

The 1st KOSEN Research International Symposium



March 1-2 , 2023

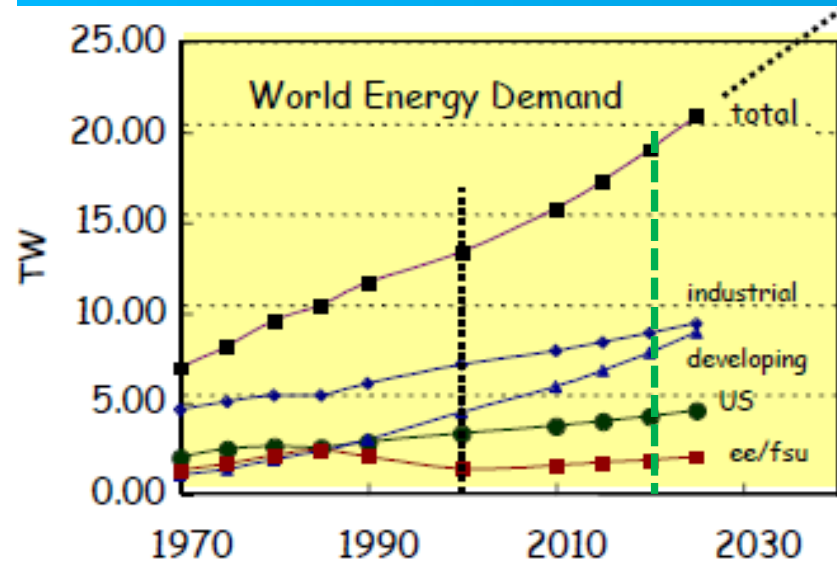
Molecular Passivation for High-Efficiency and Stable Methylammonium-Free Perovskite Solar Cells with Fluorinated Supramolecules

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

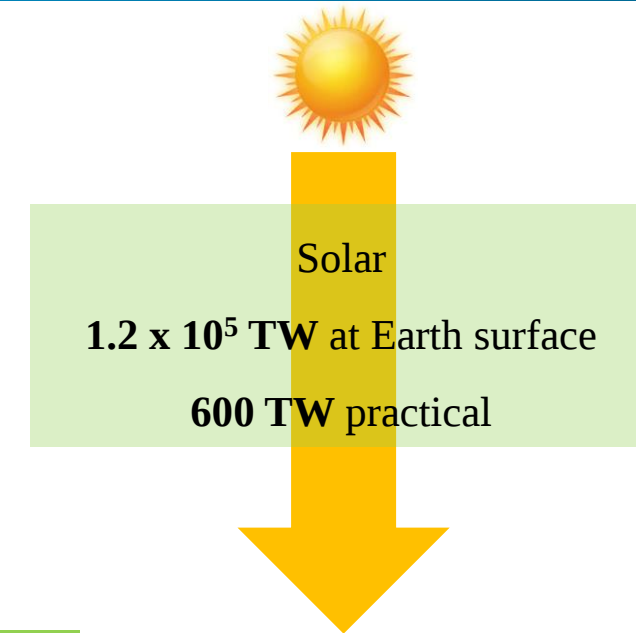
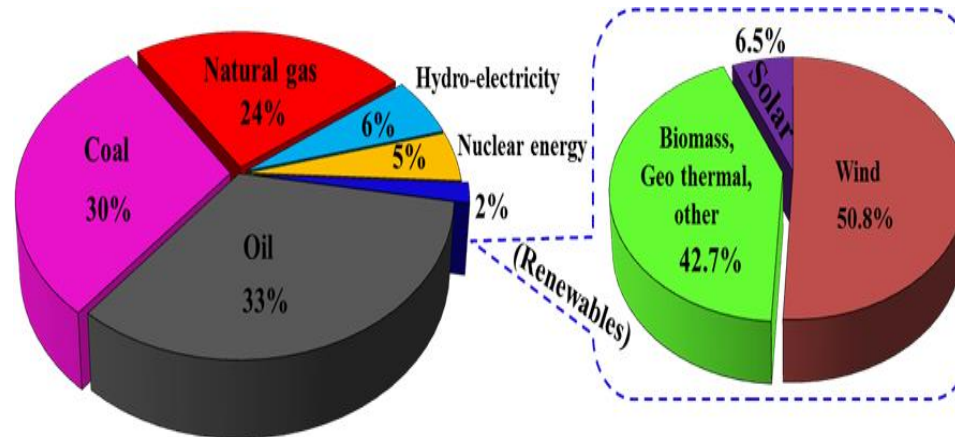
Photovoltaic Materials Group

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

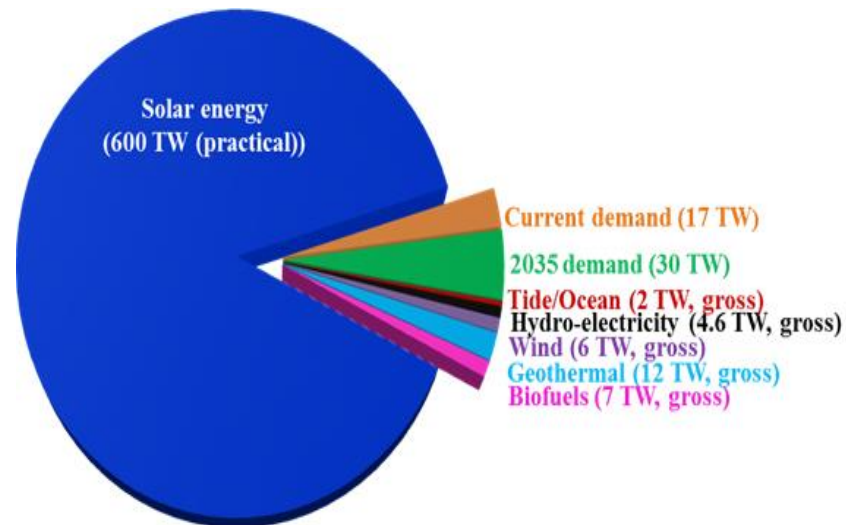




To meet energy demand



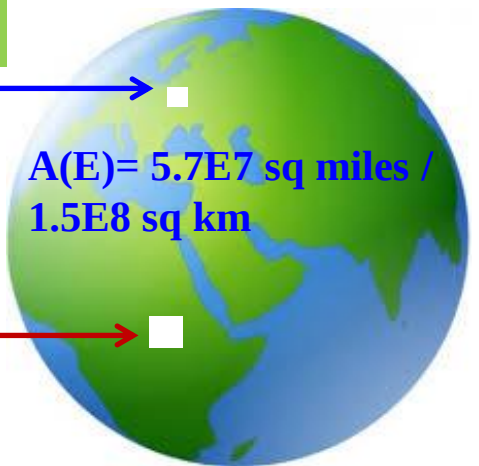
Potential of renewable energy



PV cell having PCE of 10%

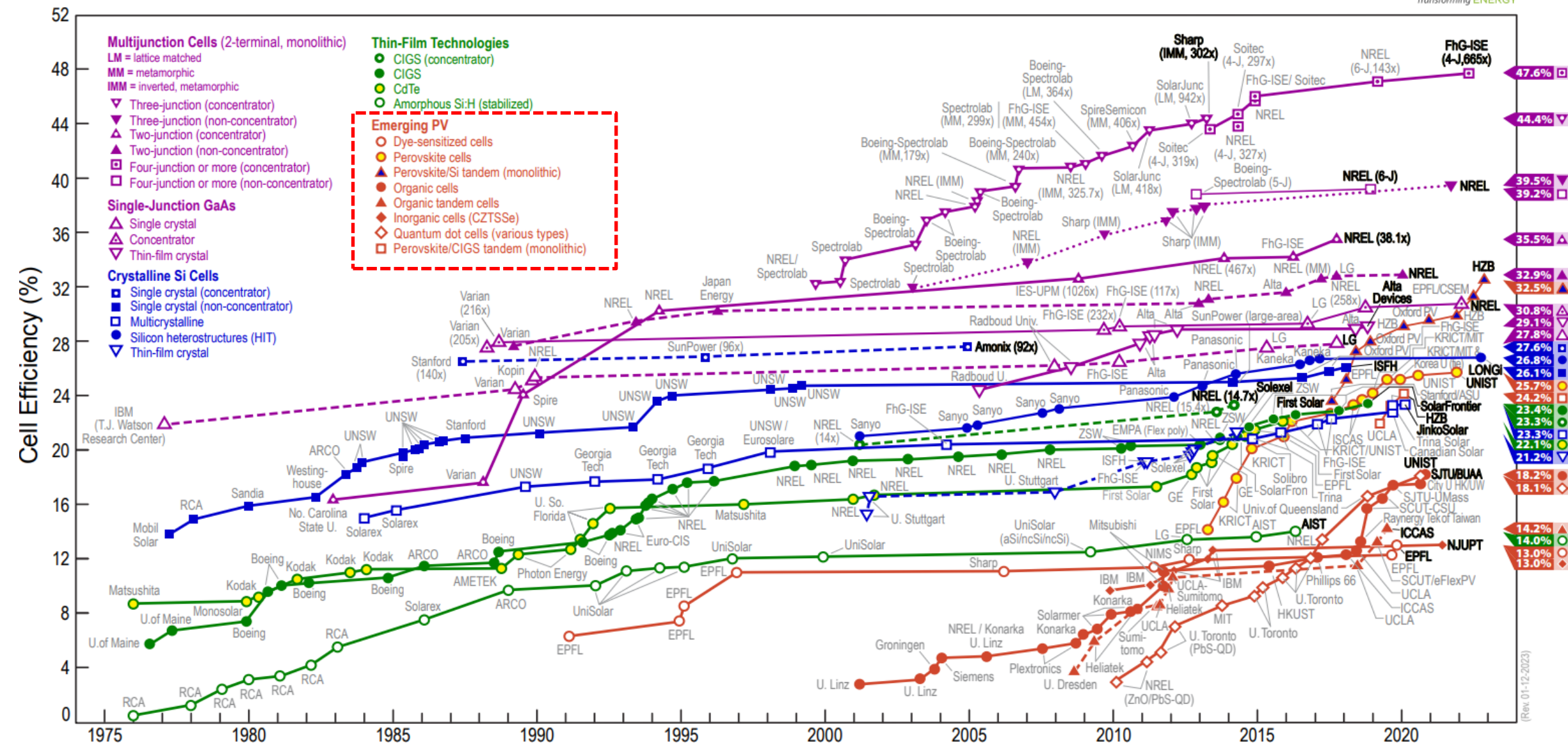
Current demand; 15-18 TW
[0.19% of land area (540x540 km²)]
[JPN-3,77,930 km²; ¾ of Jpn]

2040 energy demand; 30-35 TW
[0.97% of land area (1200x1200 km²)]



<http://www.eia.doe.gov>

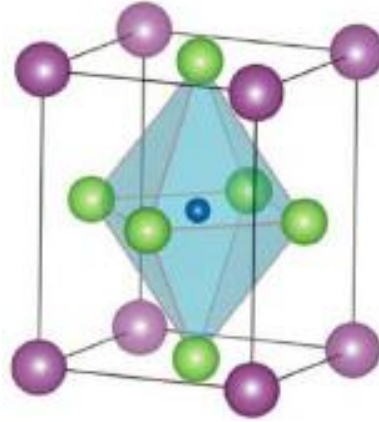
NREL
Transforming ENERGY



Halide perovskite: promising for light harvesting

CsPbX_3 (1892)

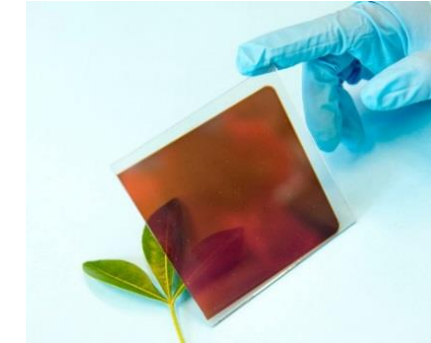
$\text{CH}_3\text{NH}_3\text{PbI}_3$ -
Dieter Weber in 1978



A- MA, FA, Cs,

B- Pb, Sn, Ge

X- Cl, Br, I



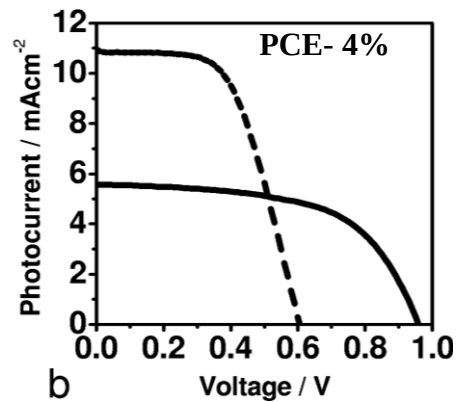
$$E_g = 1.55 \text{ eV}, \alpha = 10^4 - 10^5 \text{ cm}^{-1}$$

$$L_D > 1 \mu, E_{\text{ext}} < kT, \text{ bipolar carriers}$$

2009: First perovskite solar cells;

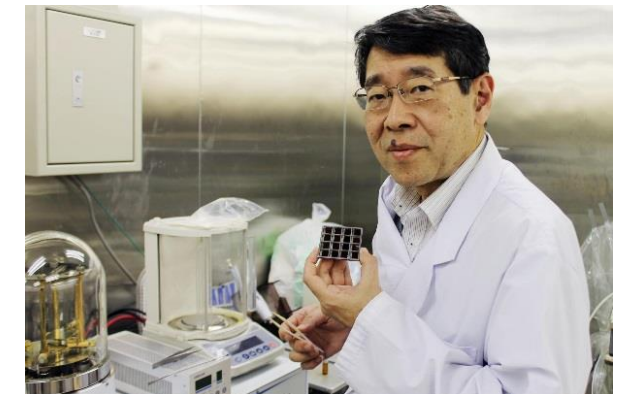
J | A | C | S
COMMUNICATIONS

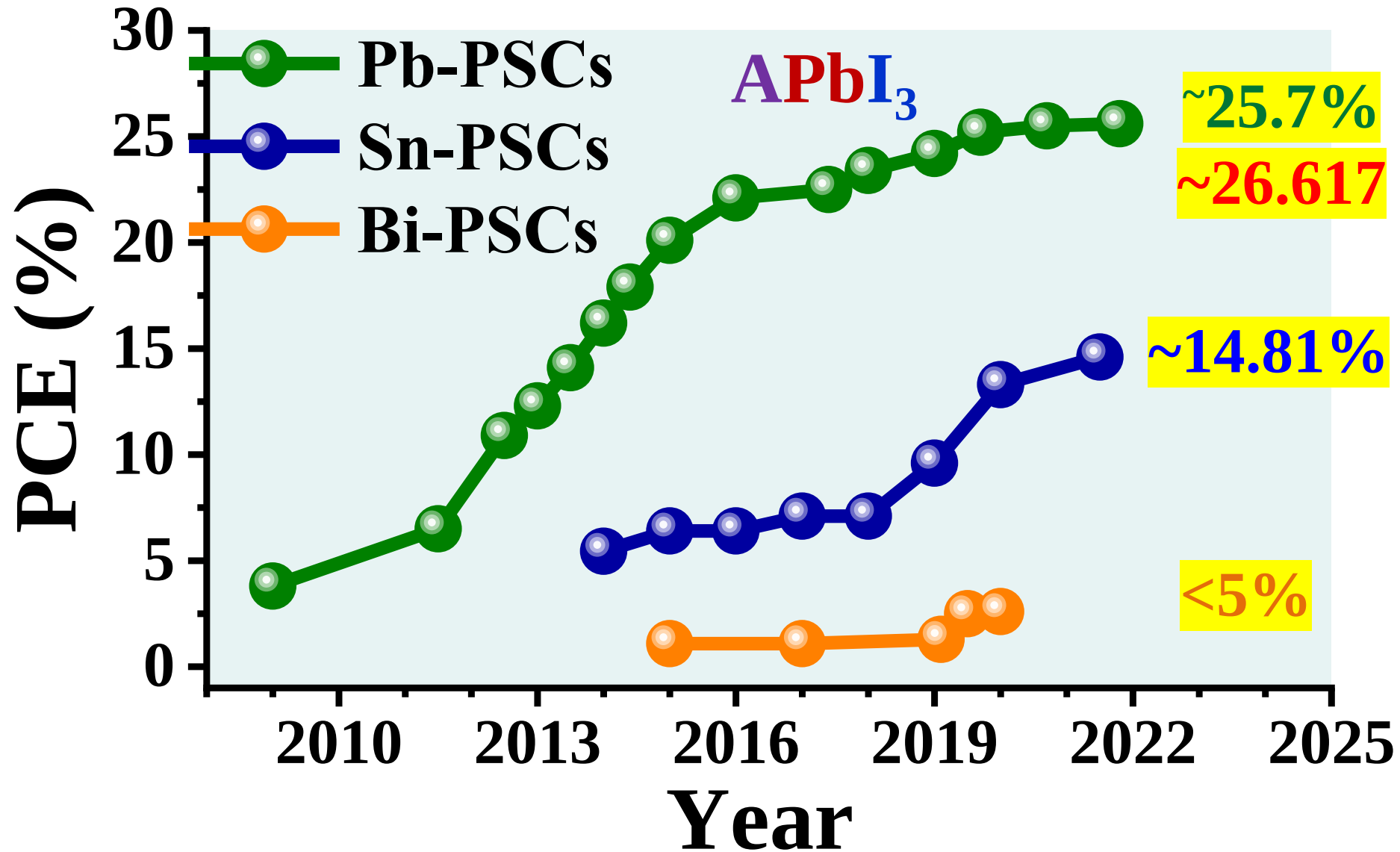
$\text{CH}_3\text{NH}_3\text{PbBr}_3/\text{TiO}_2$ (solid line)
 $\text{CH}_3\text{NH}_3\text{PbI}_3/\text{TiO}_2$ (dashed line).



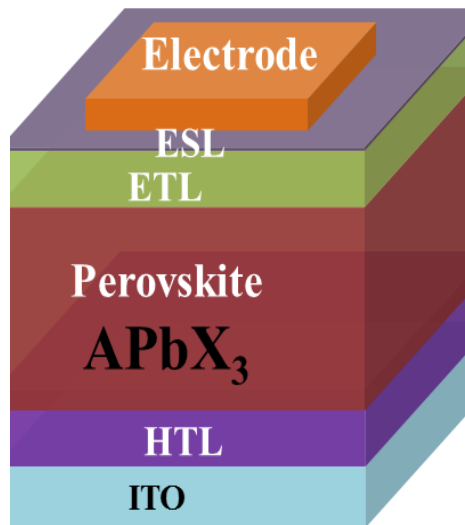
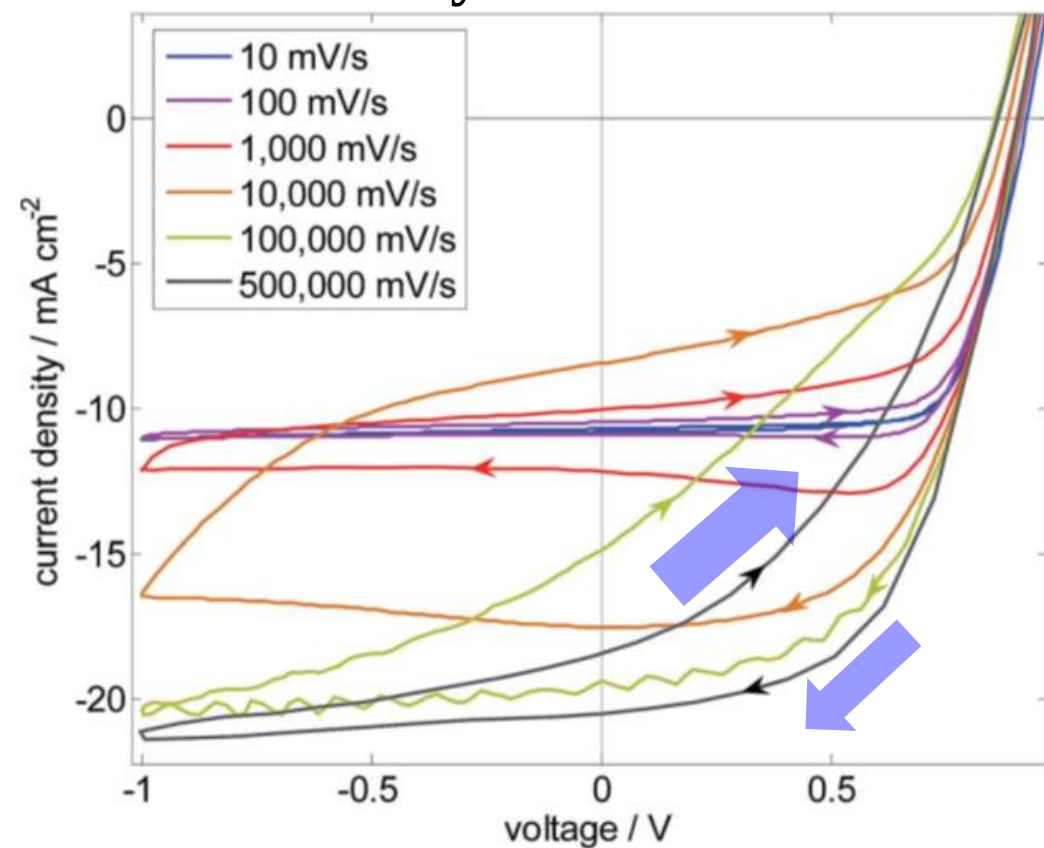
Dye sensitized structure:
4% efficiency

Prof. Tsutomu Miyasaka ;
Toin University of Yokohama

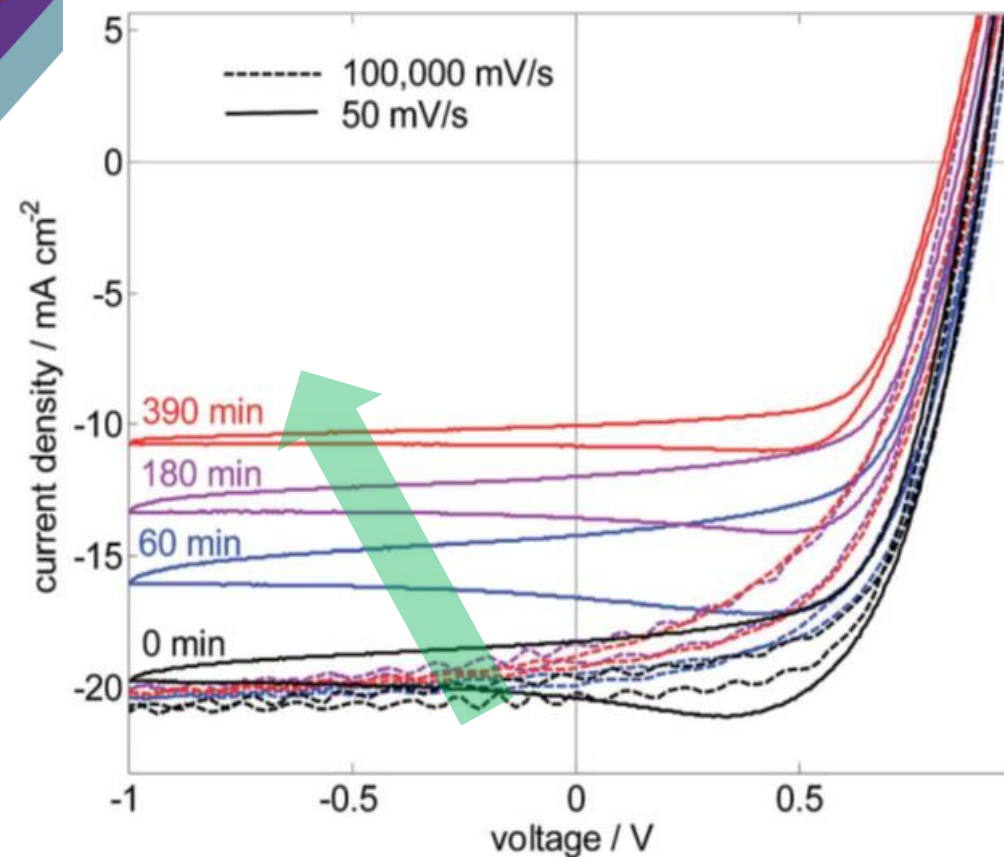




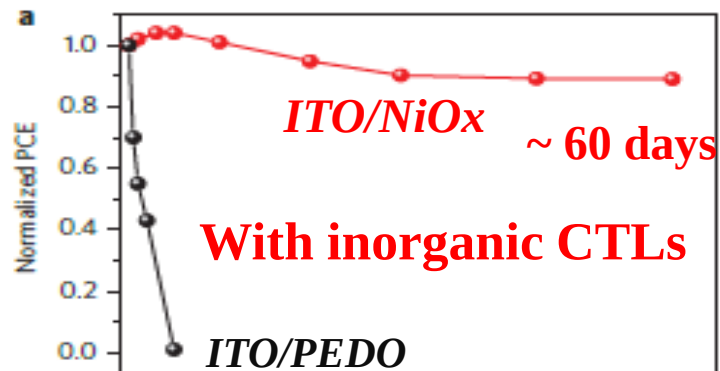
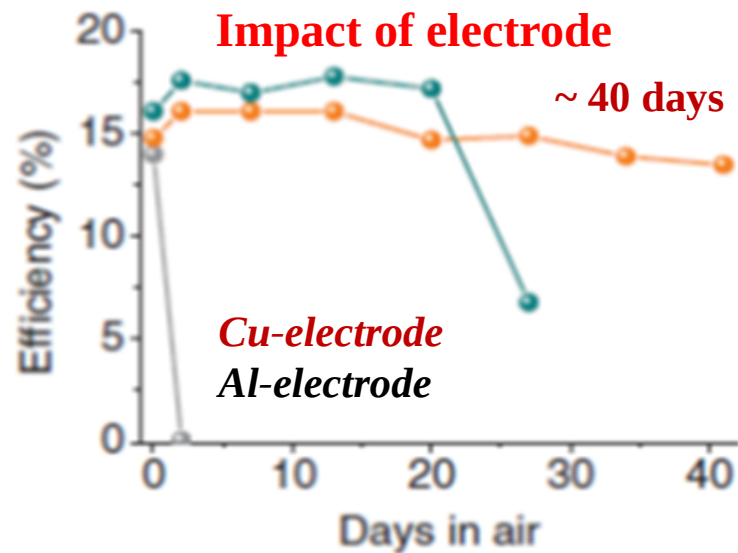
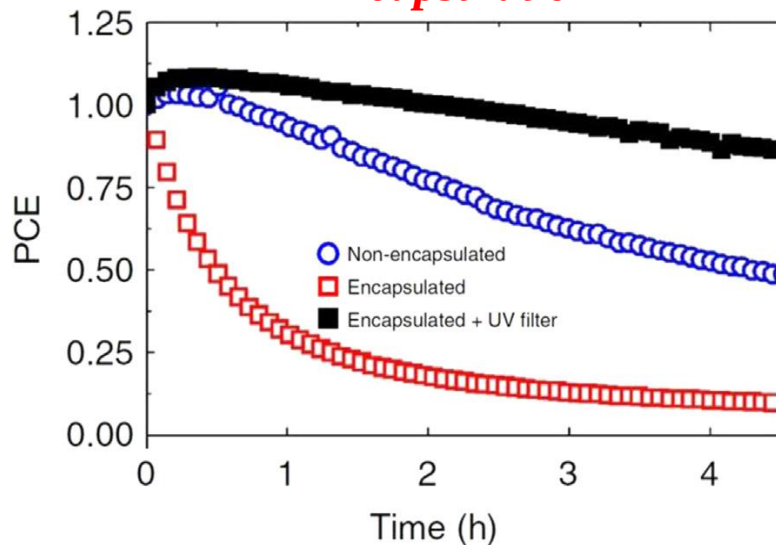
J-V hysteresis



Device degradation

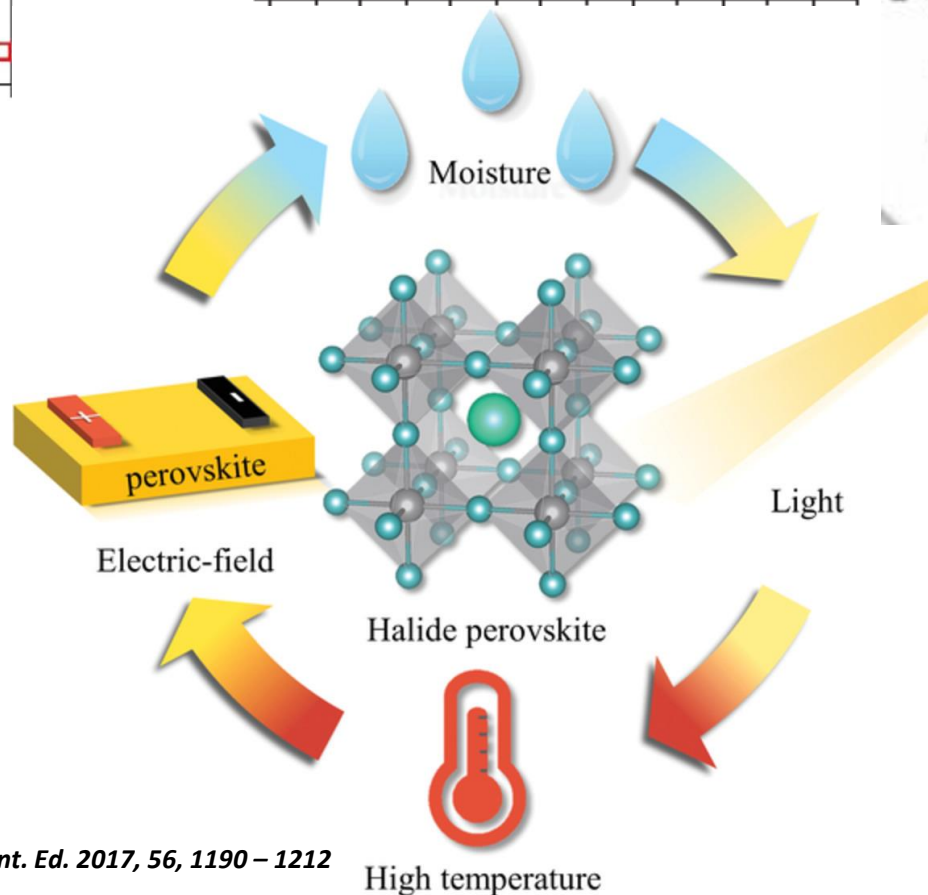
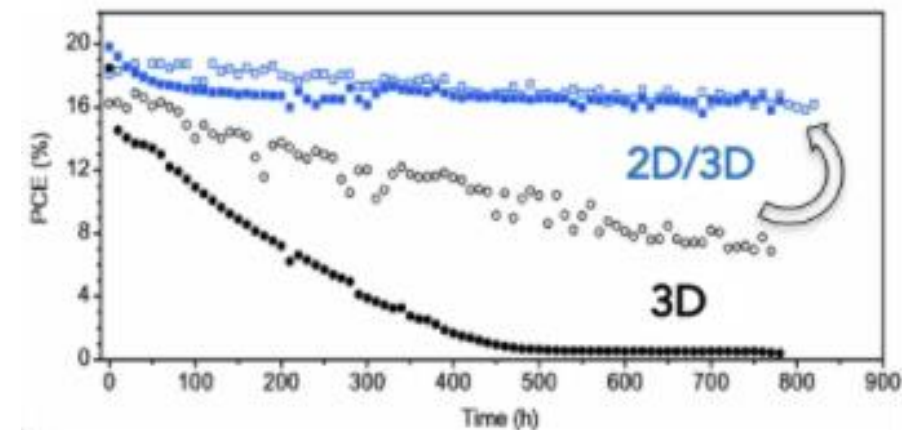


Encapsulation

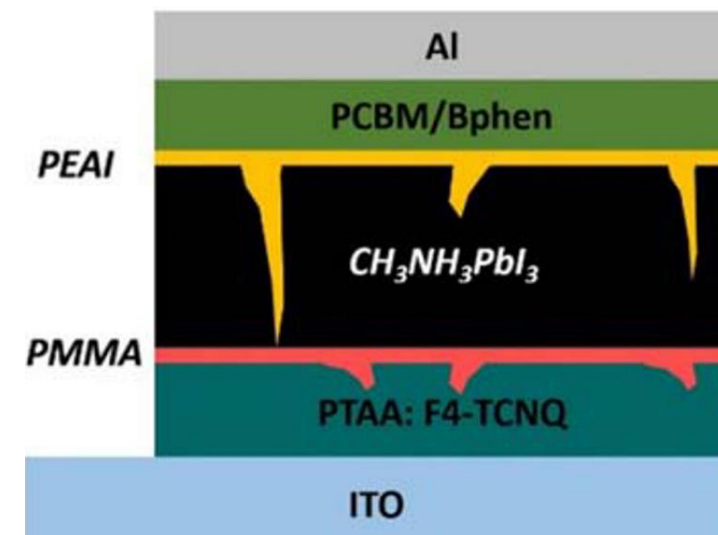


Standard: 85C/85%- RH; 1000 hours

Improved Stability

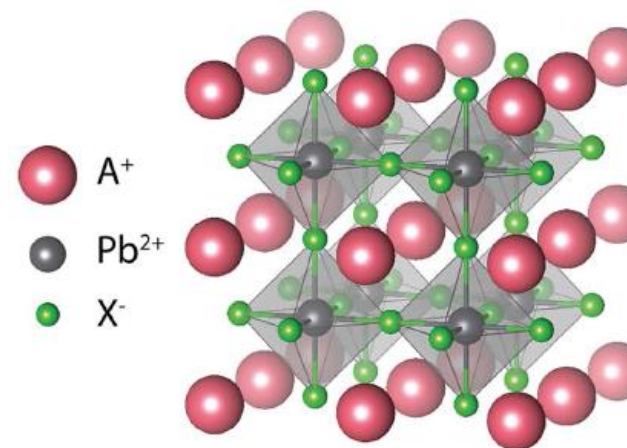
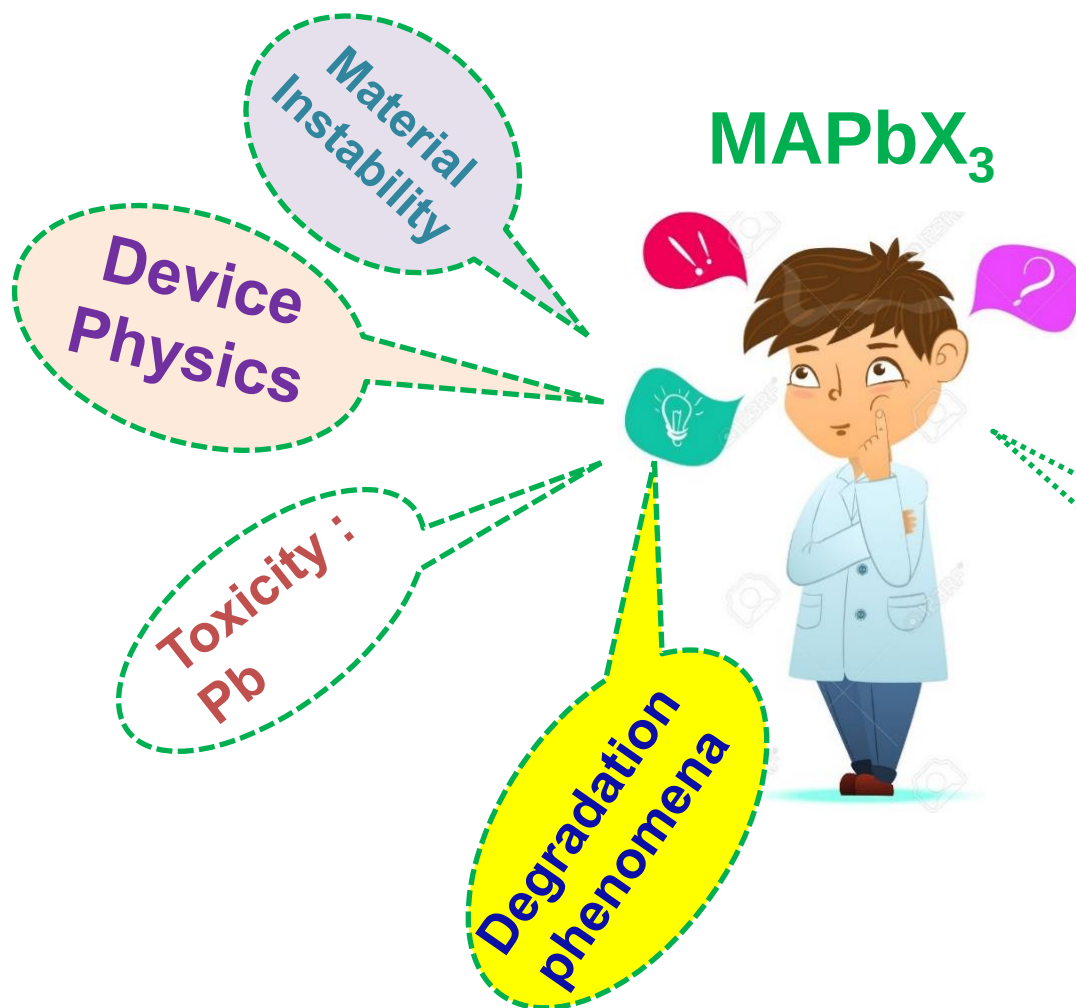


Interfacial passivation



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

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

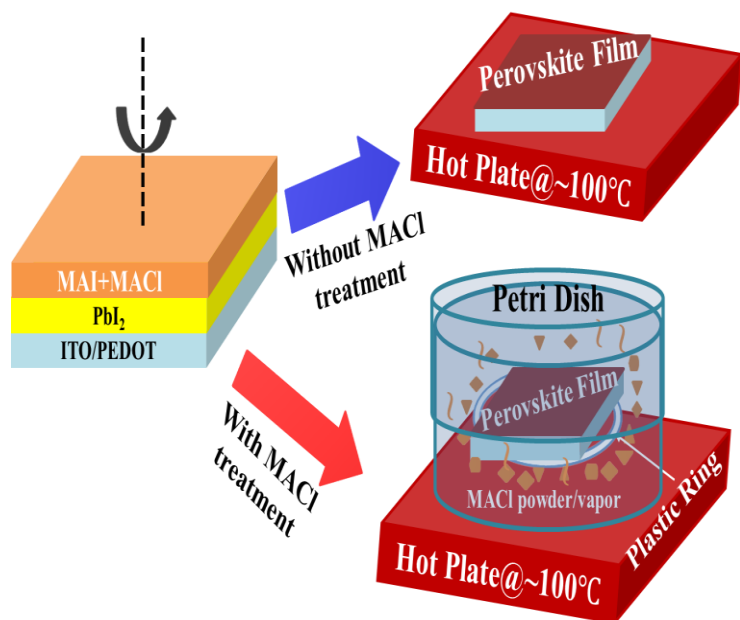


Underlying physics

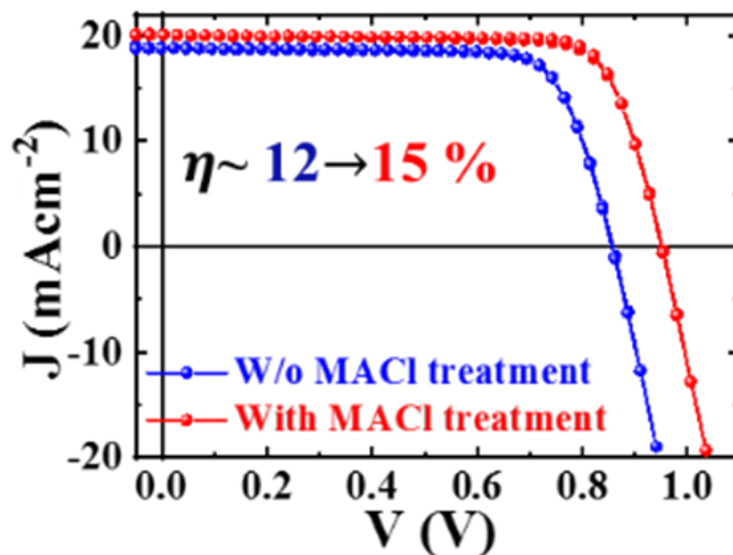
Exploration on

- Material properties
- Interface quality with the contact layer
- Carrier dynamics
- Ionic migration
- Defect physics

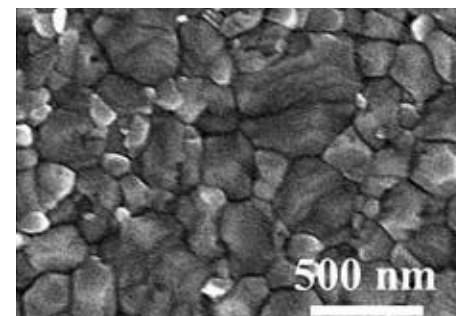
Film crystallization



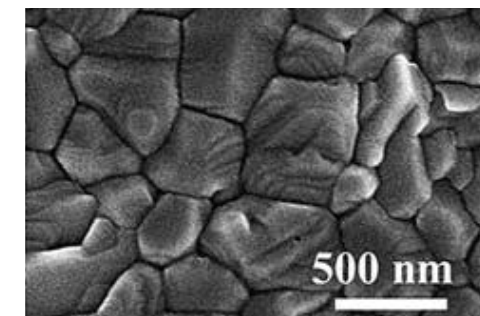
PCE- Improved



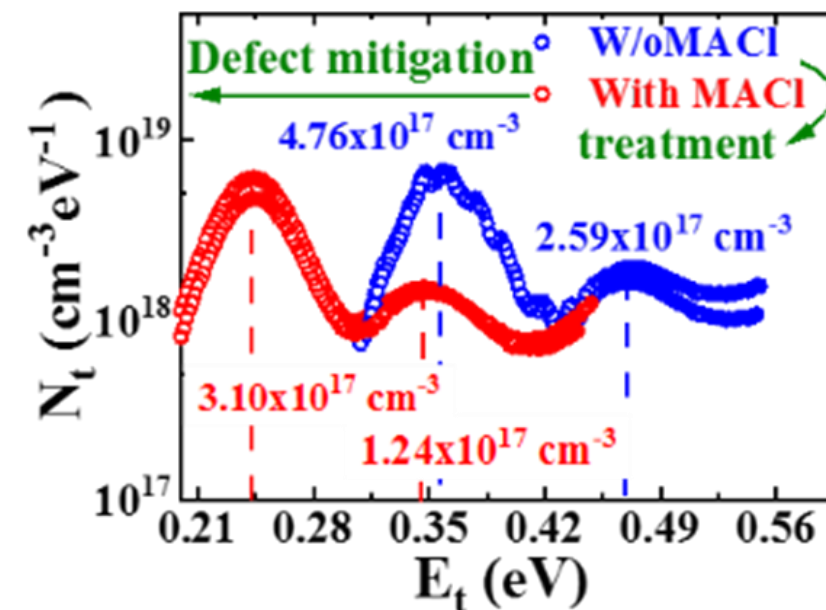
Control



MAI-treated

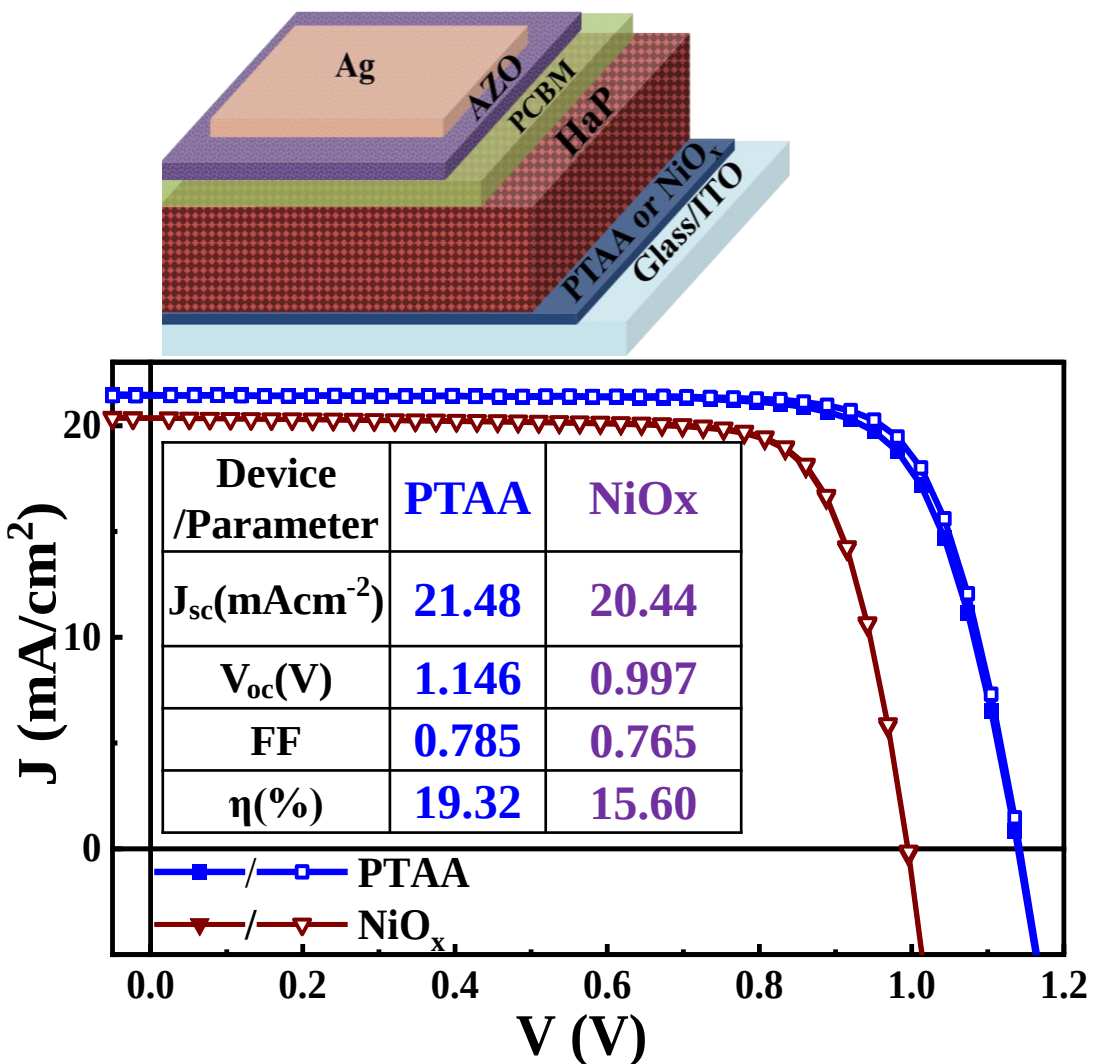
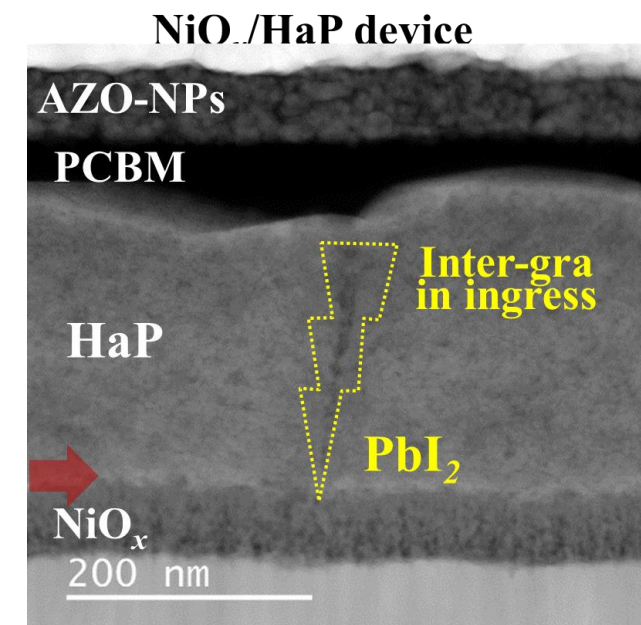
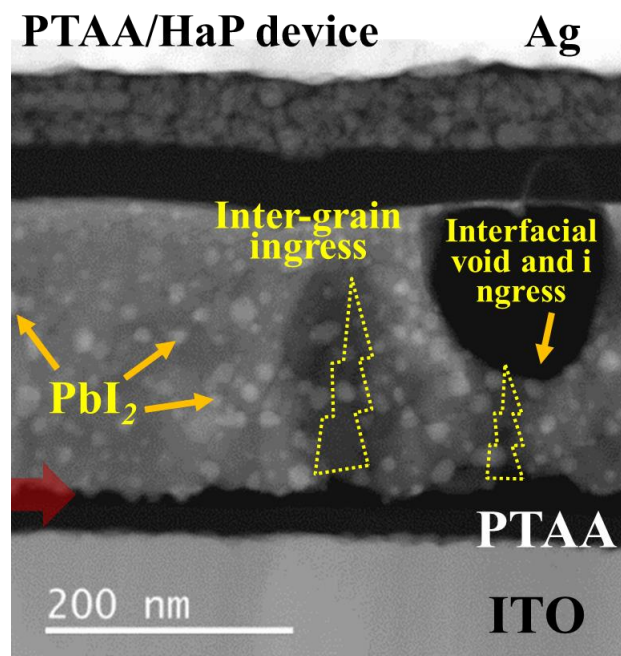
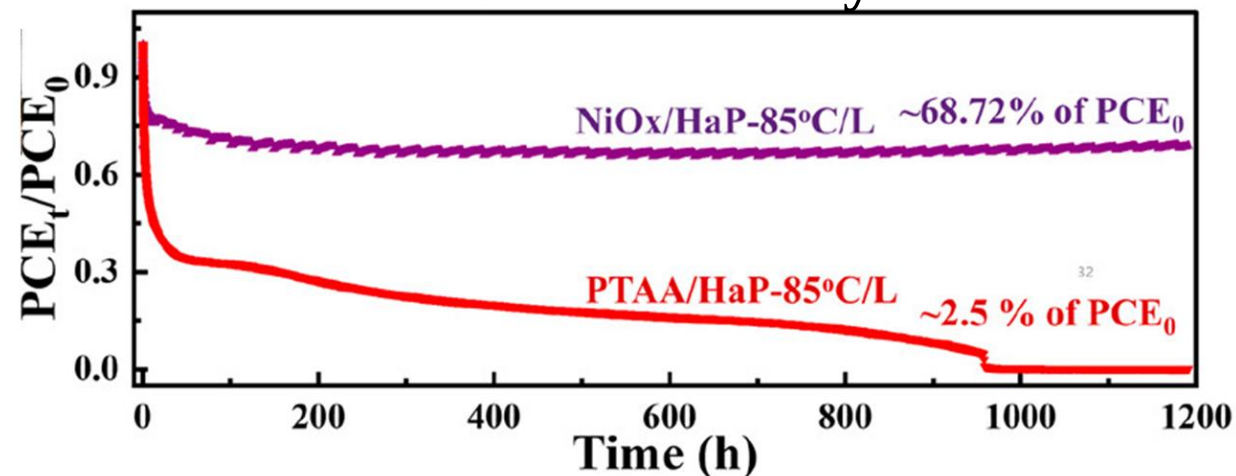


Defect passivation



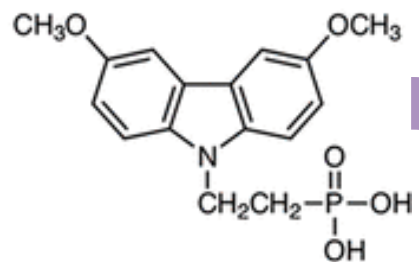
- Khadka et al., *Sustain. Energy Fuels*, 2017, 1, 755
- Khadka et al., *J. Mater. Chem. C*, 2017, 5, 8819

Device stability

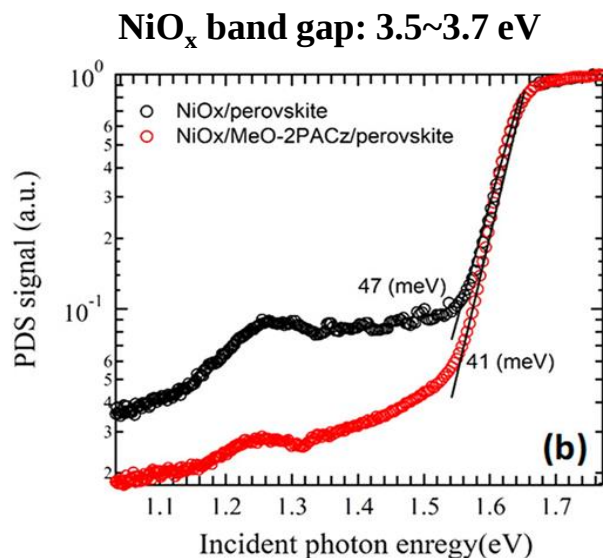
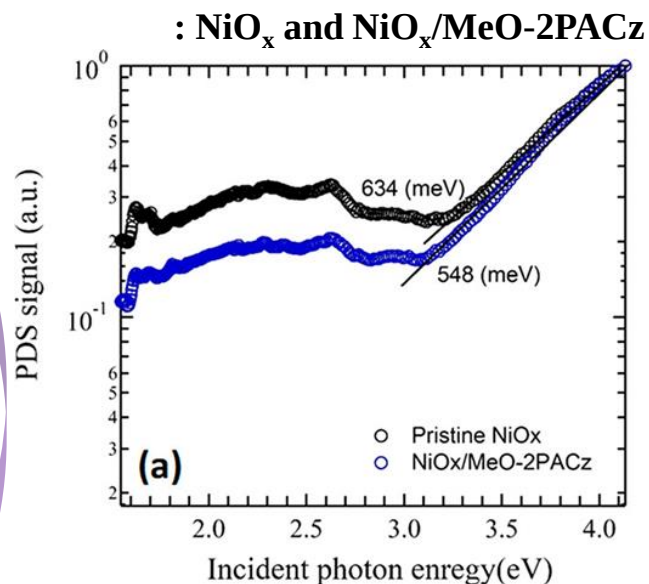
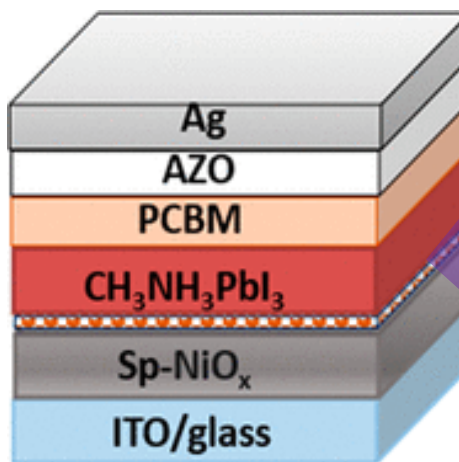


- Khadka et al. ACS Appl. Energy Mater. 2021, 4, 10, 11121
- Khadka et al. ACS Appl. Mater. Interfaces, 2018, 11, 7055
- Khadka et al, ACS Appl. Mater. Interfaces, 2018,10, 22074
- Khadka et al., J. Mater. Chem. C, 2018, 6, 162-170

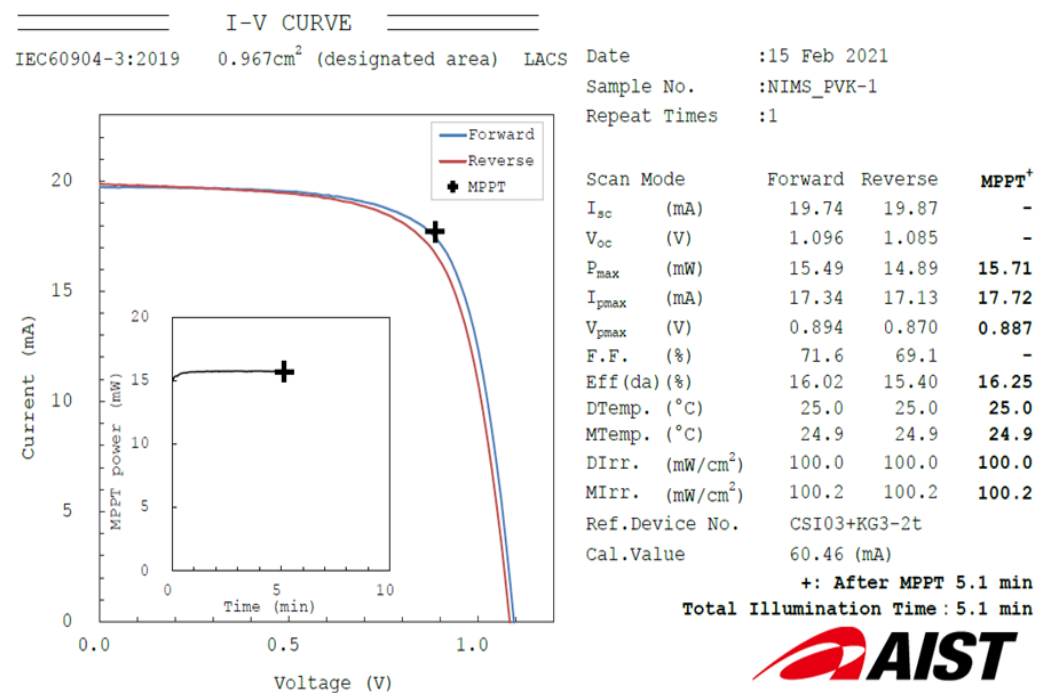
Photothermal Deflection Spectroscopy



MeO-2PACz



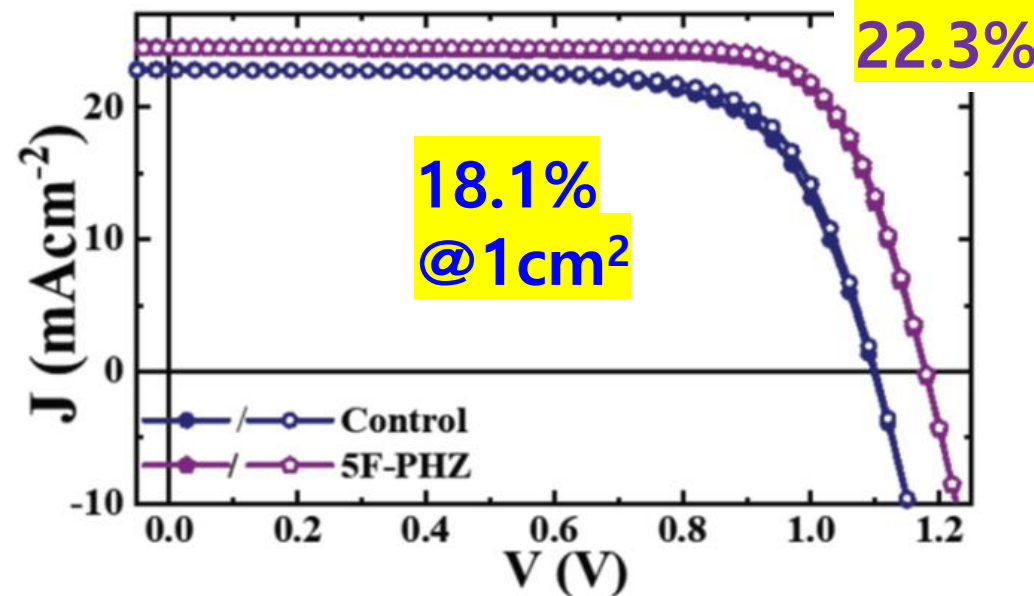
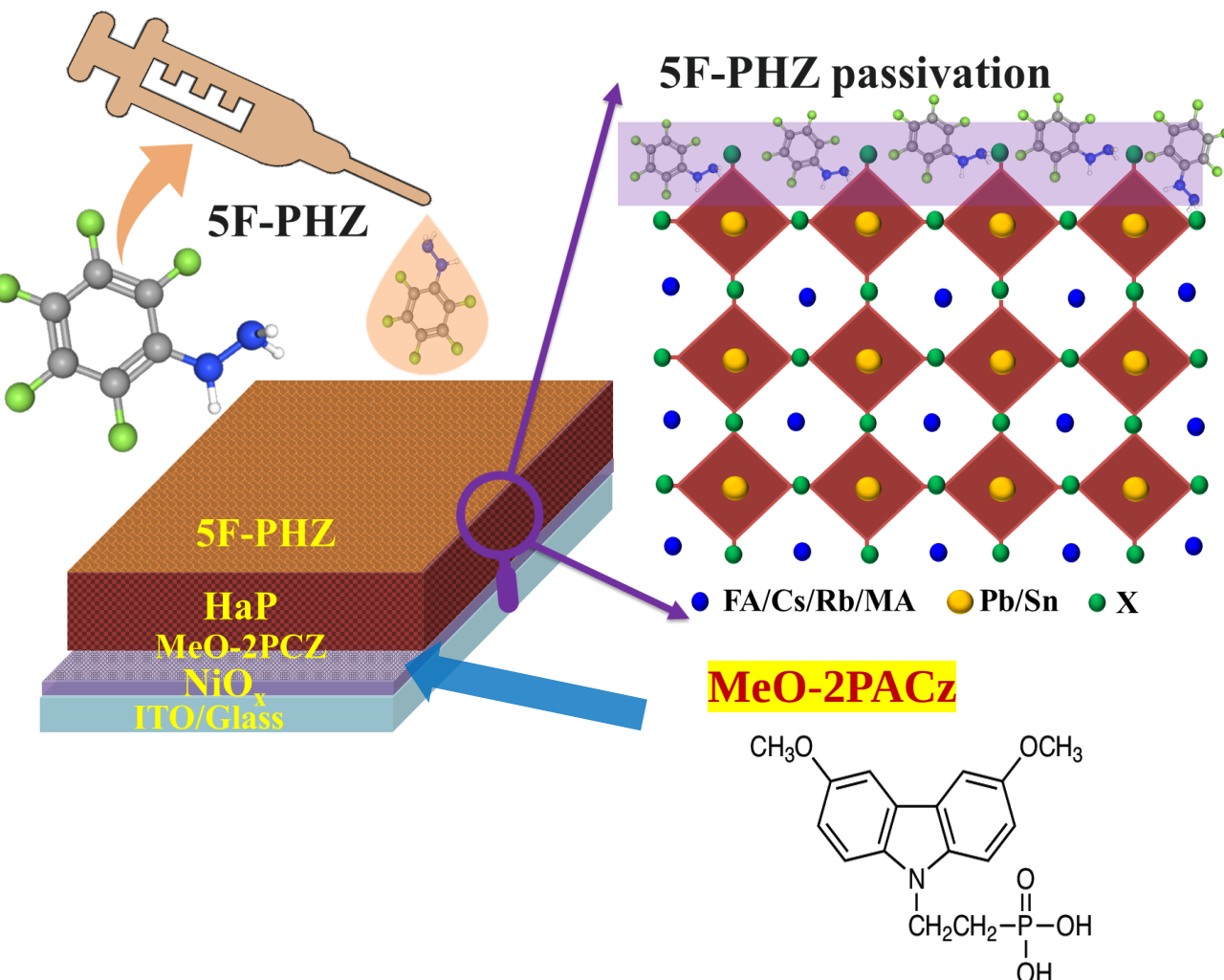
- ✓ PCE: 15.60 → 17.2%
- ✓ Certified PCE → 16.3% @ 1 cm²
- ✓ MAPI device with ~ 270 nm



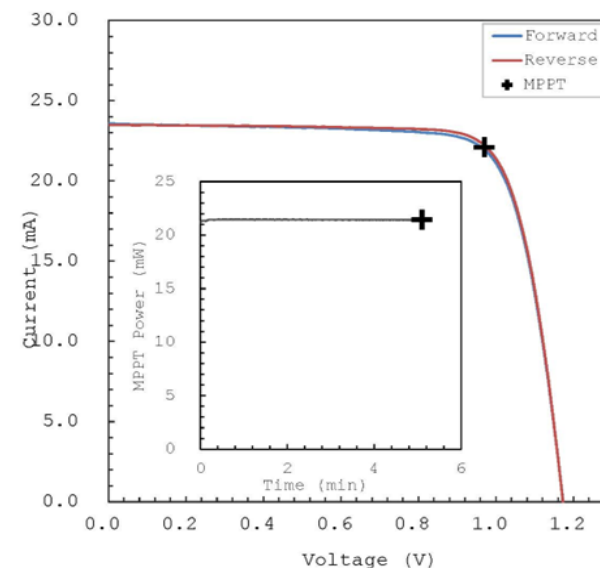
- Miyano and co-workers, ACS Omega 2022, 7, 12147.

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

✓ $\text{MAPbI}_3 \rightarrow \text{FA}_{0.84}\text{Cs}_{0.12}\text{Rb}_{0.04}\text{PbI}_3$

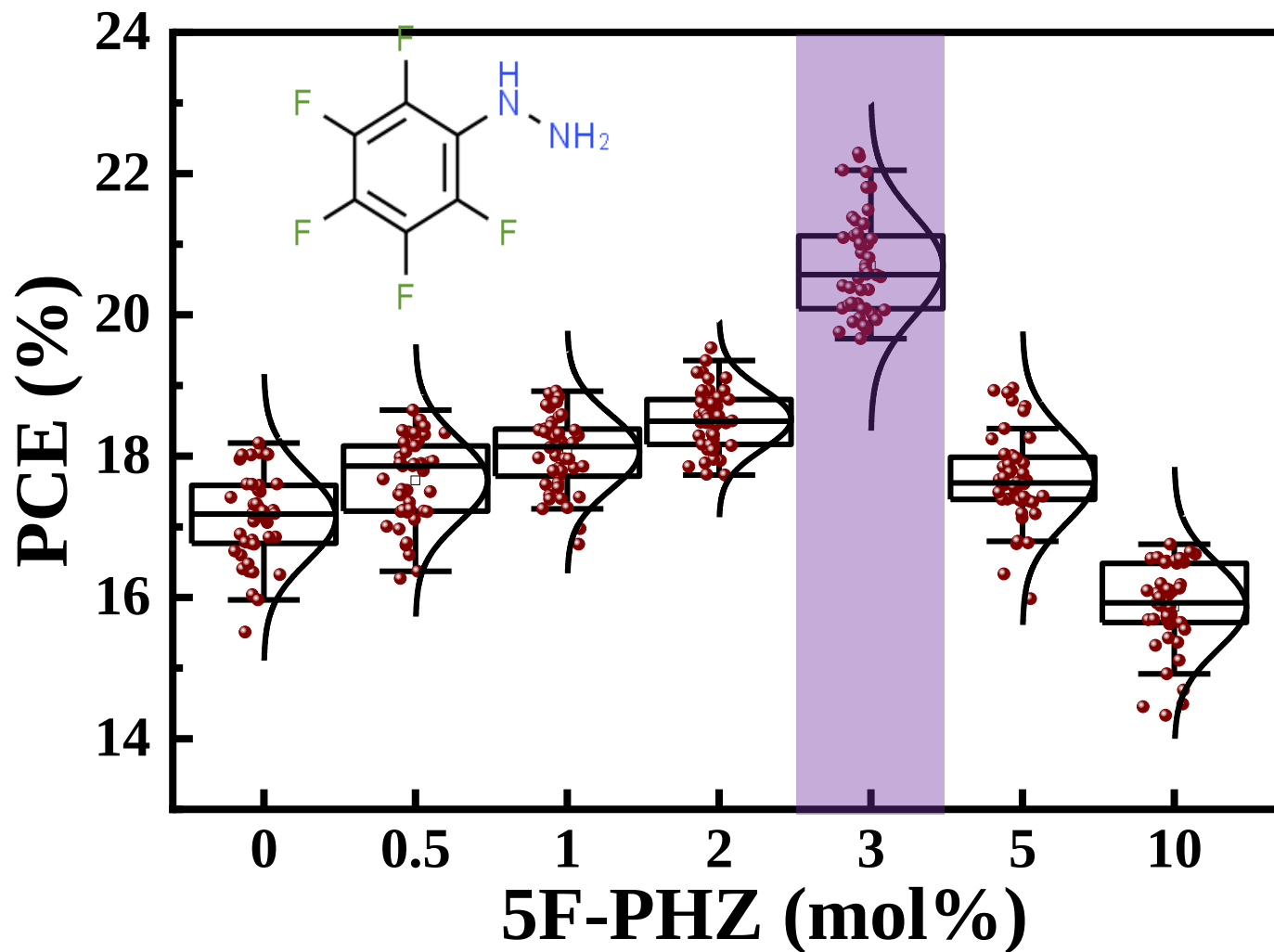
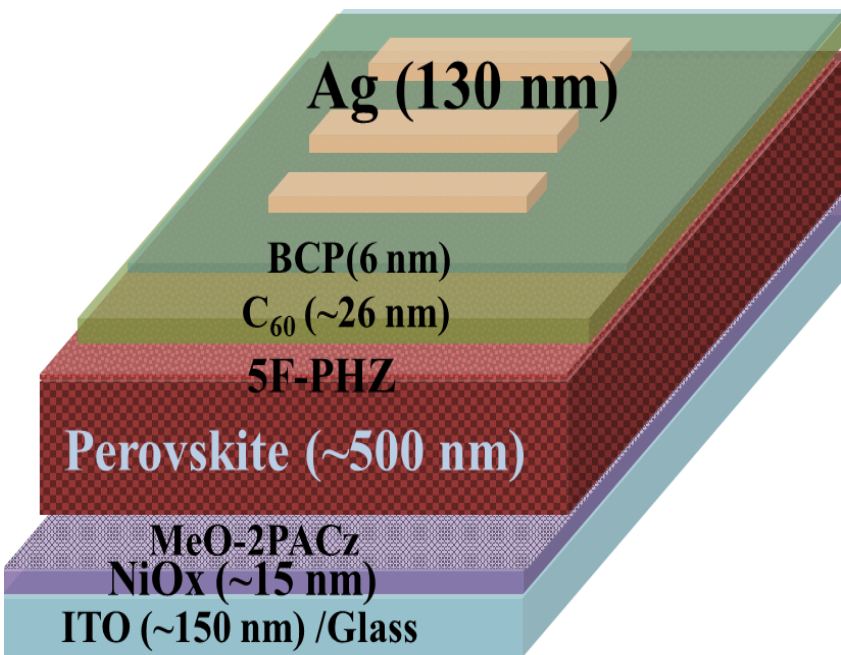
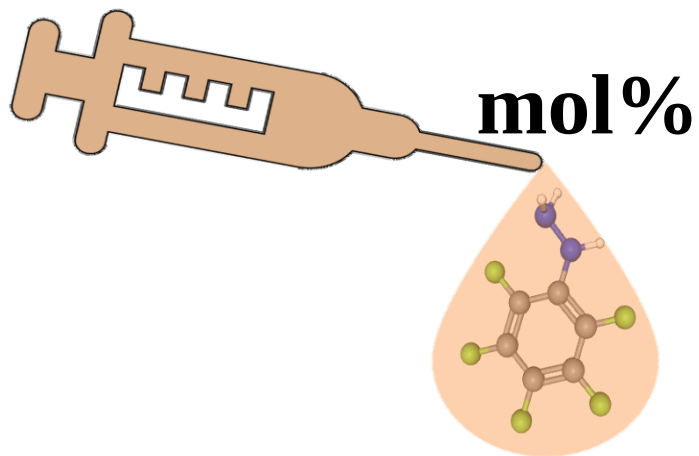


IEC 60904-3:2019 1.026 cm^2 (designated area) LACS

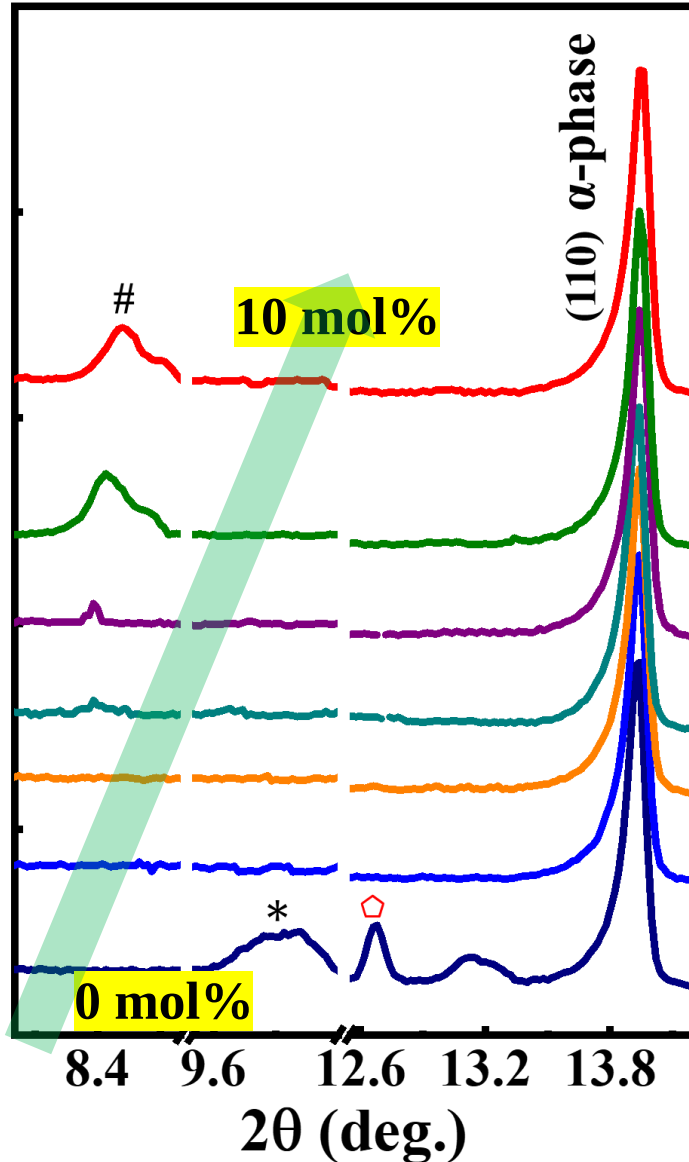


Date : 14 Feb 2022
Sample No. : NIMS_FAPVK-3
Repeat Times : 1

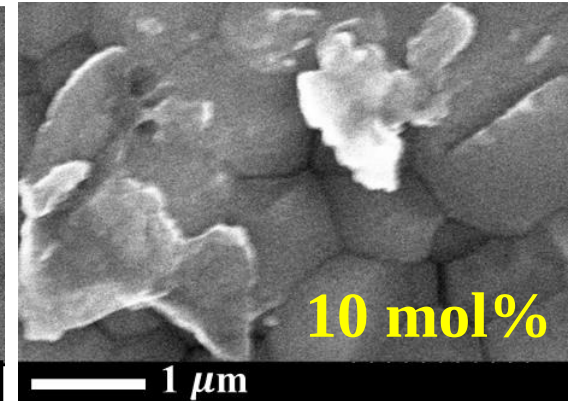
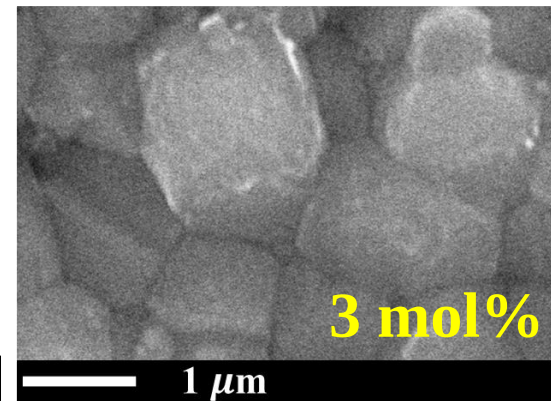
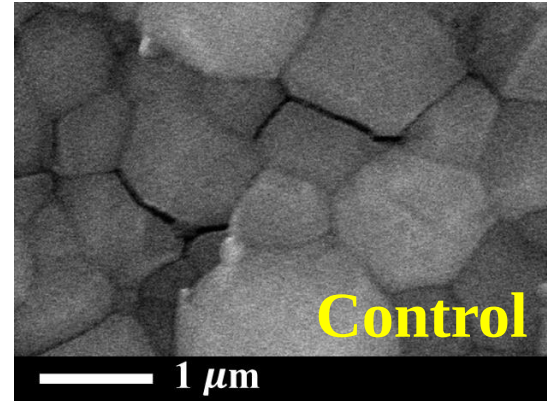
Scan Mode	Forward	Reverse	MPPT ⁺
I _{sc} (mA)	23.58	23.50	-
V _{oc} (V)	1.173	1.173	-
P _{max} (mW)	21.31	21.56	21.44
I _{pmax} (mA)	21.89	22.17	22.11
V _{pmax} (V)	0.973	0.973	0.970
F.F. (%)	77.0	78.2	-
Eff (da) (%)	20.77	21.01	20.90
DTemp. (°C)	25.0	25.0	25.0
MTemp. (°C)	25.2	25.2	25.2
Dirr. (mW/cm ²)	100.0	100.0	100.0
Mirr. (mW/cm ²)	99.6	99.6	99.6
Ref.Device No.	CSI03+KG3-2t		
Cal.Val.of Ref.	60.22 (mA at 100mW/cm ²)		
	+: After MPPT 5.1 min		
	Total Illumination Time : 5 min		



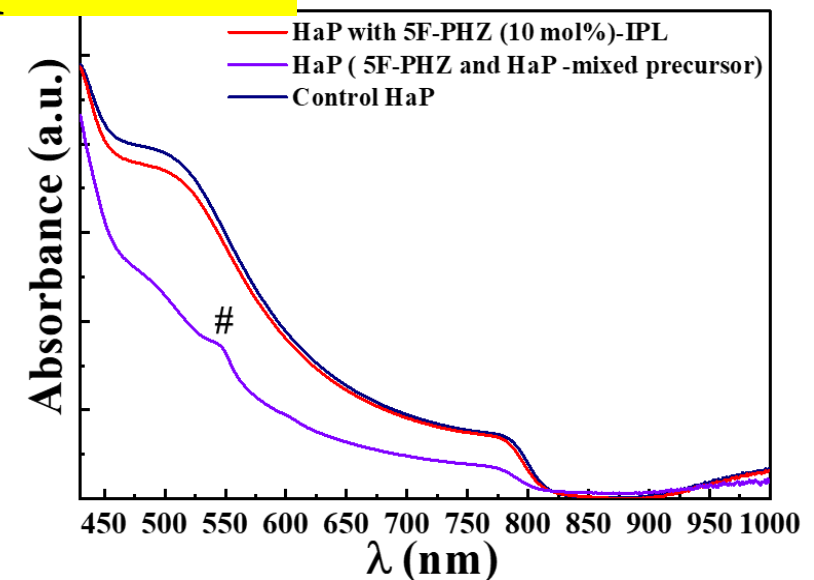
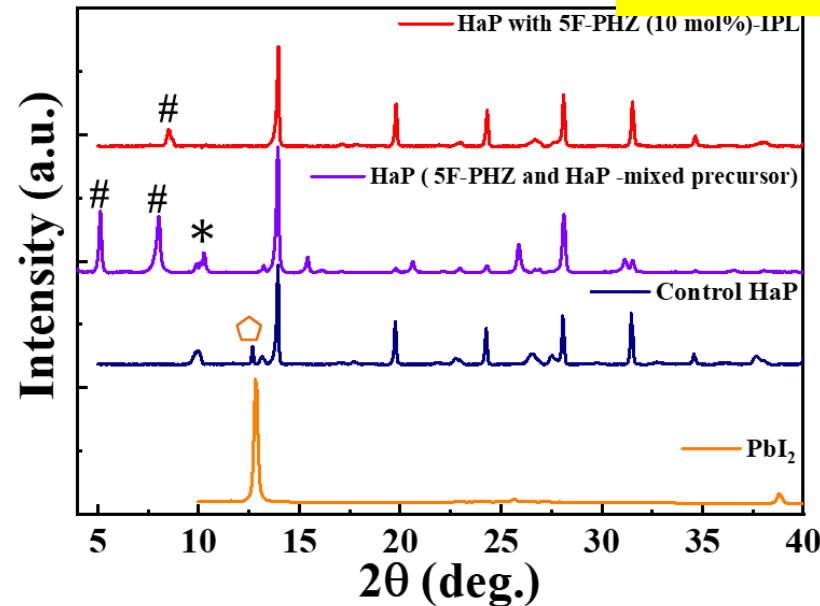
XRD results



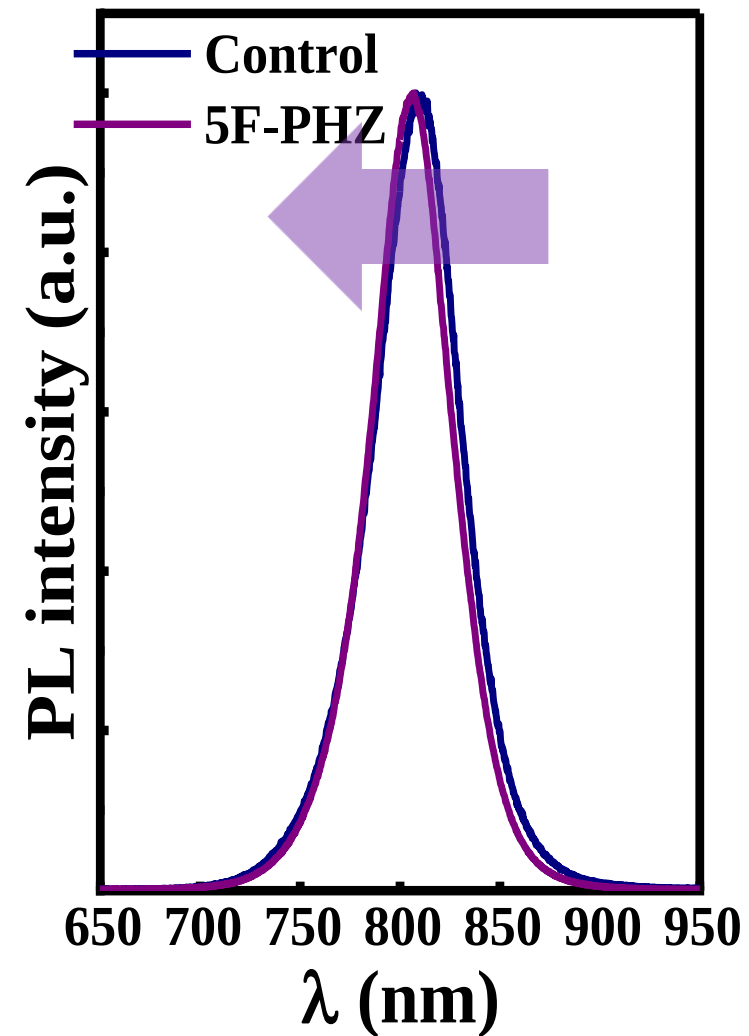
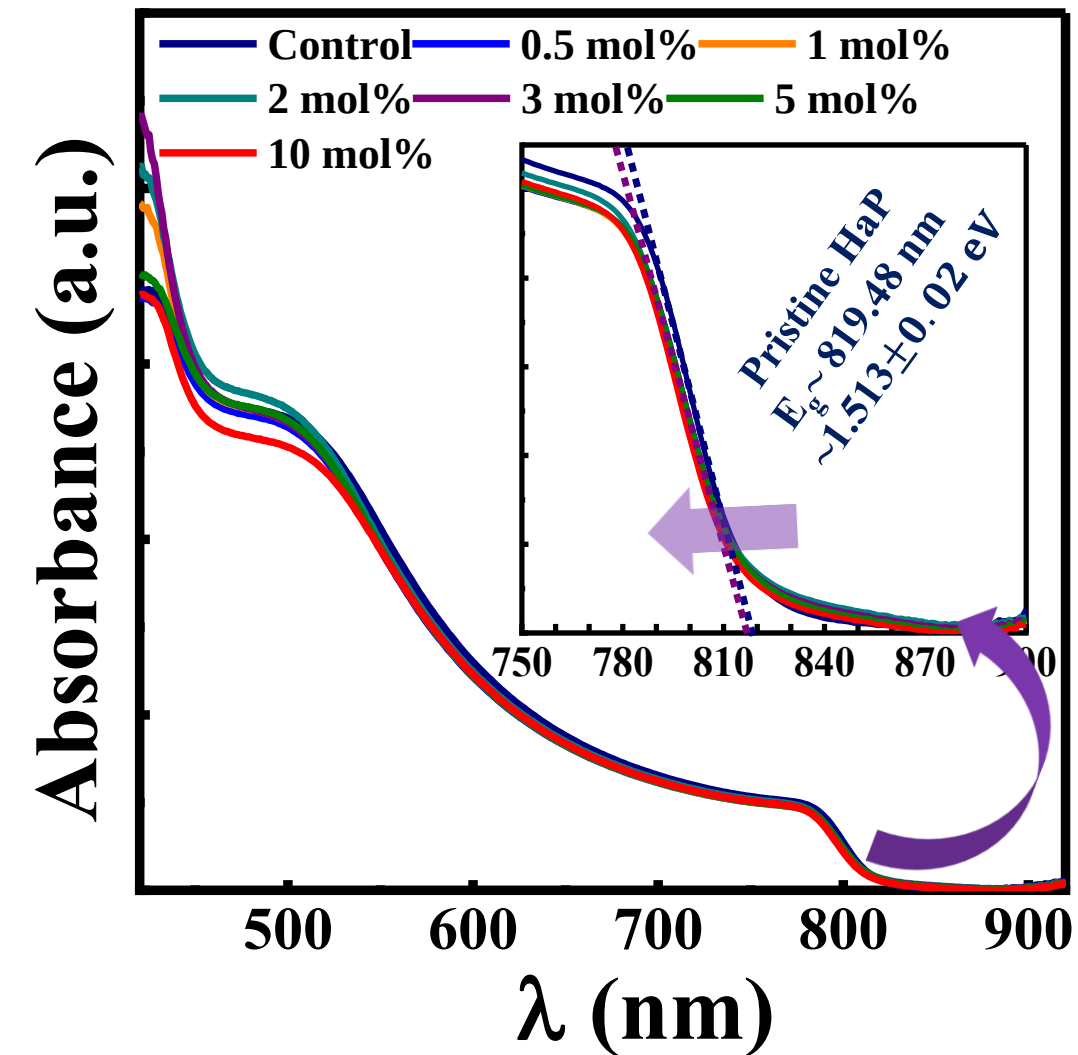
✓ 5F-PHZ additive: well coverage on the surface



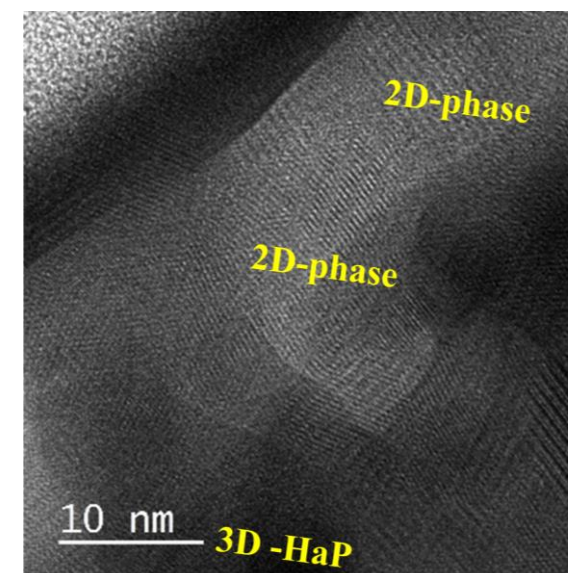
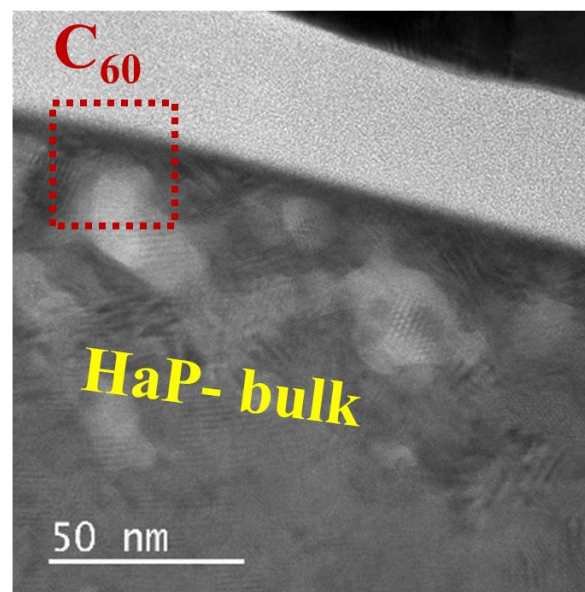
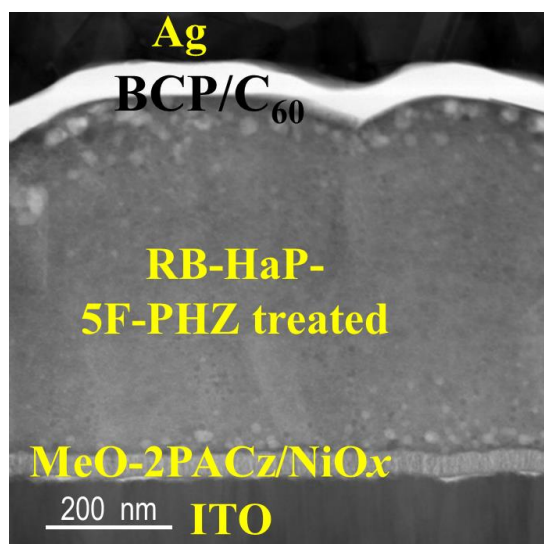
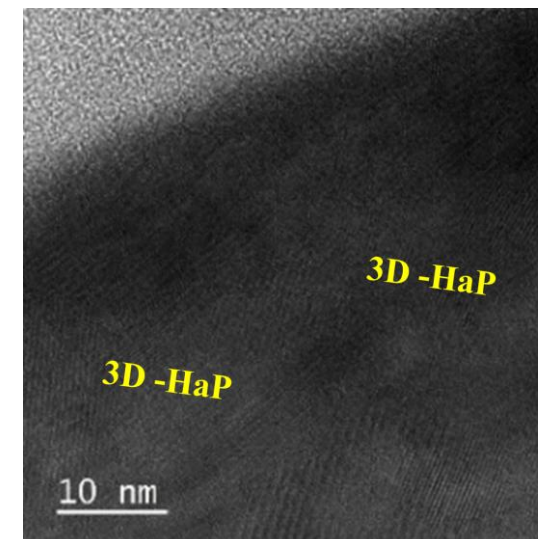
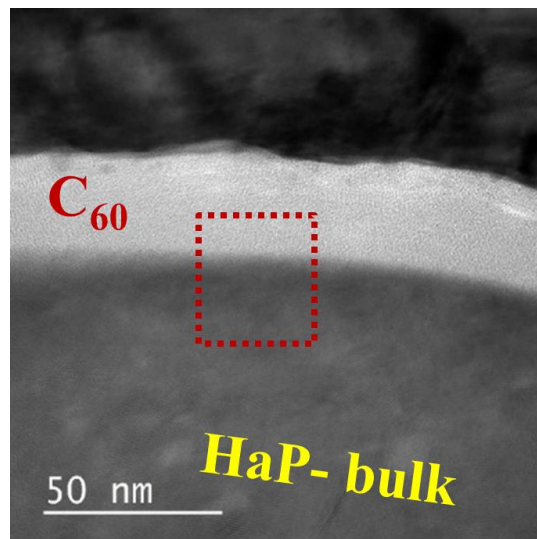
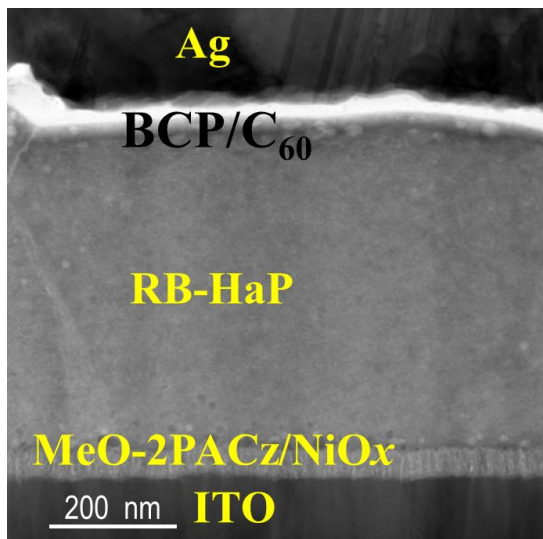
Mixed precursor

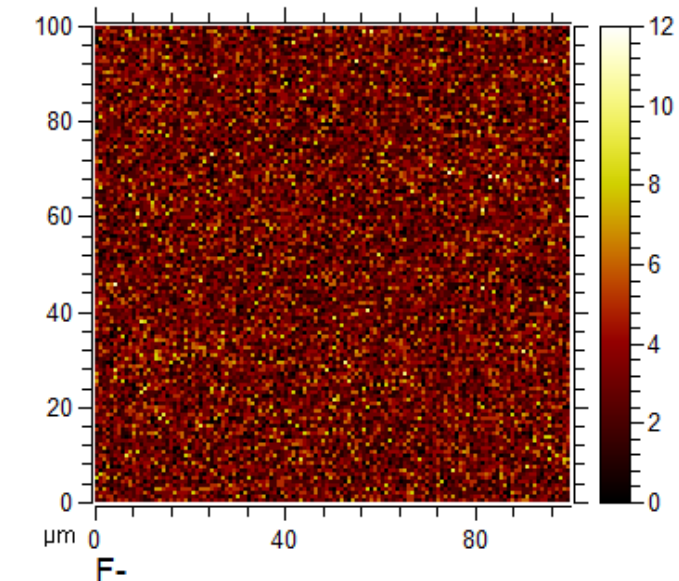
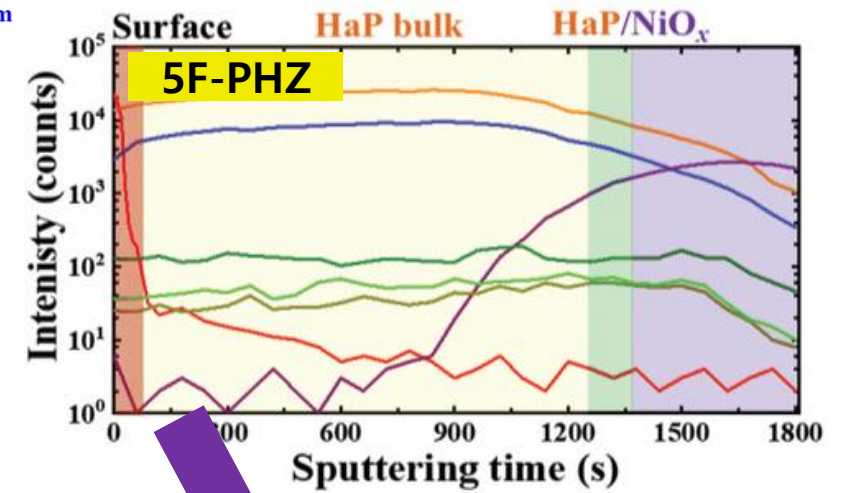
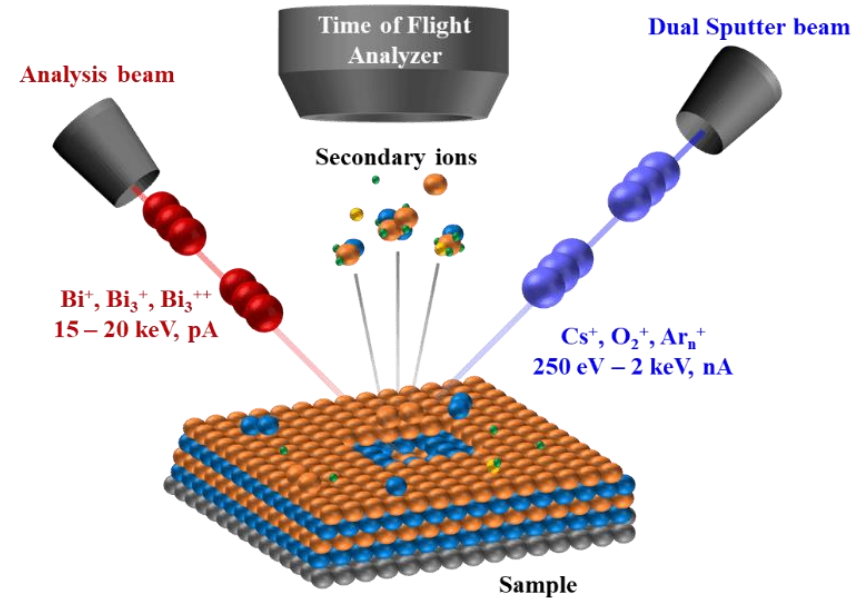
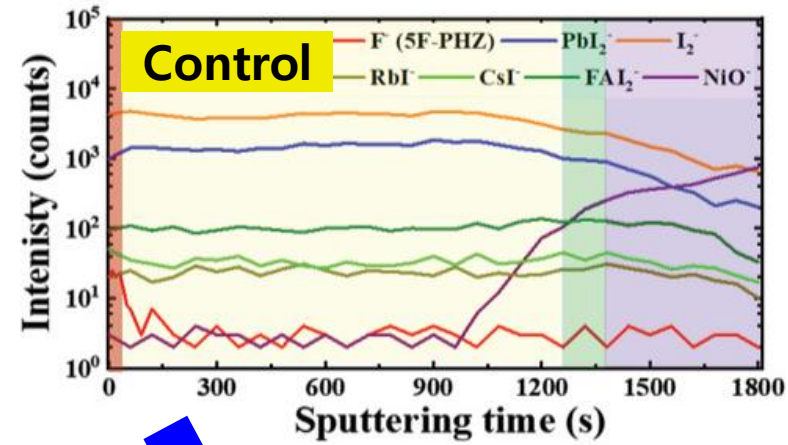


✓ Absorption spectra

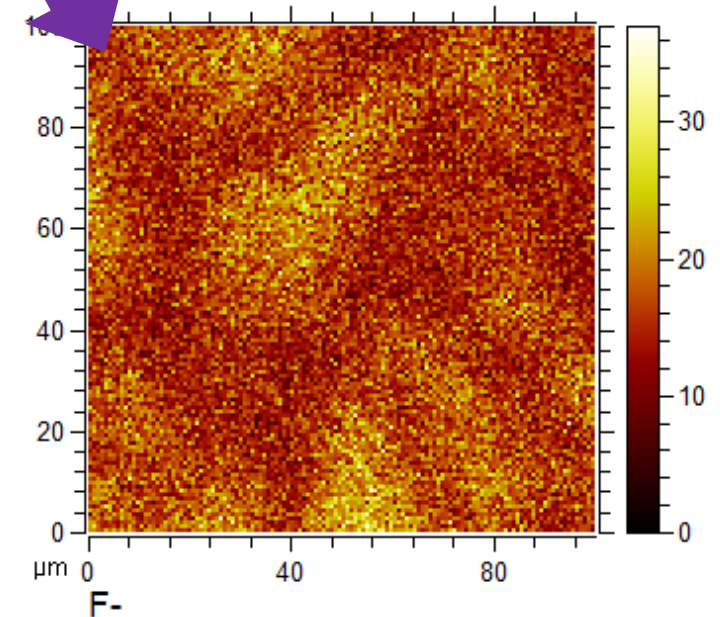


- ✓ PL characteristics peak
- ✓ Blue shift with 5F-PHZ

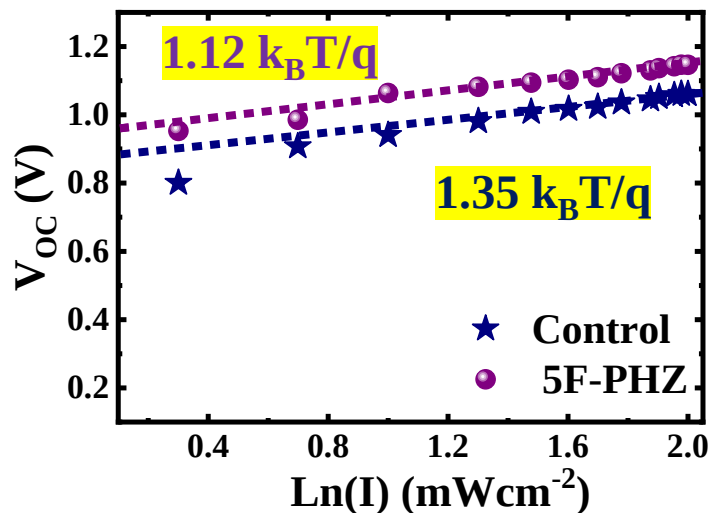




ToF-SIMS; 5F-PHZ
2D images

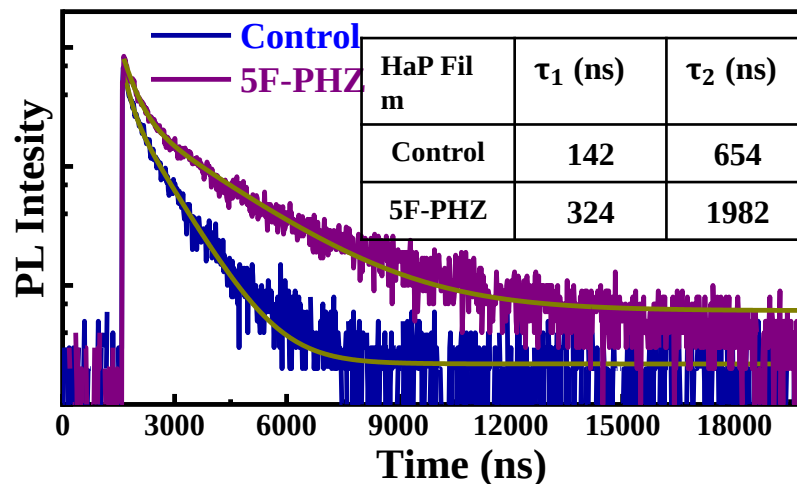


V_{OC} -I analysis

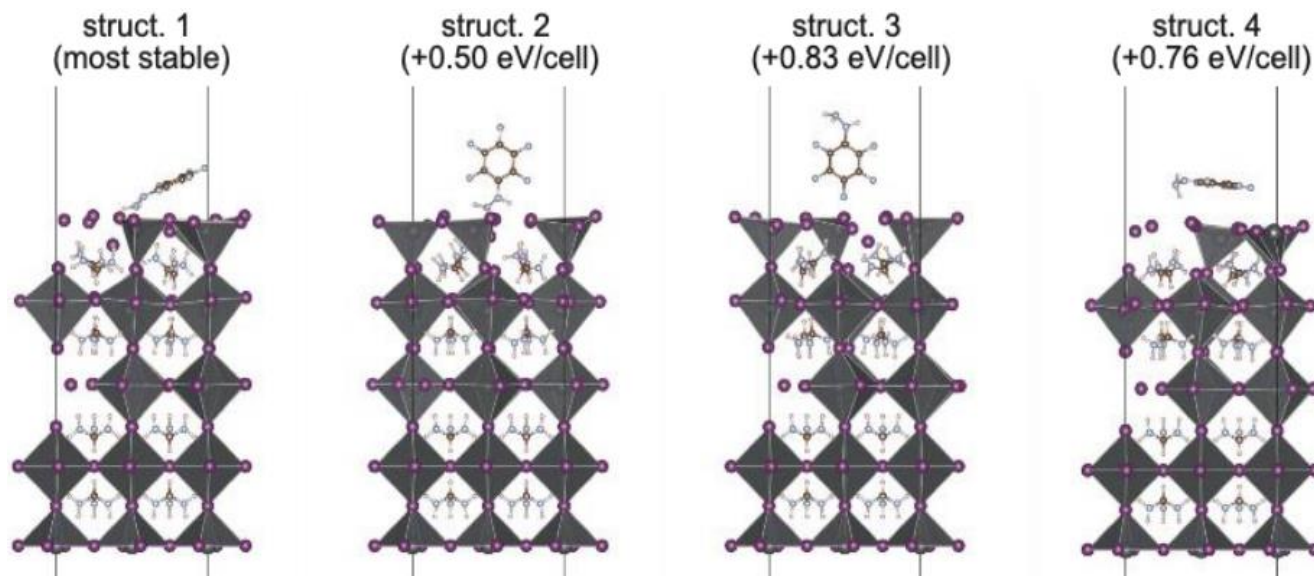
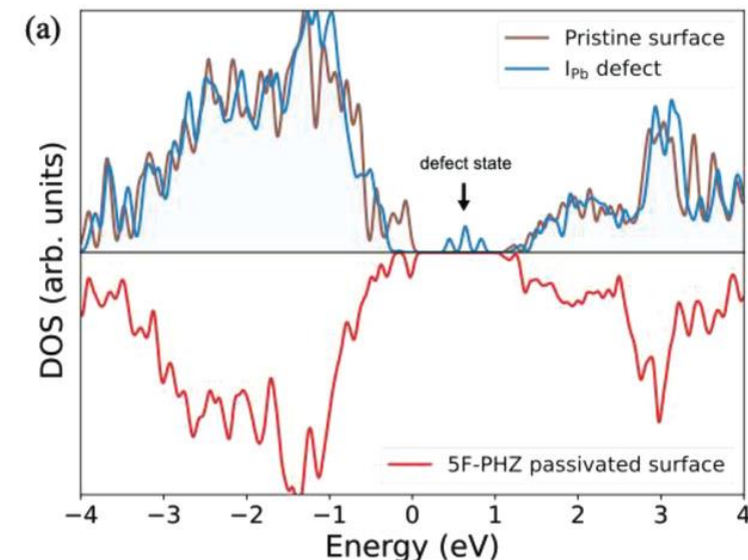


TRPL results

Longer carrier lifetime



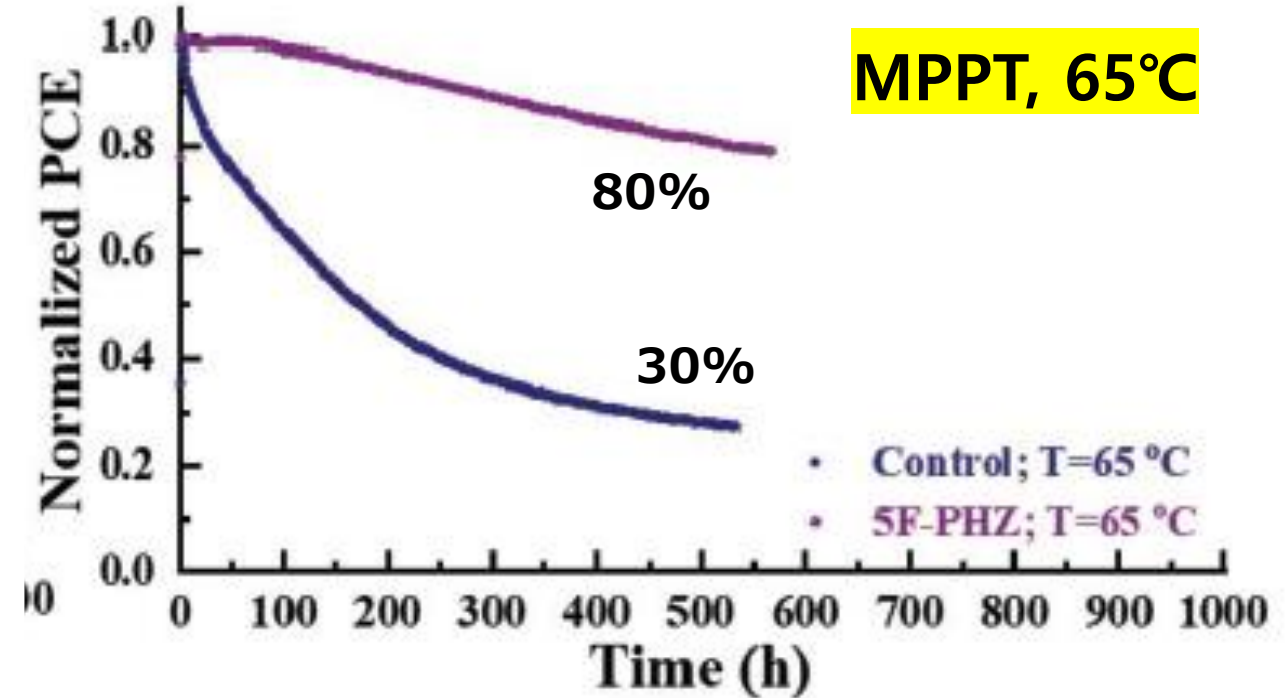
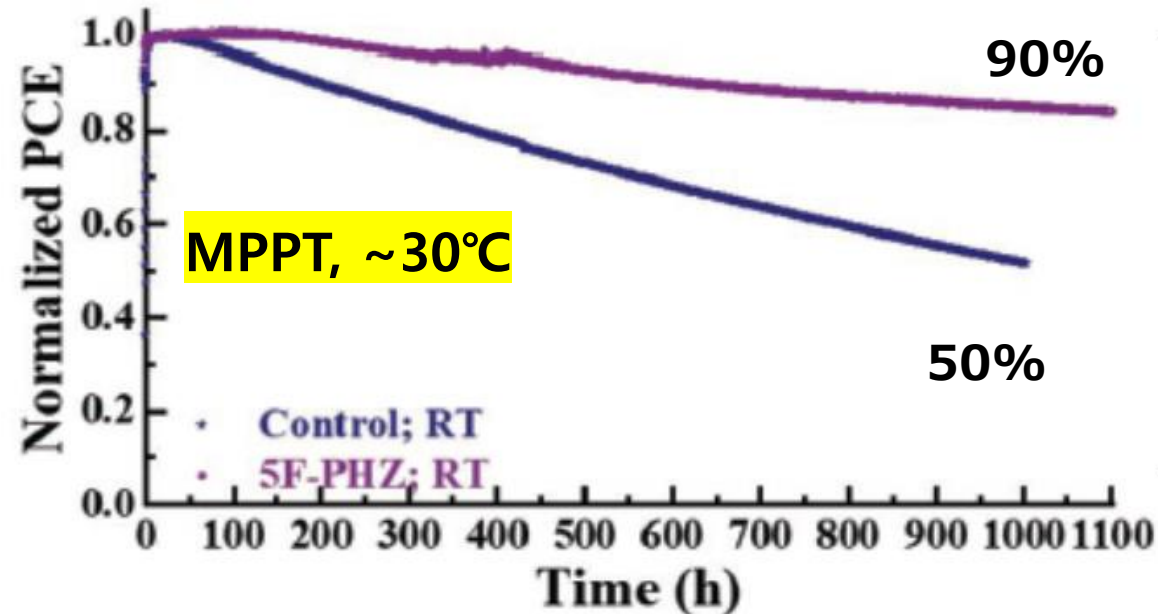
DFT calculations



Terumasa Tadano,
Spin Theory Group

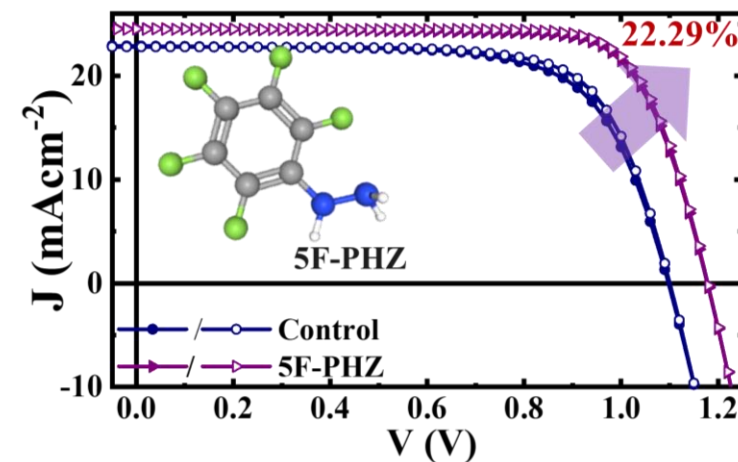
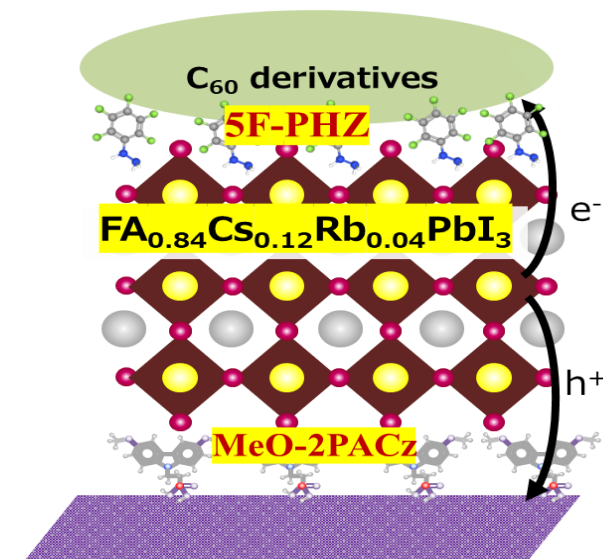
**Over 22 % @1 cm²
Maintain 20% after 1000 hr**

High Stability



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*



Photovoltaic Materials Group

Thank you for your attention



Our team

Oral Session D

14:40-14:55	120	Mitsuhiro	Technology, Nara College	Phosphonium-Cation- Based Ionic Liquids
-------------	-----	-----------	--------------------------	---

Session No.
D-O-2

15:05-16:10, Wednesday, March 1, 2023

Chairperson TSUNASHIMA Katsuhiko (Wakayama KOSEN)

Login required →

◀▶ If the table is cut off in the middle, scroll left or right.

Time	KRIS No.	Speaker	Affiliation	Title
D-O-2-1 15:05-15:25	84	NAGATA Takahiro Invited Speaker	National Institute for Materials Science (NIMS)	Electronic state modification of (Ga _x In _{1-x}) ₂ O ₃ solid solution thin film by combinatorial method
D-O-2-2 15:25-15:40	40	PARK Jongdoc	National Institute of Technology (KOSEN), Oshima College	Practicing Self-sustainable Renewable Energy System by Using Natural Energy Sources
D-O-2-3 15:40-15:55	83	KHADKA Dhruba B.	National Institute for Materials Science (NIMS)	Molecular Passivation for High-Efficiency and Stable Methylammonium-Free Perovskite Solar Cells with Fluorinated Supramolecules
D-O-2-4 15:55-16:10	30	SANGAROON Siriyaoporn	Maharakham University, Thailand	Characterization of CLYC7 scintillation detector in wide neutron energy range