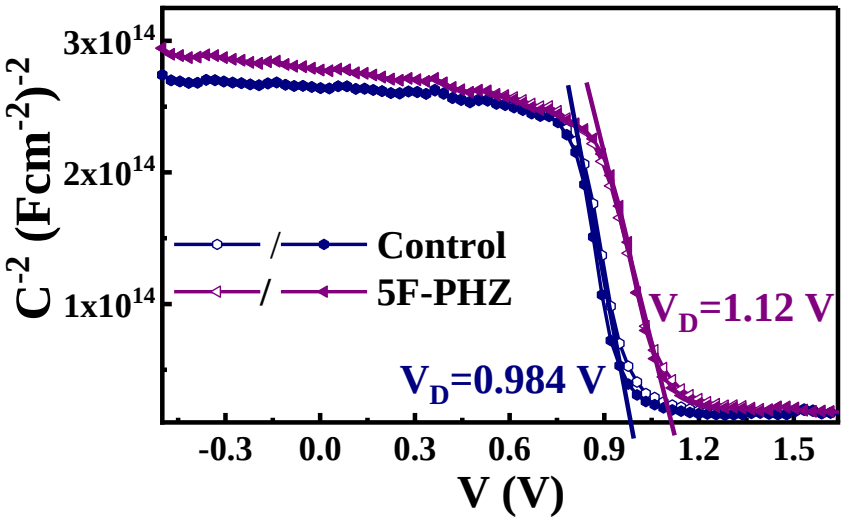


HaP Film	τ_1 (ns)	τ_2 (ns)
Control	142	654
5F-PHZ	324	1982

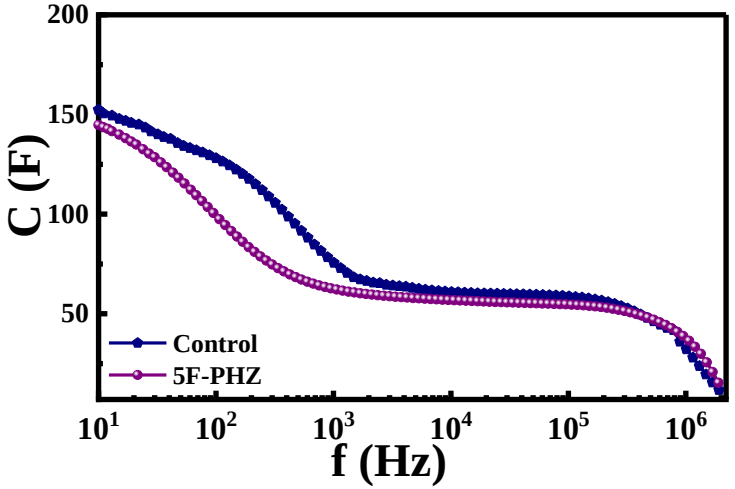
PSCs: Capacitance-Analysis

➢ **Mott-schotky plot**

$$C(V)^{-2} = -\frac{2}{q\varepsilon_0\varepsilon_s N_A(x)}(V + V_D)$$



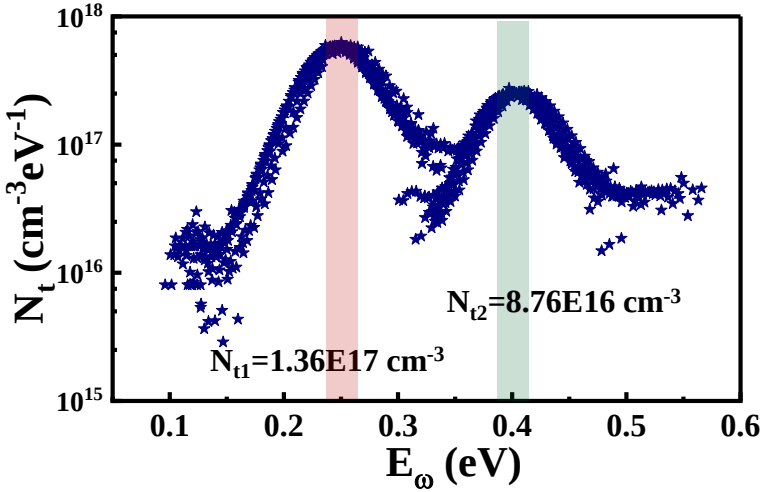
➢ **C-f spectra**



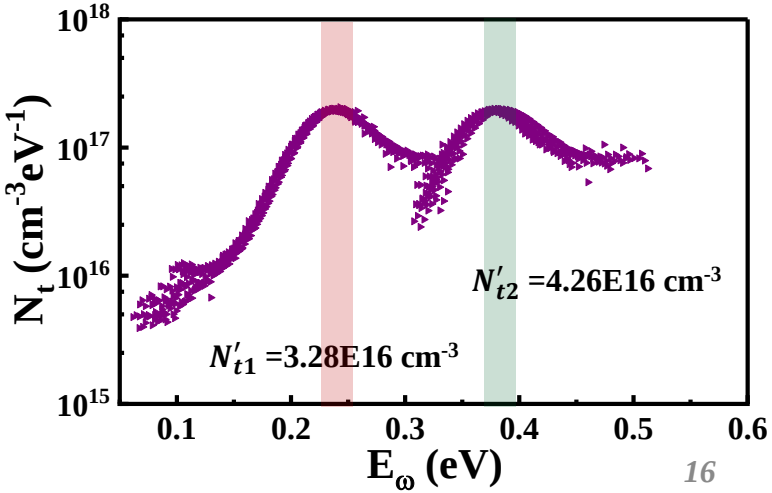
➢ **C-f-T analysis**

➢ **Defect profile**

$$N_t = -\frac{V_{bi}}{ew}\left(\frac{\omega}{k_B T}\frac{dC}{d\omega}\right)$$



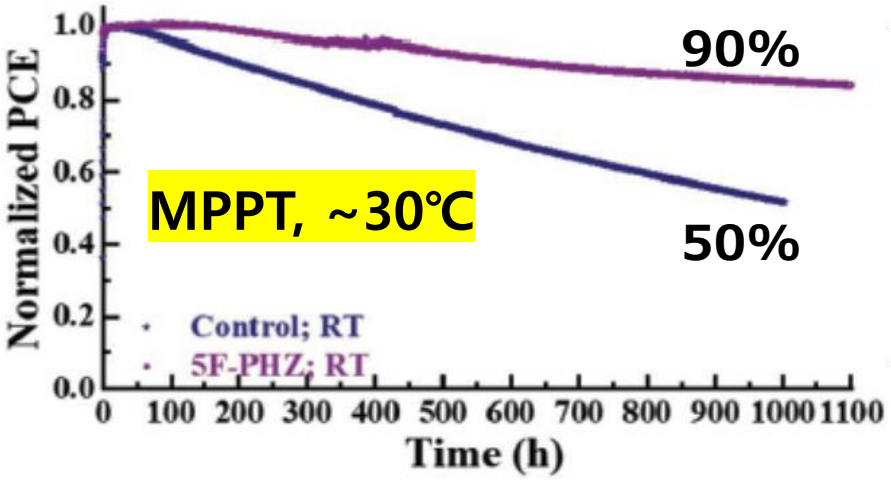
➢ **Defect densities- attenuated**

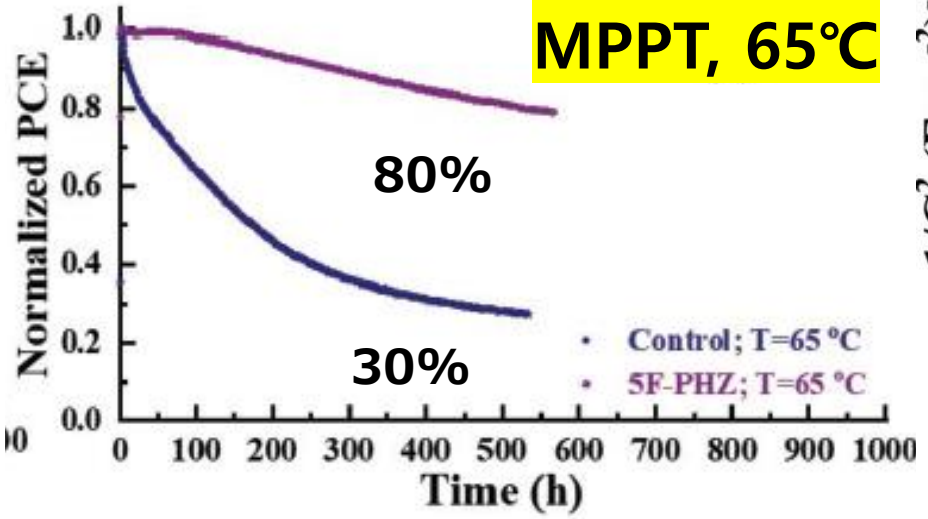


➢ **Increase in diffusion potential (V_D)**

5. PSCs- Surface passivation: device stability/ capacitance

High Stability

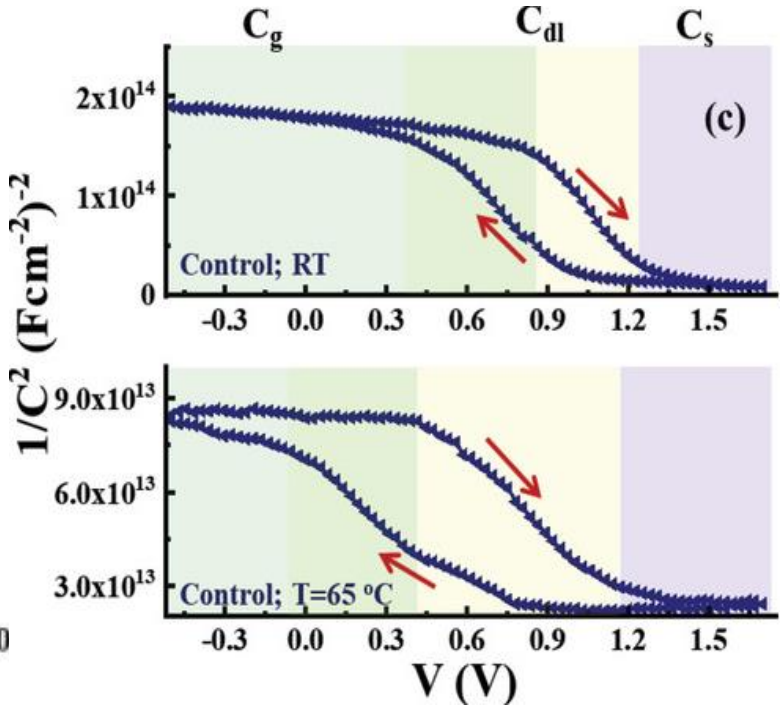




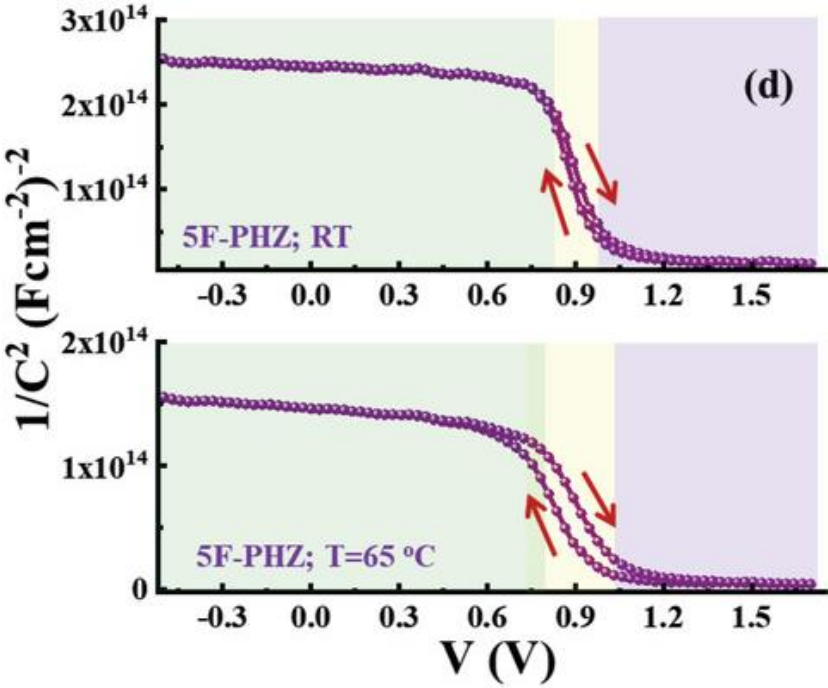
Over 22 % @1 cm^2
Maintain 20% after 1000 hr

- ***Capacitance Spectra***
- ***Degradation trend***

Hysteresis:
Ionic or charge carrier accumulation



Retain- intrinsic properties



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6. PSCs: perovskite system passivation method

➢ **Passivation method is applicable to different band gap perovskite devices**

Perovskite composition	Condition	E_g^a [eV]	J_{SC} [mAcm^{-2}]	V_{OC} [V]	FF	PCE [%]	(E_g^a/q -V_{OC}) [V]
$Rb_{0.04}Cs_{0.12}FA_{0.84}PbI_3$ (RG-HaP)	Control	1.514	22.88	1.096	0.722	18.10 (17.26 ± 0.64)	0.418
	5F-PHZ	1.516	24.51	1.178	0.772	22.29 (21.03 ± 0.65)	0.338
$RbCsFAPb(I_{0.64},Br_{0.36})_3$ (WG-HaP)	Control	1.721	18.24	1.241	0.739	16.73 (15.62 ± 0.71)	0.480
	5F-PHZ	1.725	19.28	1.283	0.765	18.92 (18.32 ± 0.42)	0.442
$Cs_{0.05}MA_{0.1}FA_{0.85}(Pb_{0.5},Sn_{0.5})I_3$ (NG-HaP)	Control	1.246	30.72	0.758	0.722	16.81 (15.23 ± 0.98)	0.488
Note: PEDOT:PSS for HTL	5F-PHZ	1.246	31.16	0.831	0.747	19.34 (18.74 ± 0.57)	0.415

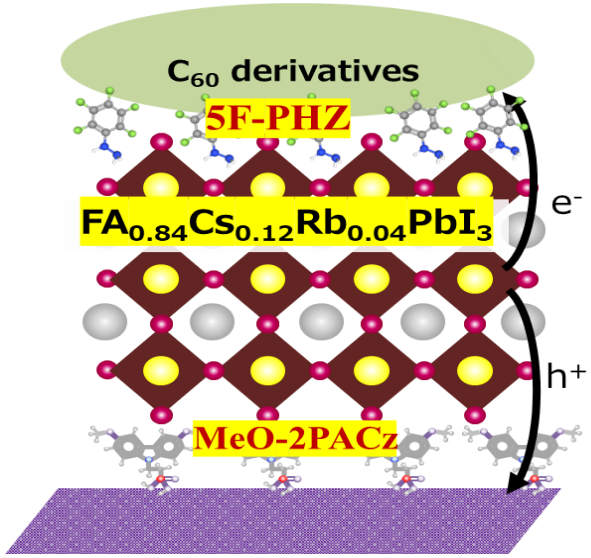
✓ **Highly efficient semi-transparent devices with wide-bandgap perovskite devices (V_{OC}-1.32V, PCE>17%)**

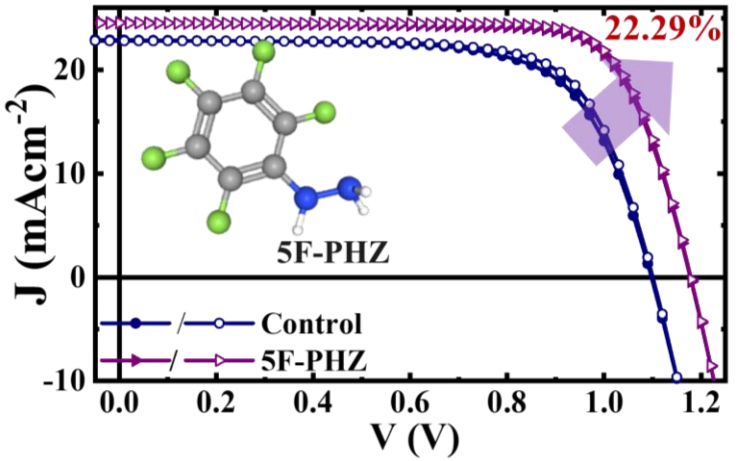
✓ **Possibility achieve all-perovskite tandem devices with wide- and narrow-band gap devices**

Report Summary

5F-PHZ passivation in Pb-HaP

- *Interface modulation with fluoroarene functional derivatives*
- *Form interfacial embedded 2D-layers*
- *Attenuate defect densities and suppress of ion migration*
- *PCE increase from 18% to > 22 % - with superior stability*





Team/ Acknowledgements

Photovoltaic Materials Group

Thank you for your attention



Our team



nanoGe Home Program Location Social dinner Sponsor Space COVID Protocol Important dates and information Sponsorship Contact Us

Registration

Signup Login

Schedule

	Sunday, Jan 22	Monday, Jan 23			Tuesday, Jan 24		
8:00 - 8:45		Registration					
8:45 - 8:55		Opening					
8:55 - 9:00					Announcement of the day		
9:00 - 9:45		Ryan, James			Snaith, Henry		
9:45 - 10:15		Nguyen, ThucQuyen			Hayase, Shuzi		
10:15 - 10:45		Fabregat-Santiago, Francisco			Ho-Baillie, Anita		
10:45 - 11:15		Coffee Break			Coffee Break		
11:15 - 11:45		Kovalenko, Maksym			Miyasaka, Tsutomu		
11:45 - 12:15		Freitag, Marina			Mhaisalkar, Subodh		
12:15 - 12:20		Tanabe, Taro			Justianto, Madeleine		
12:20 - 12:50		Murakami, Takurou			Han, Liyuan		
12:50 - 12:55		Sorbello, Luca			Li, Natalie Lok Kwan		
12:55 - 13:25		Kanemitsu, Yoshihiko			Shin, Hyunjung		
13:25 - 15:00		Lunch break			Lunch break		
15:00 - 15:30		PERRIN, Lara	Bessho, Takeru	Jung, Hyun Suk	Shen, Qing	Kogo, Atsushi	Saeki, Akinori
15:30 - 15:45		Habazaki, Hiroki	He, Yakun	Bodnarchuk, Ma...	Ishikawa, Ryo	KHADKA, DHRU...	Rajamanickam, ...
15:45 - 16:00		Tsuji, Ryuki	Sharma, Romika	Shen, Zhongjin	Pitaro, Matteo	Jenatsch, Sandra	Jeon, Jihun
16:00 - 16:15		Valsalakumar, Sr...	Cabas Vidani, An...	Neild, Amy	Zargar, Fatemeh	Flores-Diaz, Natalie	Nakamura, Tomoya
16:15 - 16:30		Kawaraya, Masa...	Luo, Xinhui	Murdey, Richard	Wang, Shuanglong	Raifuku, Itaru	Wu, Tianhao
16:30 - 17:00		Poster session			Coffee Break		
17:00 - 17:15	Registration				Diau, Eric Wei-Guang		
17:15 - 17:30	Welcome drink						
17:30 - 18:00					Park, Nam-Gyu		
18:00 - 18:15							
18:15 - 18:30					Closing		
18:30 - 19:00							