2025 MRS SPRING MEETING & EXHIBIT
April 7-11, 2025 | Seattle, Washington

Molecular Passivation of Wide Bandgap Tin Perovskite Solar Cells With Multifunctional Hydrazide Derivative

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

9th April , 8- 8:15 am

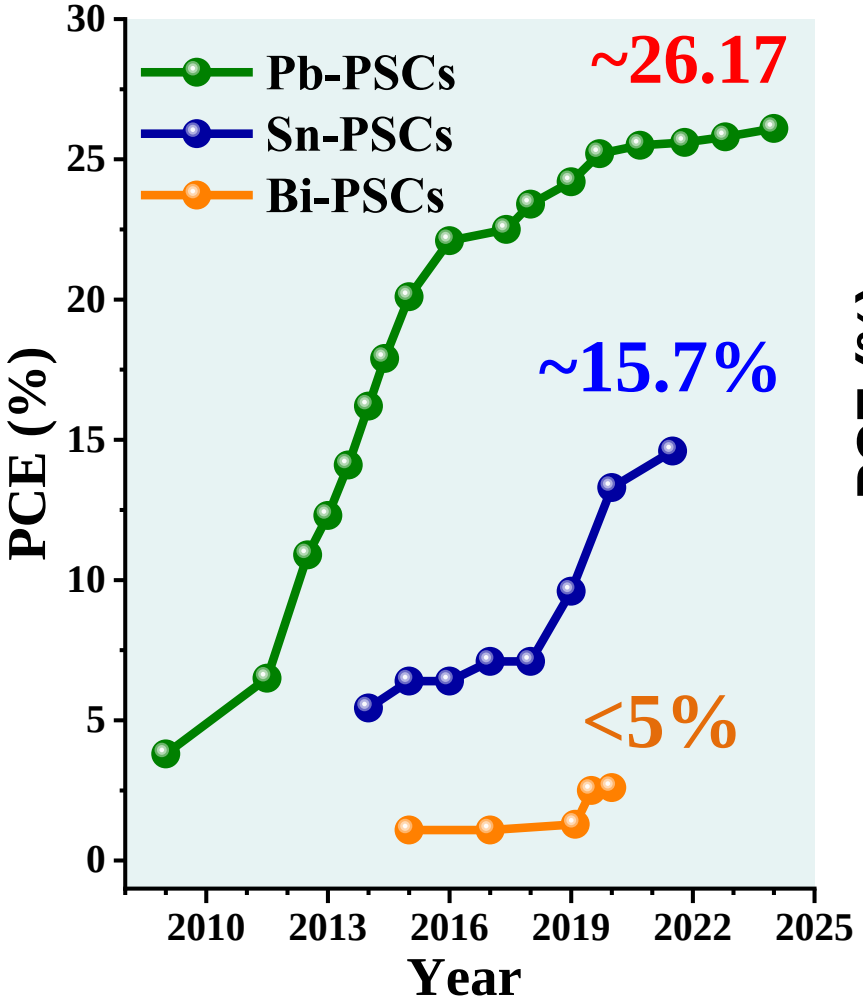
Photovoltaic Materials Group
Global Research Center for Environment and Energy based on Nanomaterials Science(GREEN)
National Institute for Materials Science (NIMS), Tsukuba, Japan

NIMS

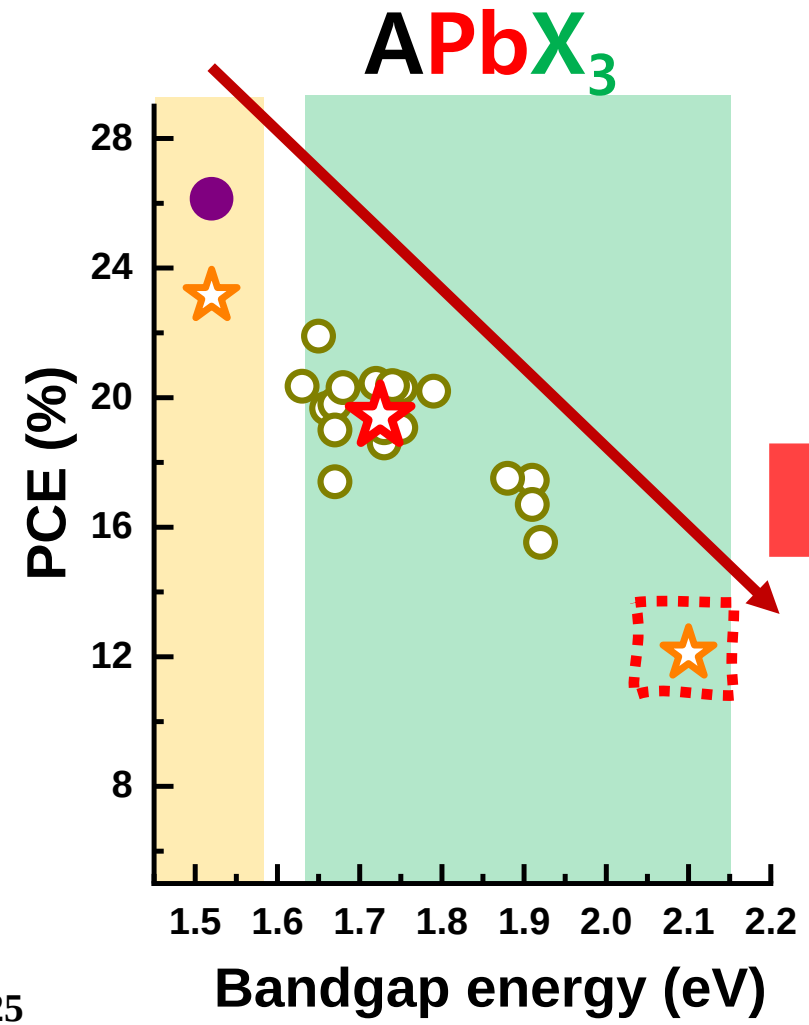
PHOTOVOLTAIC MATERIALS GROUP

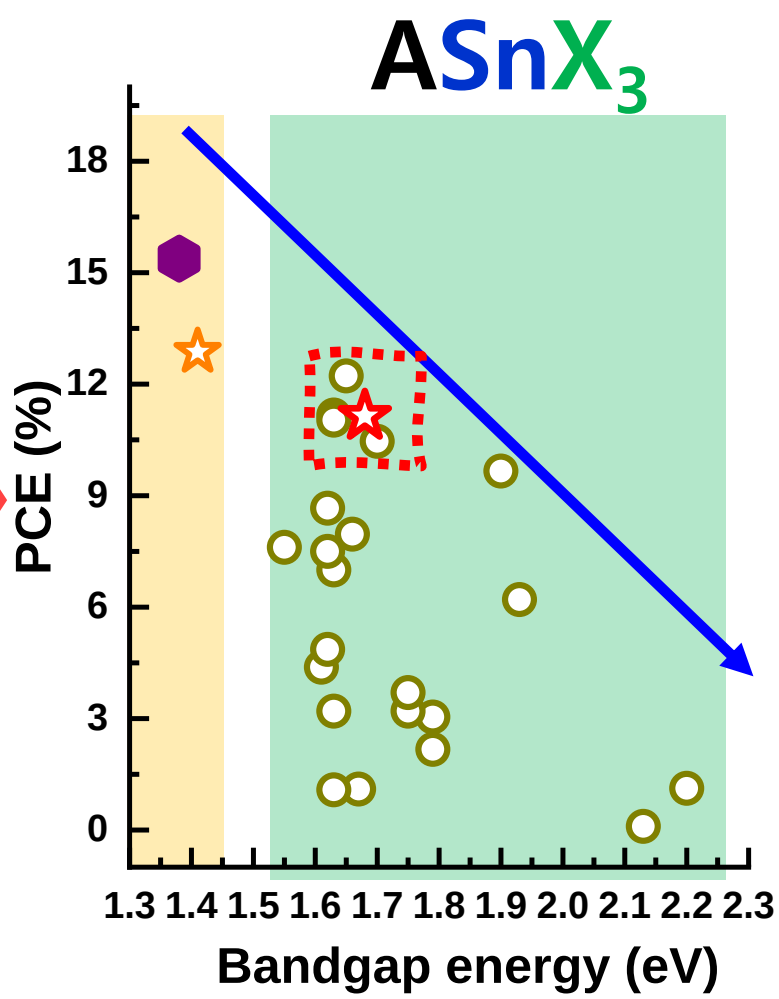
Progress in Perovskite Solar Cells

Regular Bandgap PSCs



Bandgap vs Efficiency PSCs





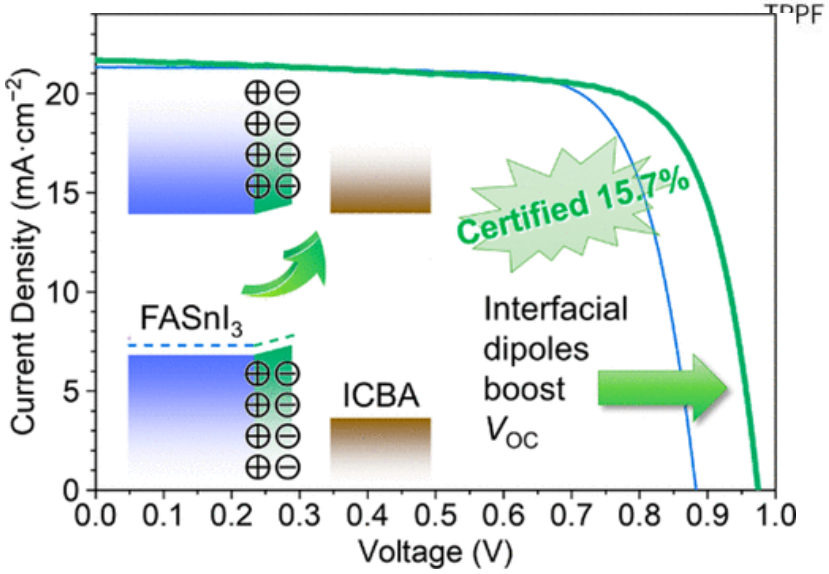
Khadka et al. Nat Commun 15, 882 (2024)

Khadka et al. Chem. Mater. 2023, 35, 4250

Sn-PSCs: Reports

Regular- Bandgap- PSCs

E_g~1.4 eV

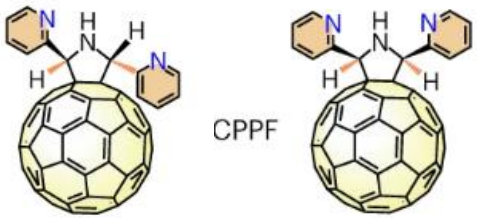


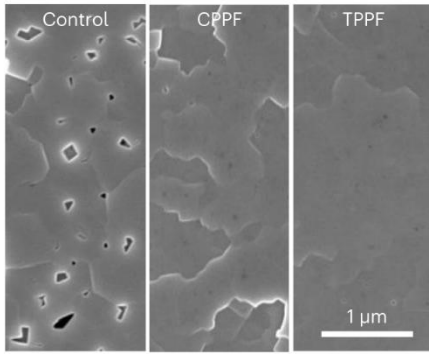
>15.7%

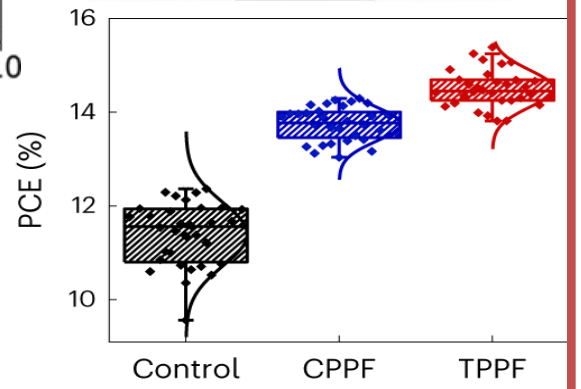
4-F-PEABr + FASnI$_3$

Mi et al., *ACS Energy Lett.* 2024, 9, 1895

Fulleropyrrolidine additives







(PEAI, FAI,SnI_2,SnF_2) precursor solution

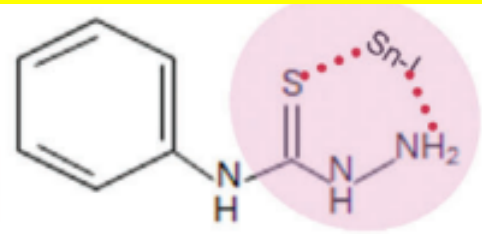
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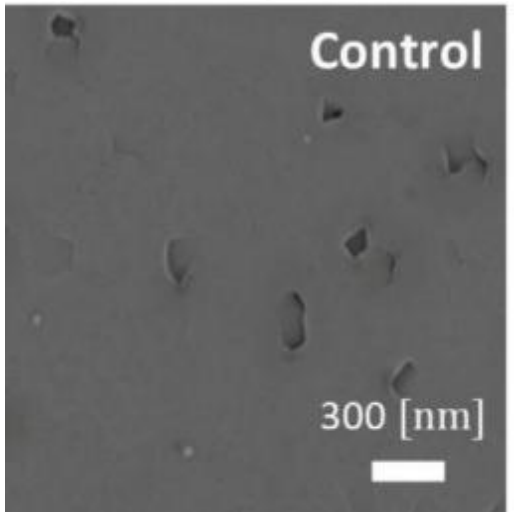
Tain and Wei group, Nat. Photon. 2024, 18, 464

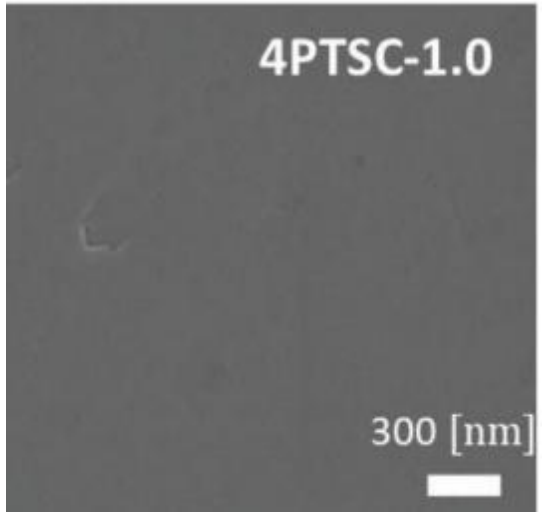
Wide- Bandgap- PSCs

E_g~1.65 eV

4-Phenylthiosemicarbazide additive





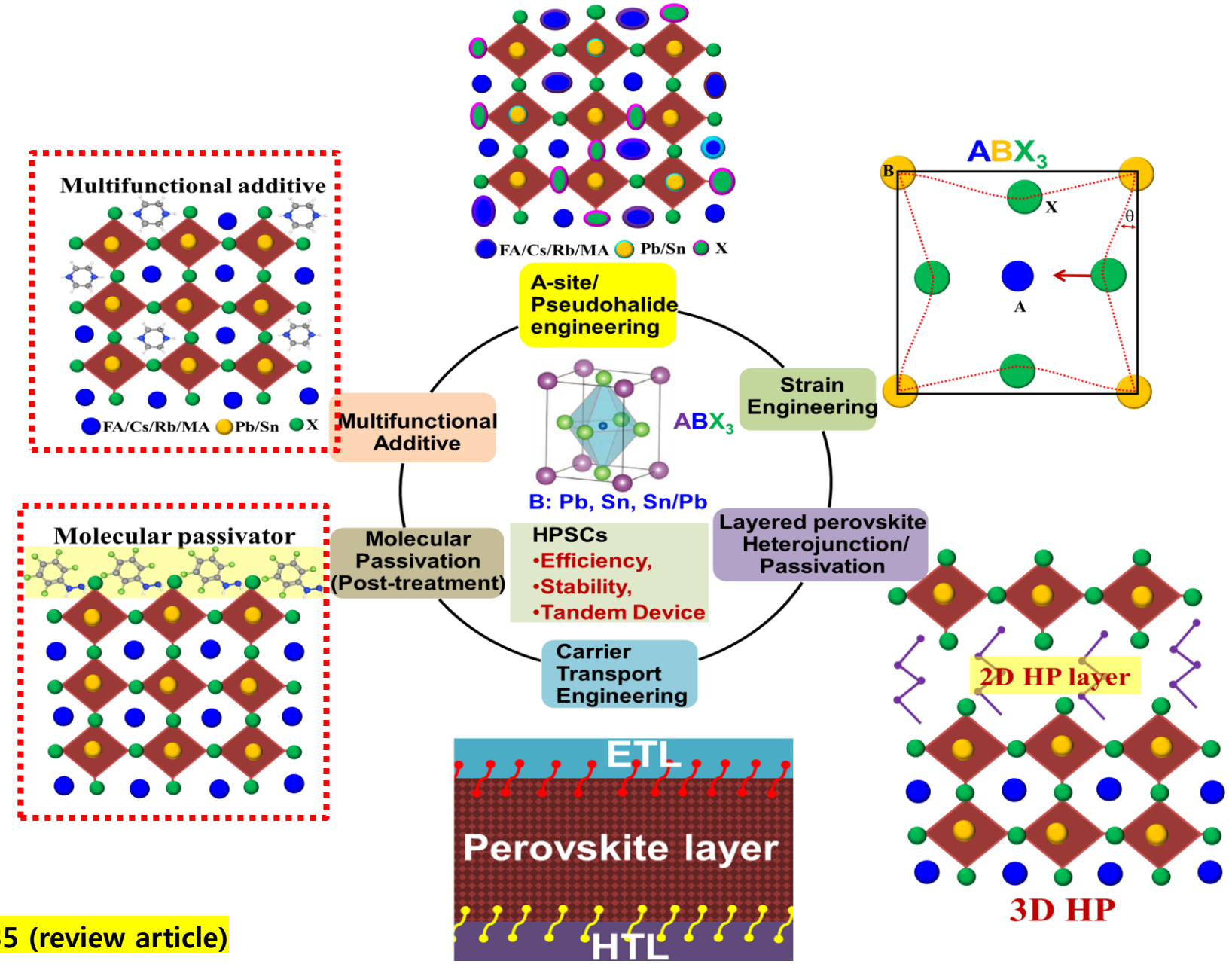


$PEA_{0.15}FA_{0.75}MA_{0.1}SnI_2Br$

>11.70%

Hayase and Khang group, Adv. Energy Mater. 2024, 14, 2401188

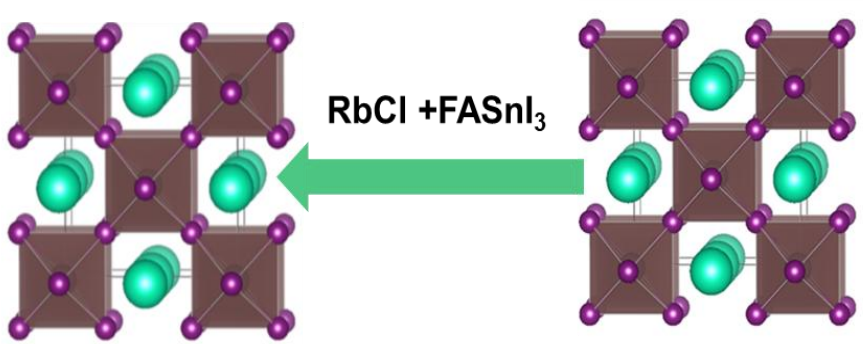
Device efficiency progress and stability



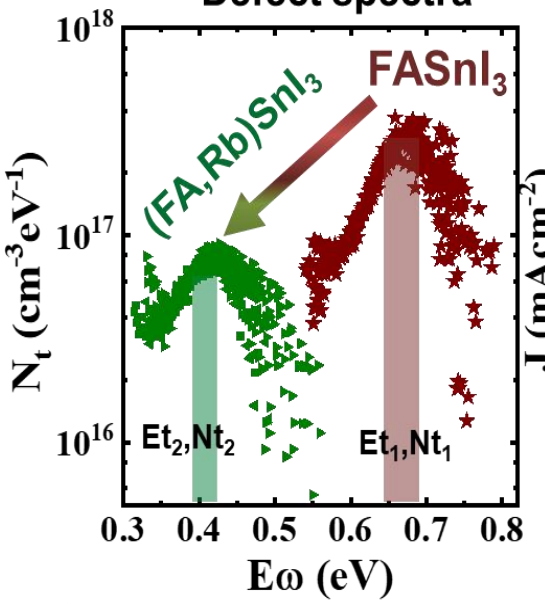
Khadka et al. Sol. RRL 2023, 2300535 (review article)

Our reports on Sn-PSCs

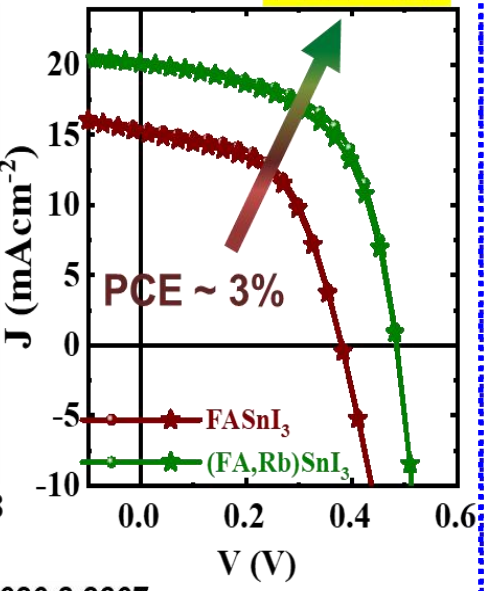
Structural regulation



Defect spectra

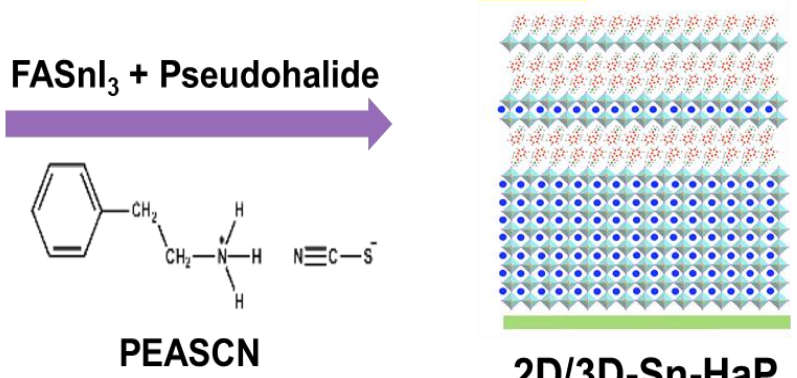


PCE~ 6%

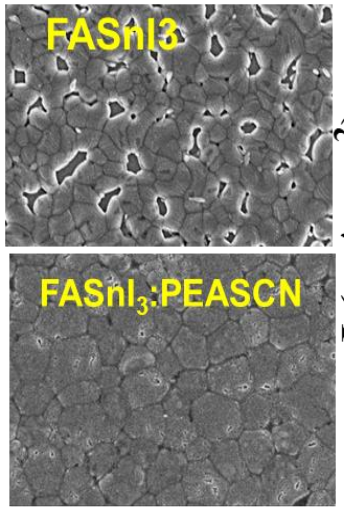


Khadka* et al. Mater. Chem. C,2020,8,2307

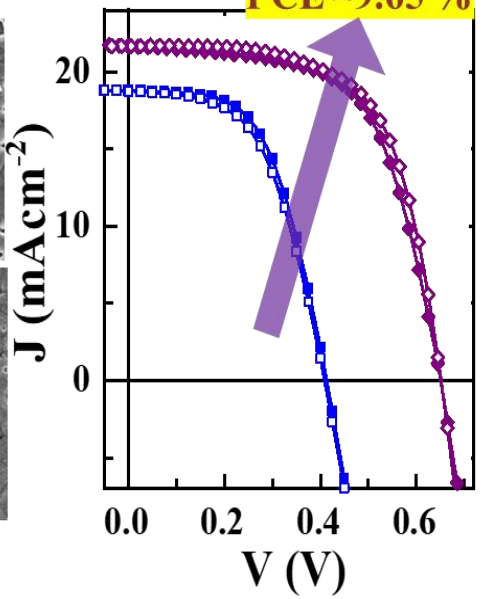
Pseudohalide additive effect



Film growth

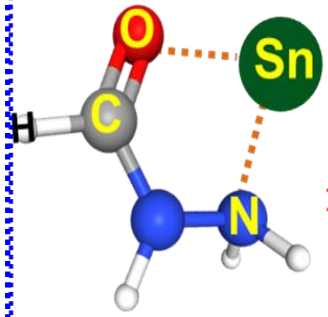


PCE ~9.65 %



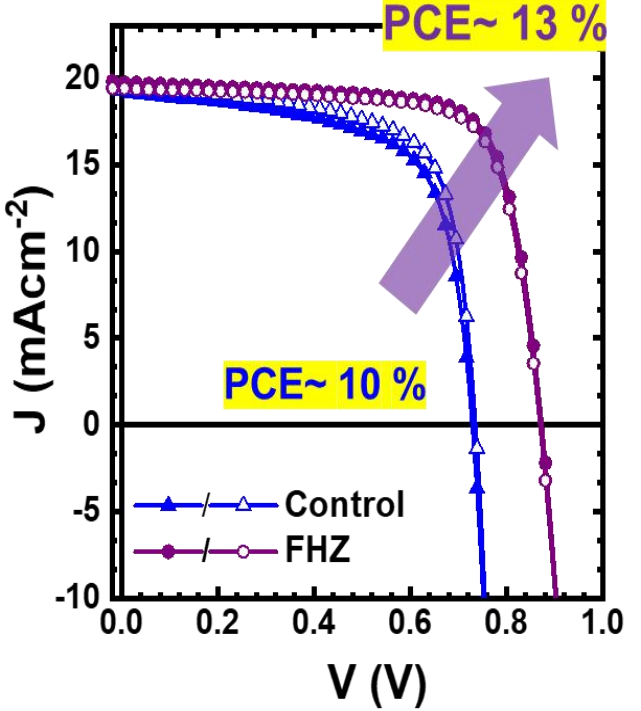
Khadka* et al. *ACS Appl. Energy Mater. 2021, 4, 12819*

Multi-functional ligand-additive



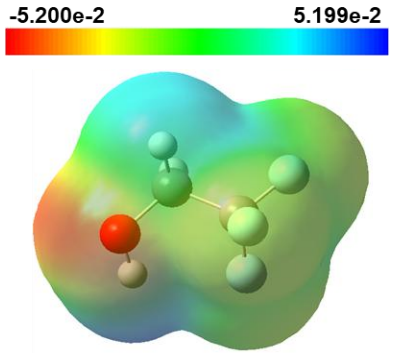
Formohydrazide (FHZ)
>Bidentate ligand

PCE~ 13 %

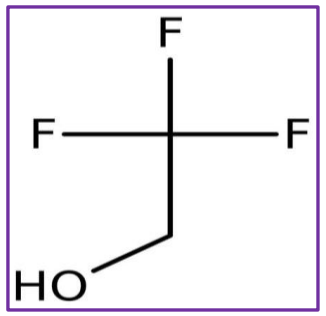


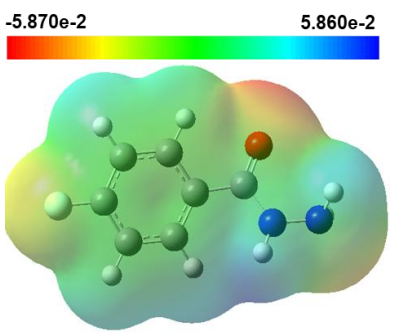
Khadka et al. Chem. Mater. 2023,35, 4250*

Additive + Surface Engineering: WB-Sn-PSCs

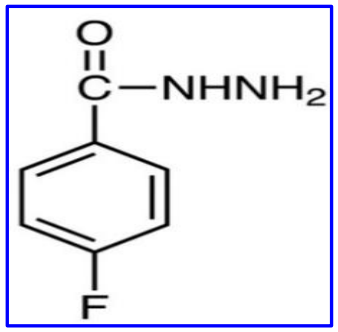


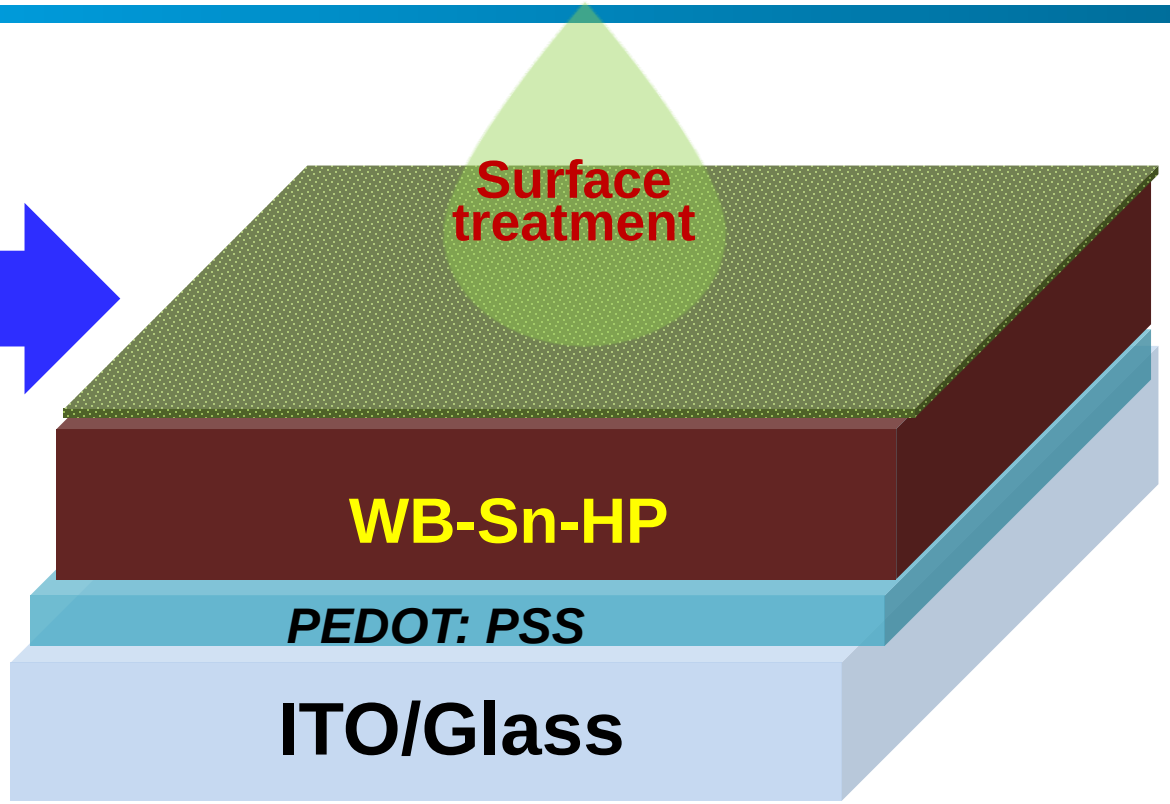
Trifluoroethanol





4-Fluoro-benzohydrazide





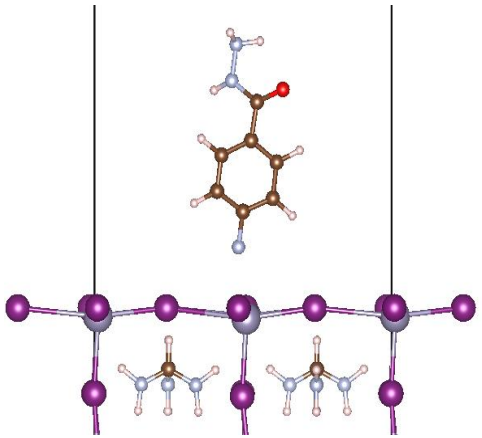
WB-Sn-perovskite

(FA, MA, PEA)SnI_2Br)
E_g ~1.68 eV

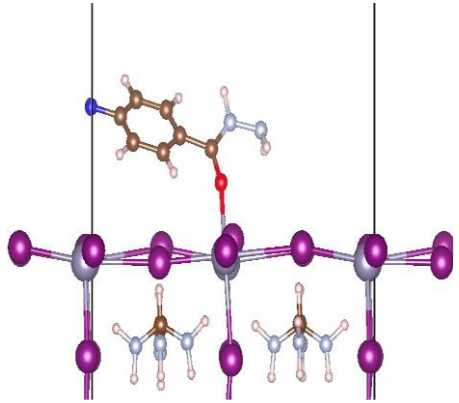
Khadka and co-workers, Small, 2024, 2410048

Molecular Interaction: F-BHZ and Sn-perovskite film

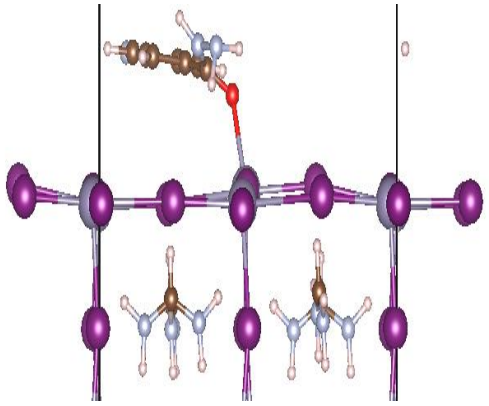
$E_{ad} = -0.62$ eV



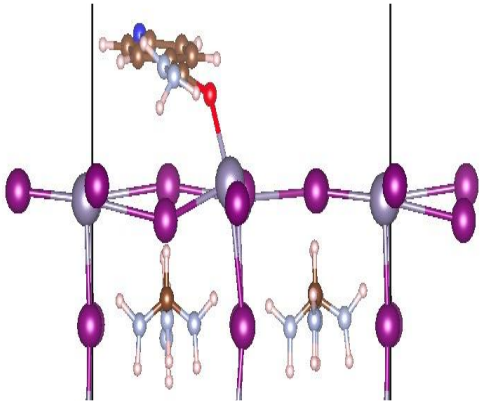
$E_{ad} = -1.27$eV

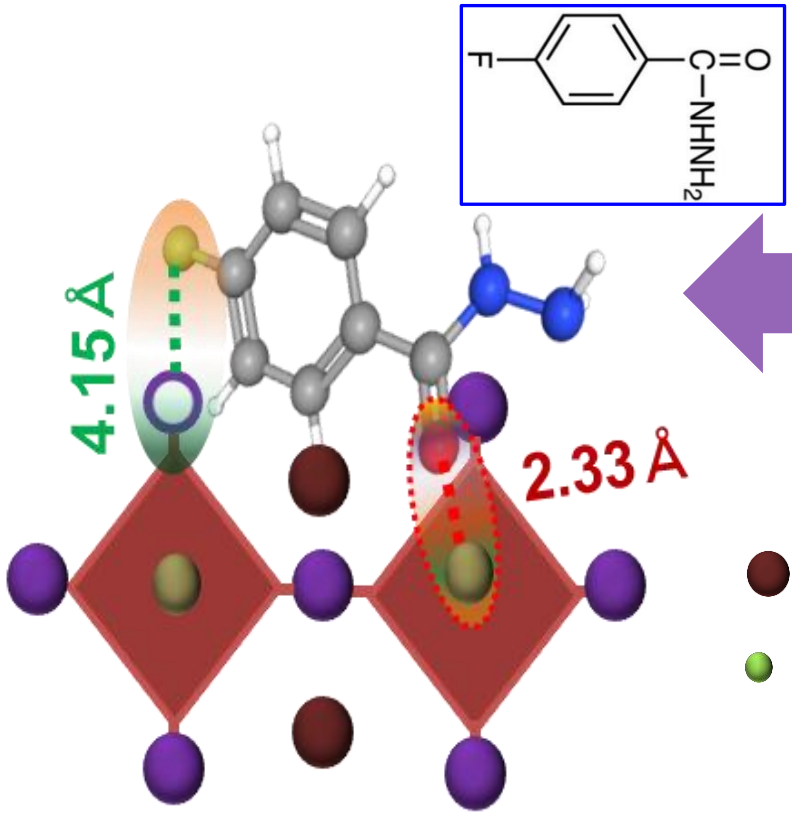


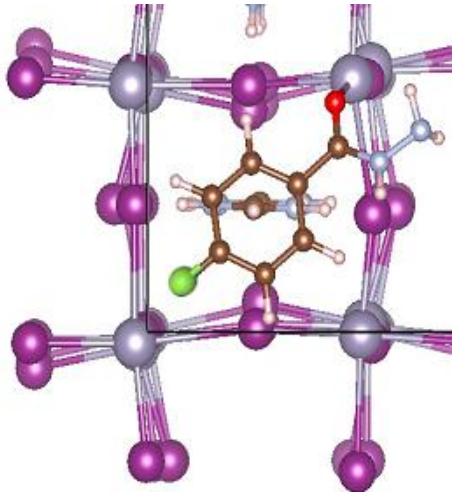
$E_{ad} = -1.47$ eV



$E_{ad} = -1.63$ eV







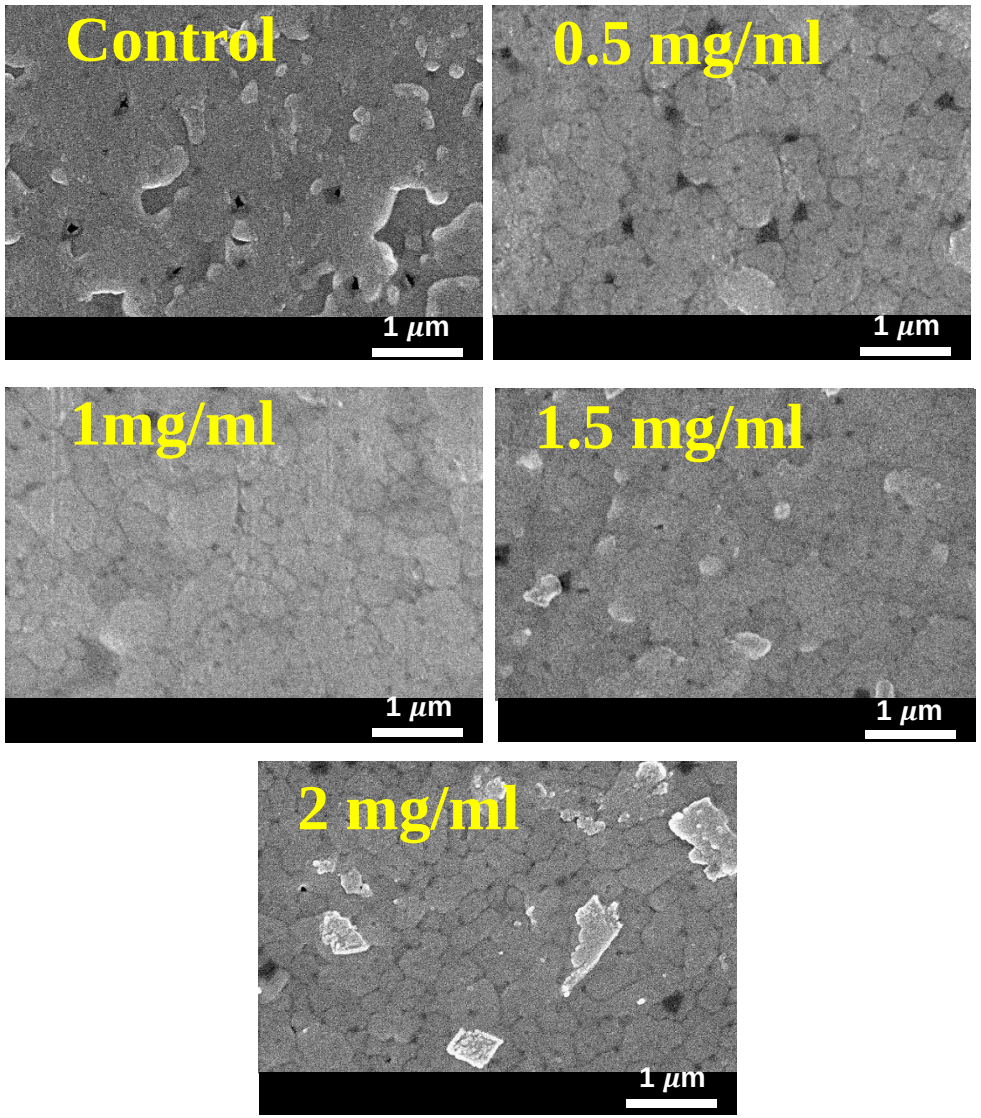
FA/MA Sn

F I/Br

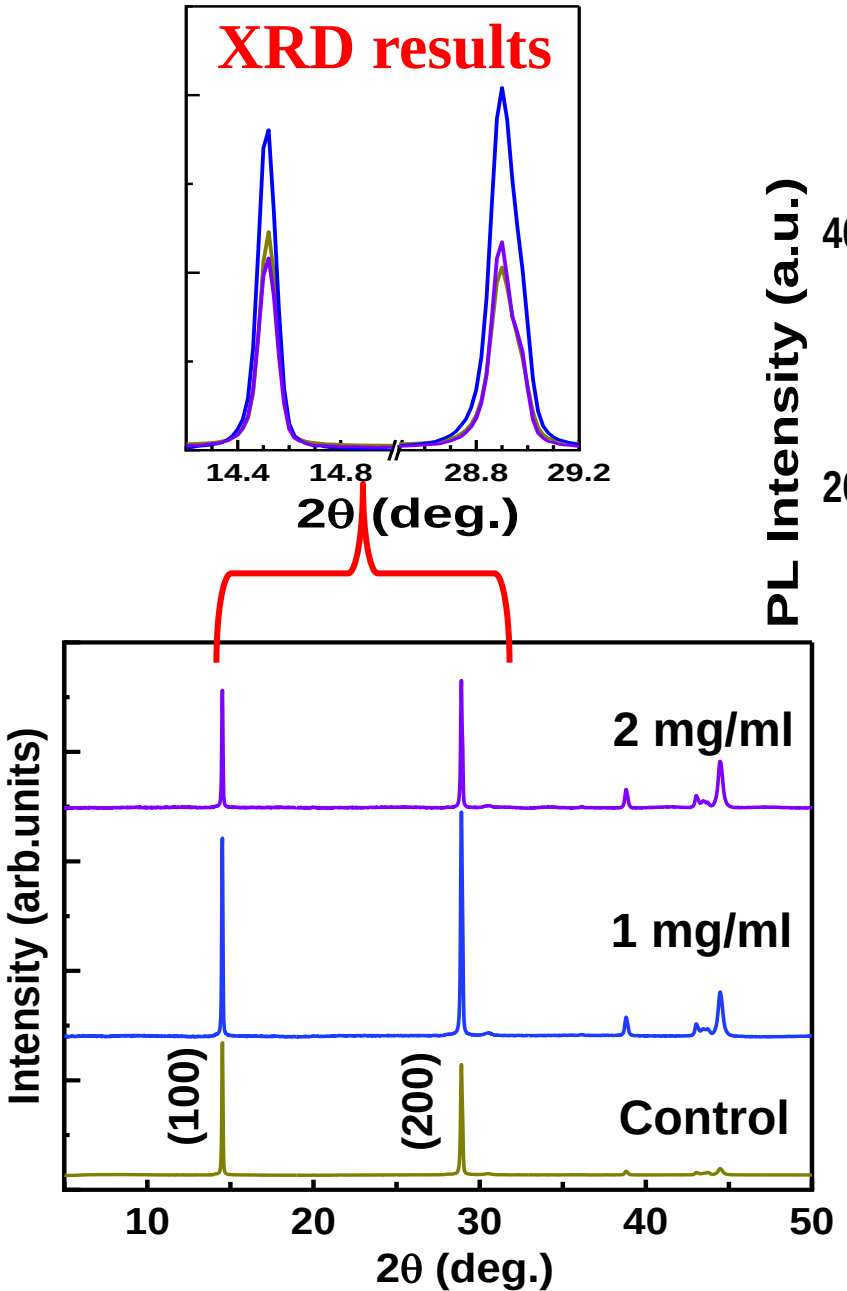
- Sn-perovskite surfaces > 2.33Å - O-Sn
  > 4.15 Å for F-I
  > 4.80 Å for F-Sn.
- strong O-Sn interaction > weak interaction of F-I

Effect of Surface Treatment >> Film Growth

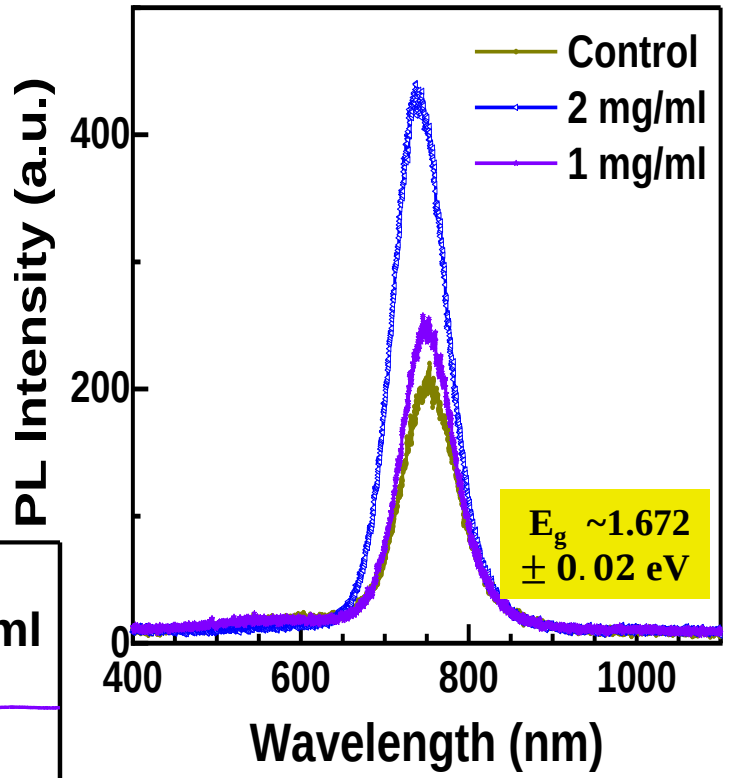
Film- morphology



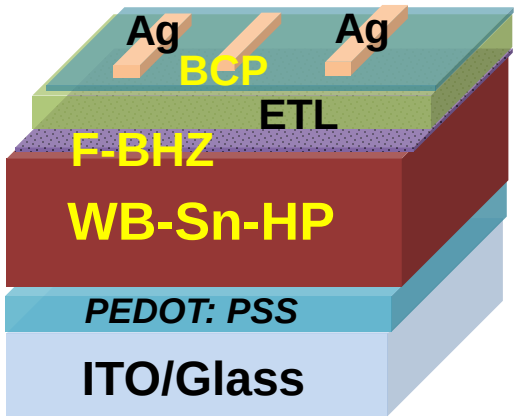
XRD results

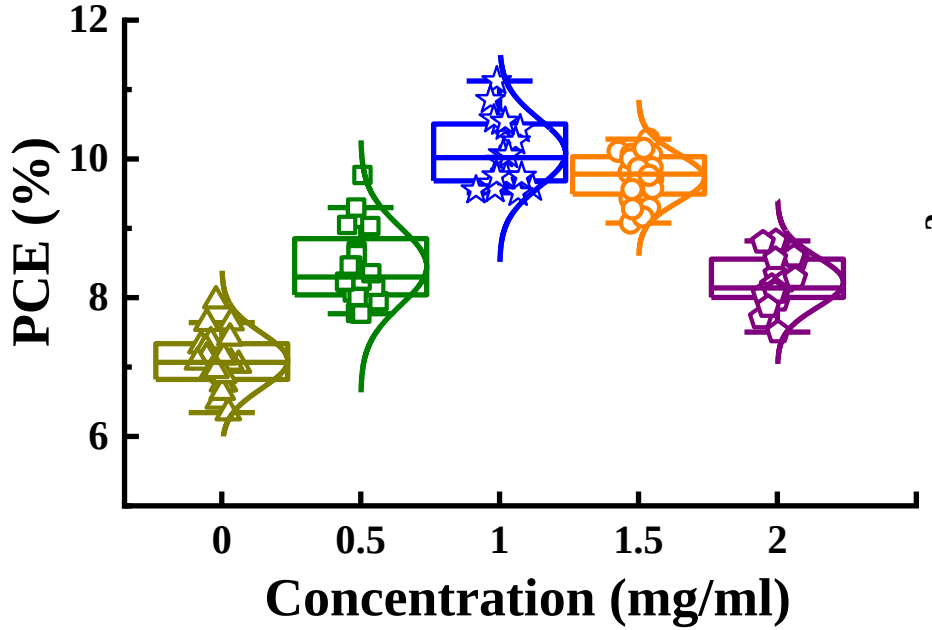


PL spectra

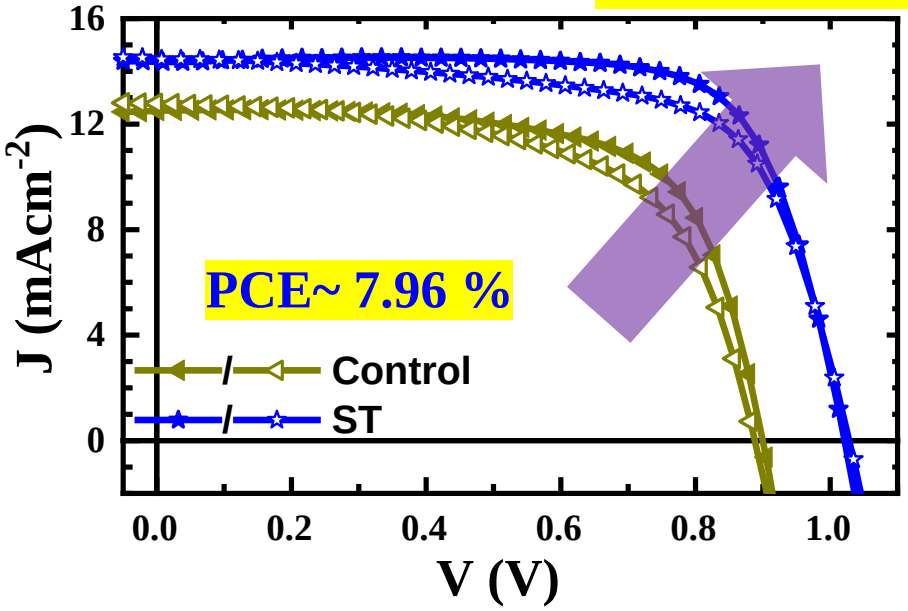


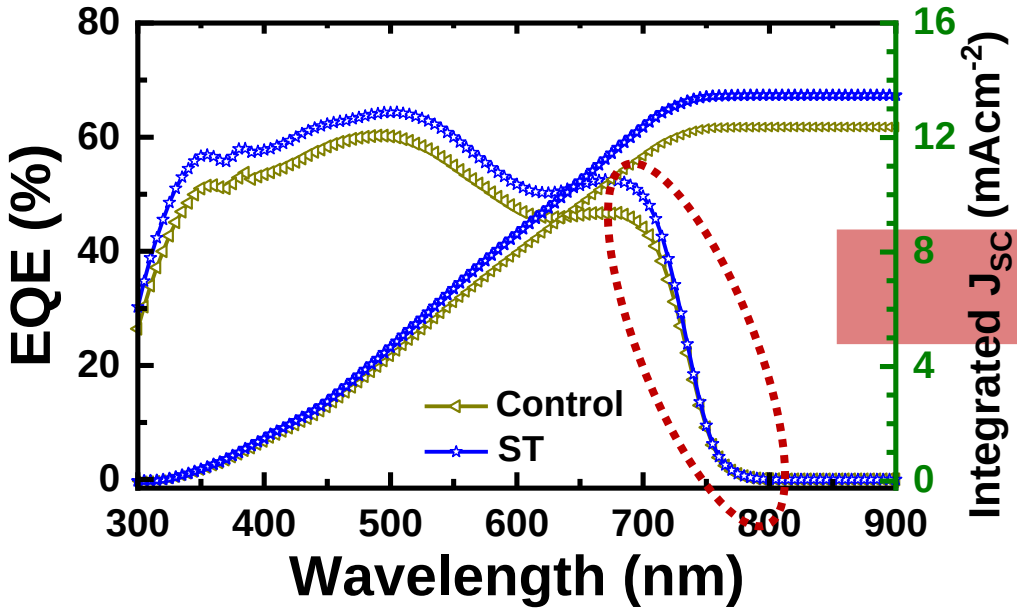
Effect of F-BHZ- passivation >> WB-Sn-PSCs

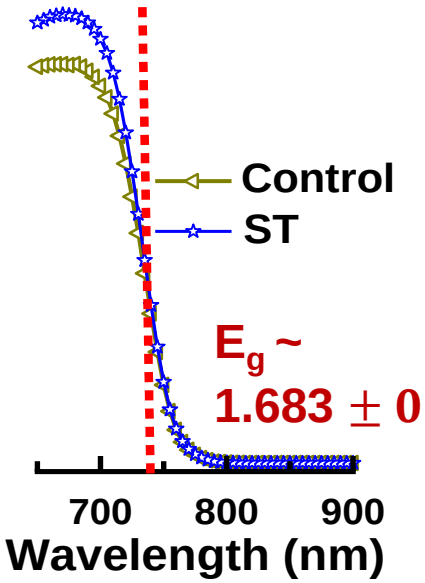




PCE~ 11.14%



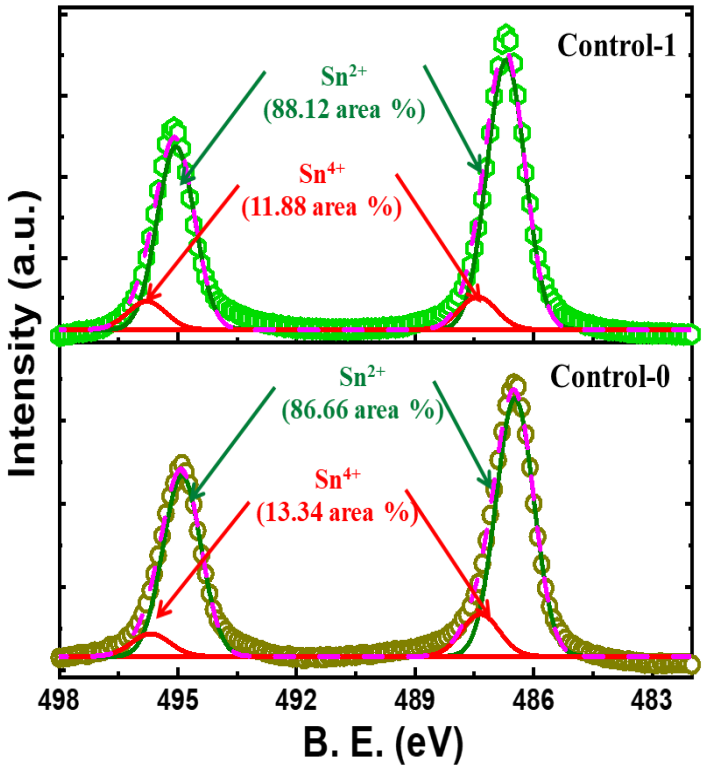


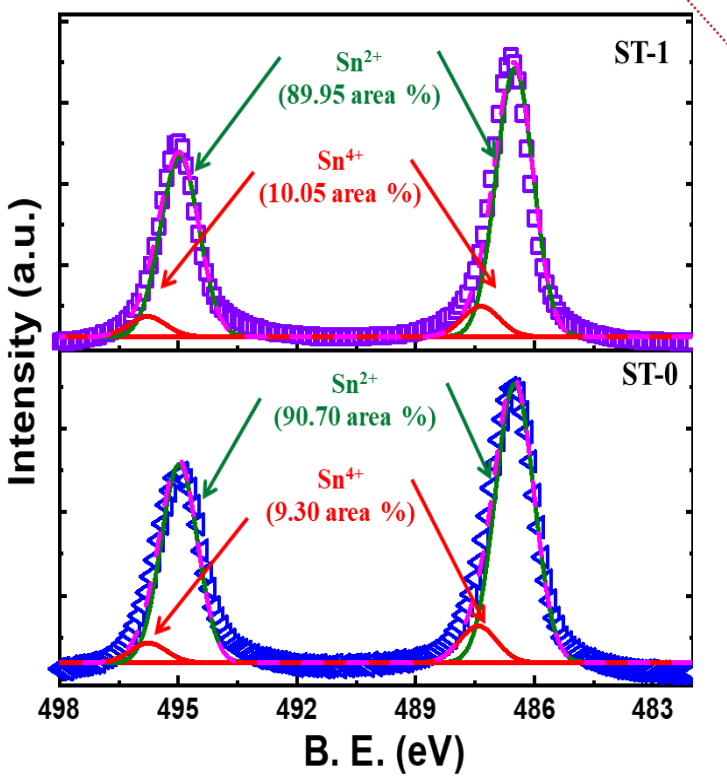


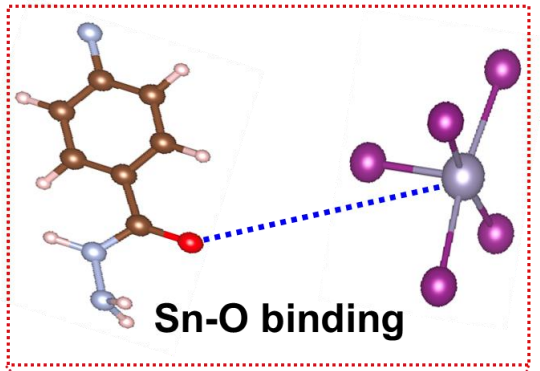
- ✓ J_{SC} -12.58 to 14.37 mA/cm^2
- ✓ V_{OC} – 0.914 to 1.024 V
- ✓ FF- 0.692 to 0.757

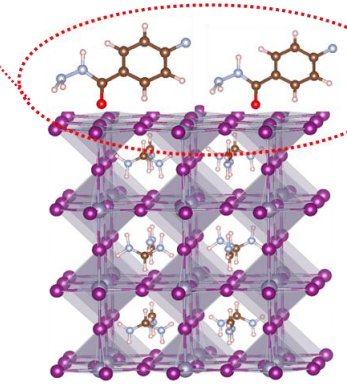
WB-Sn-HP/F-BHZ > Surface properties modulation

XPS: Suppression of oxidation



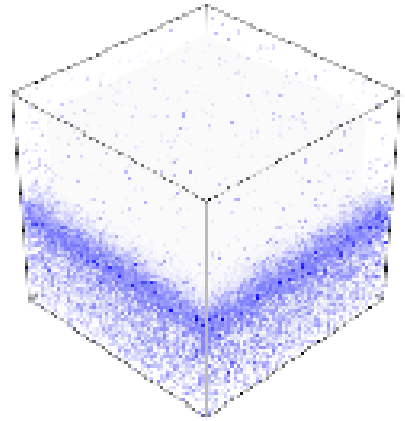




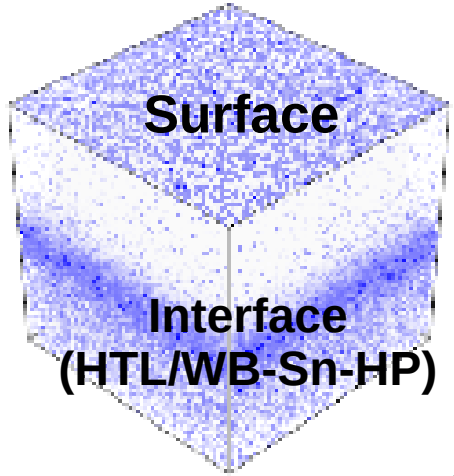


F-BHZ depth profile

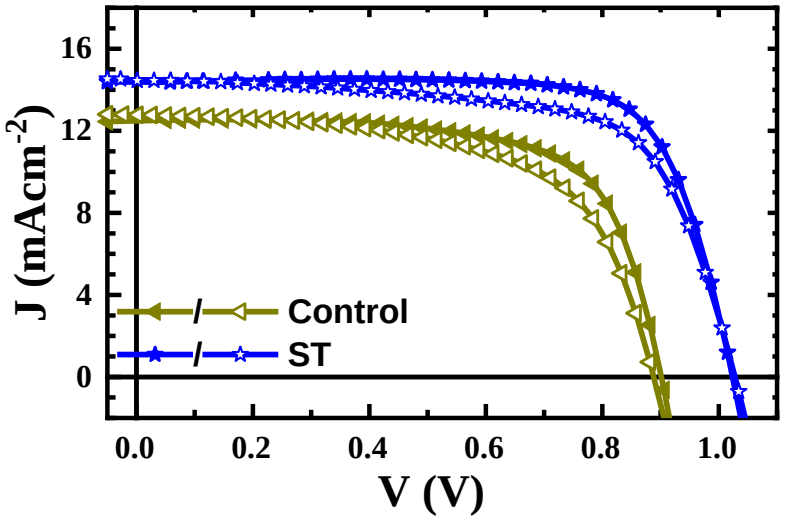
Control

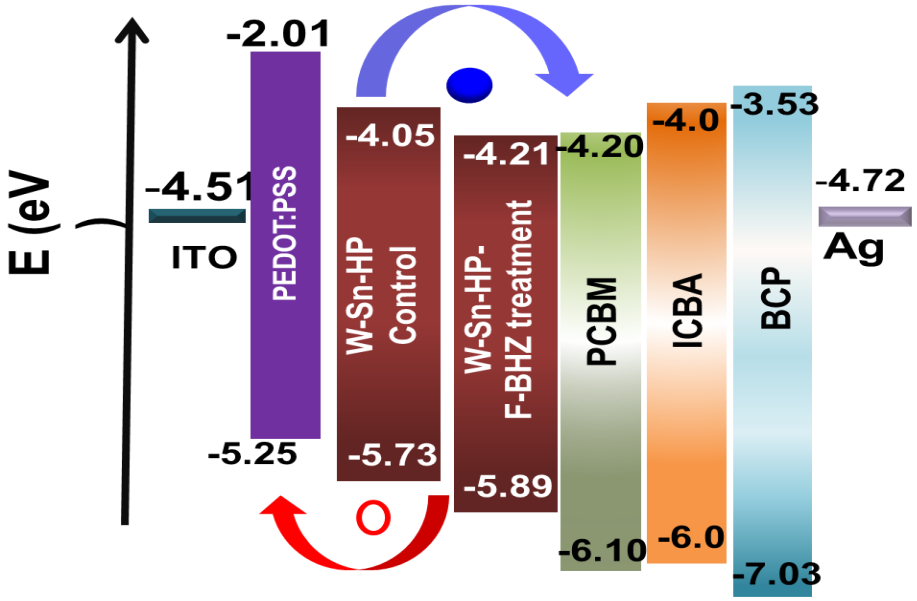


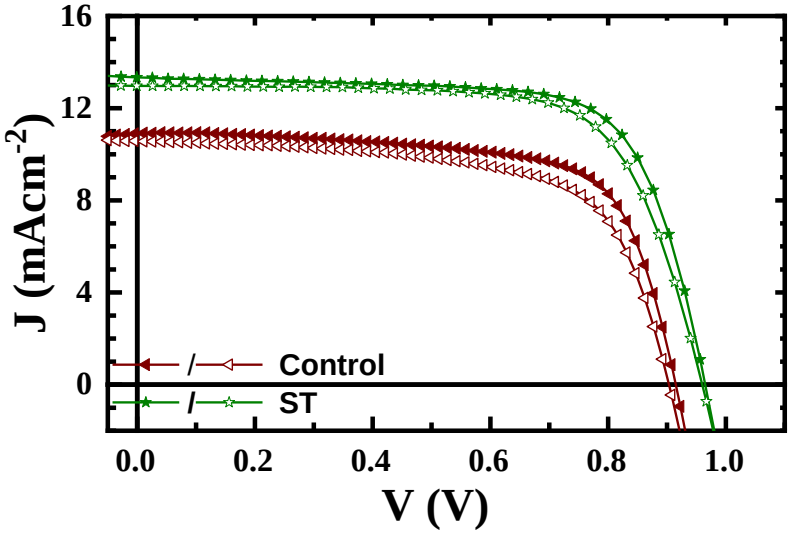
F-BHZ treated



WB-Sn-PSCs- ETL effect >> F-BHZ- effect







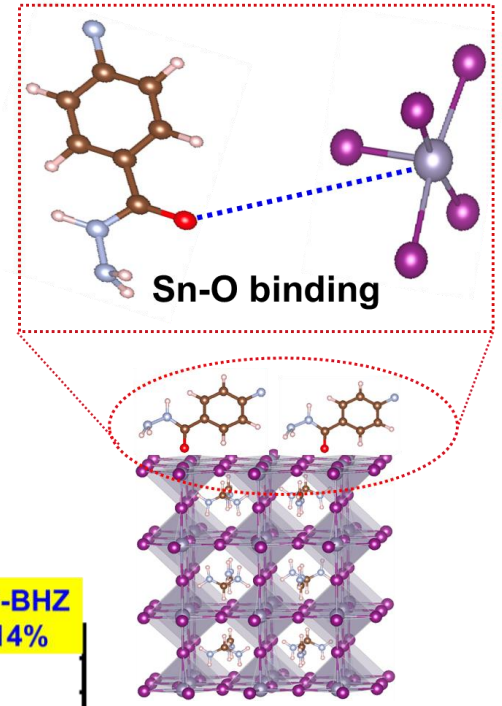
Device structure: ITO/PEDOT:PSS/WB-Sn-HP/ICBA/BCP/Ag					
Device	**Scan direction**	**J_{sc} ($mAcm^{-2}$)**	**V_{oc} (V)**	**FF**	**PCE (%)**
Control	**F**	**12.58**	**0.914**	**0.692**	**7.96**
	R	12.76	0.928	0.622	7.37
ST	**F**	**14.37**	**1.024**	**0.757**	**11.14**
	R	14.46	1.036	0.696	10.43

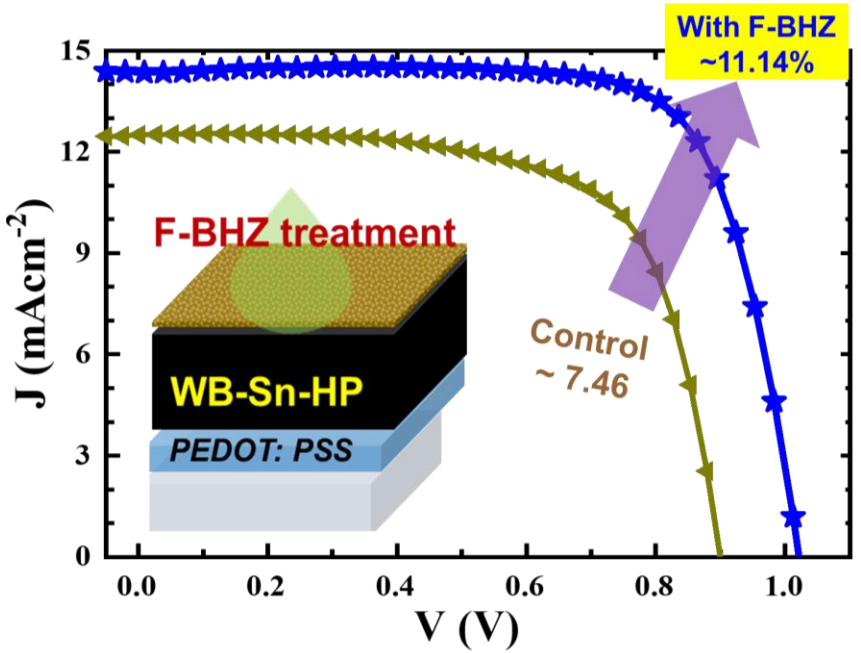
Device structure: ITO/PEDOT:PSS/WB-Sn-HP/PCBM/BCP/Ag					
Device	**Scan direction**	**J_{sc} ($mAcm^{-2}$)**	**V_{oc} (V)**	**FF**	**PCE (%)**
Control	**F**	**10.77**	**0.851**	**0.697**	**6.39**
	R	11.16	0.863	0.656	6.32
ST	F	12.95	0.959	0.717	8.90
	R	**13.41**	**0.967**	**0.706**	**9.15**

Report Summary

F-BHZ treatment:

- *Stronger interaction with Sn-perovskite surface*
- *Facilitate uniform morphology with better crystal quality*
- *Control the extent of oxidation of Sn^{2+} /Mitigation of defects*
- ***PCE > improved to 11.14 % -better stability***





Acknowledgement





Thank you for your attention