MRM2025 MATERIALS RESEARCH MEETING 2025
Dec 8-13 Yokohama
MRS-J

Sn-Perovskite Solar Cells with Terpyridine-Zinc(II) Coordination Nanosheets

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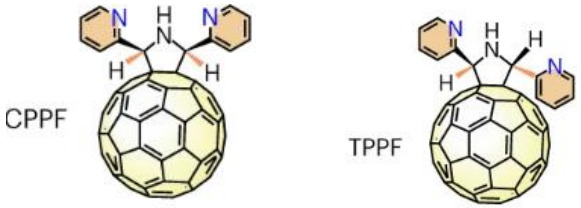
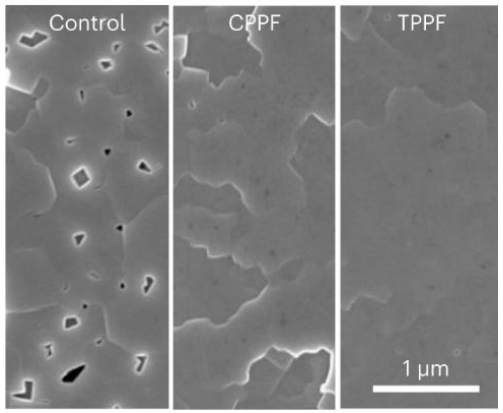
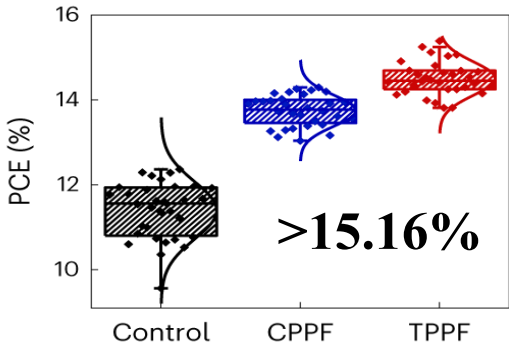
Symposium:[G-2] Metal halide perovskite solar cells
Wed. Dec 10, 2025 :11:40 AM - 12:00 PM JST: Session 18 (G221)

Sn-PSCs: Reports- Additive and Interface Engineering

Fulleropyrrolidine additives



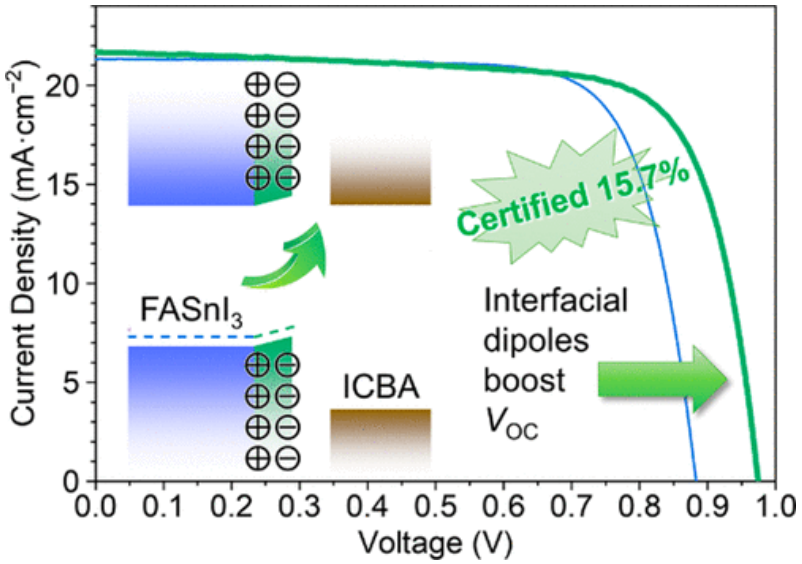




(PEAI, FAI,SnI_2,SnF_2) precursor solution

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

E_g~1.4 eV

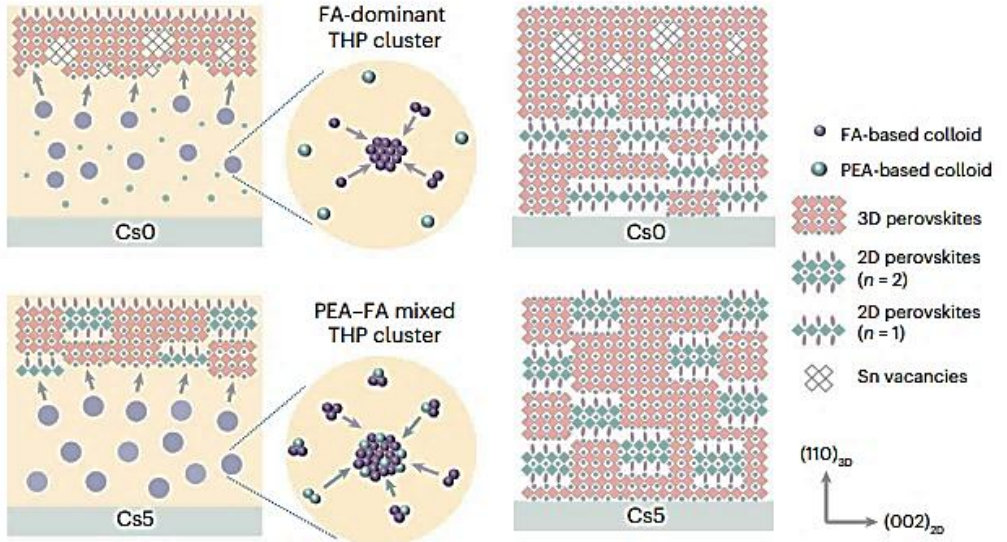


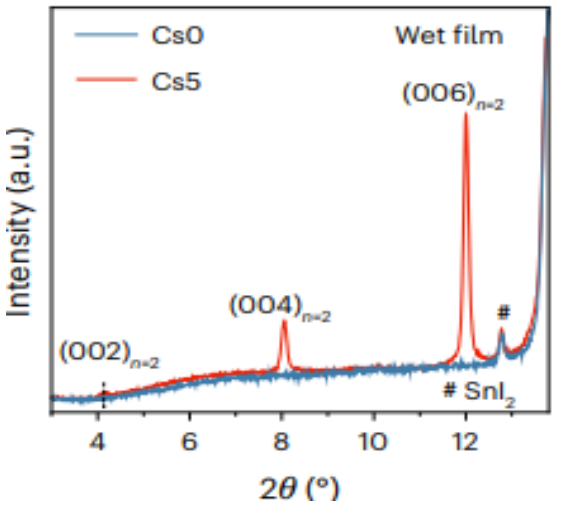
>15.7%

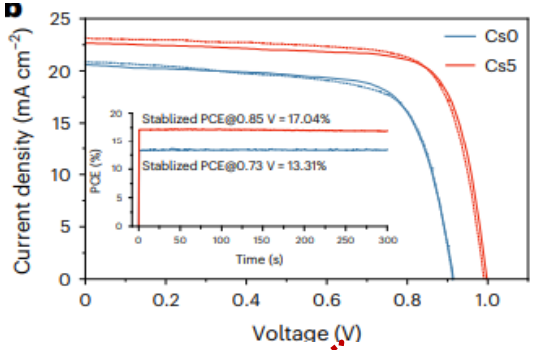
4-F-PEABr + $FASnI_3$

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

Caesium-PEA-FA –based colloid-regulated 2D/3D Sn-perovskite



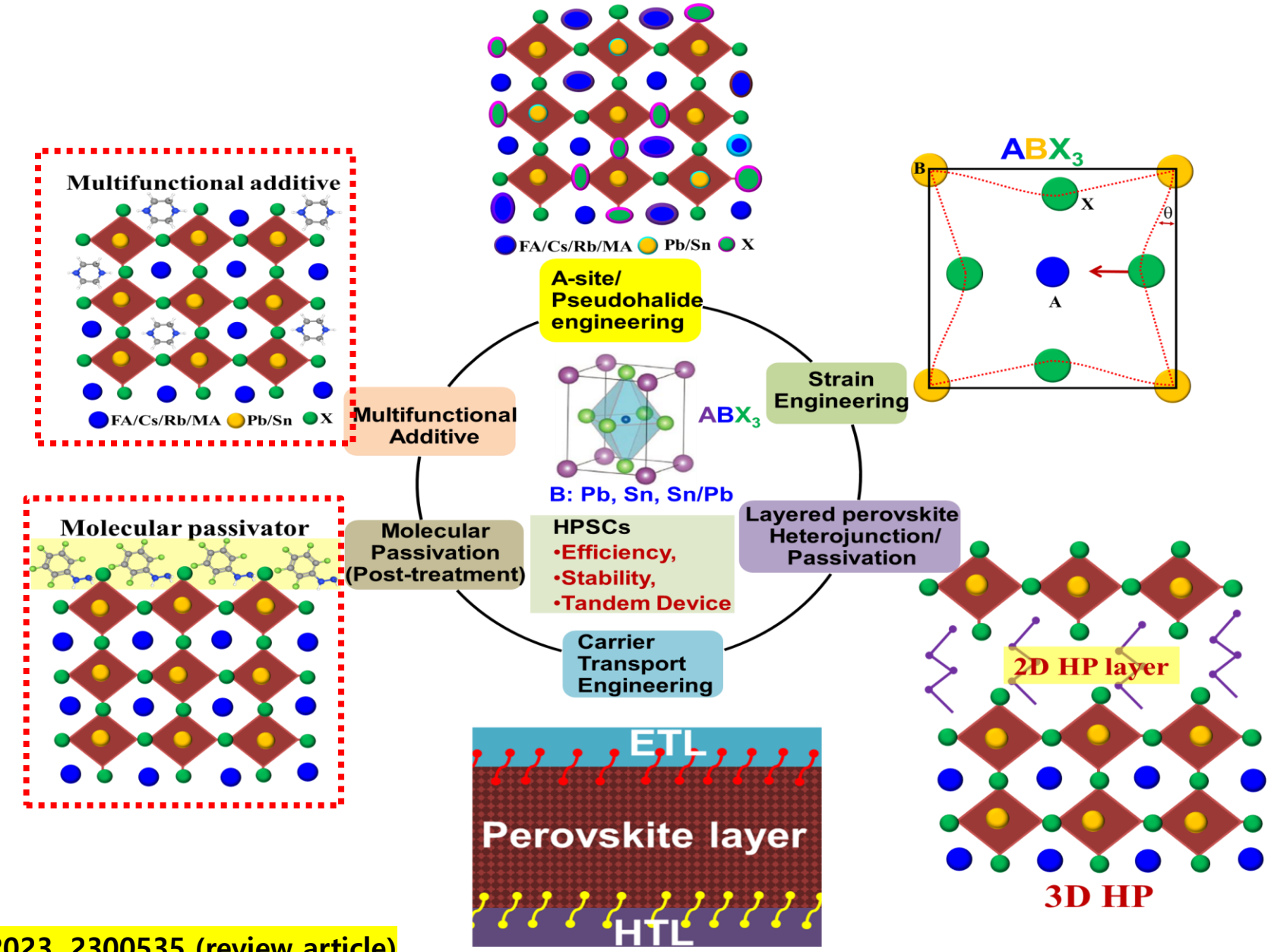




~17.13%

Wang and co-workers, Nat. Nanotechnol. 2025, 20, 779

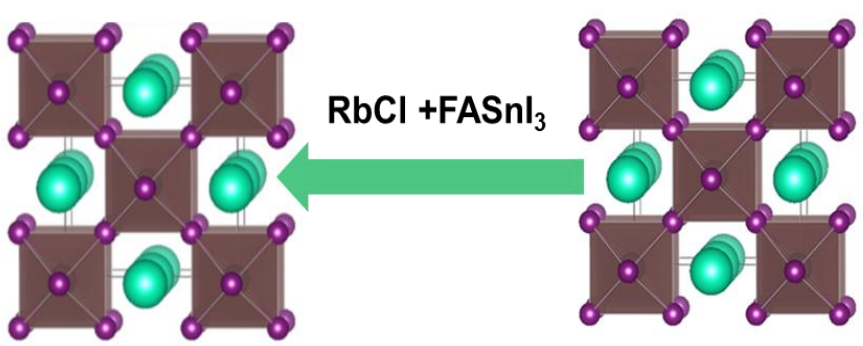
Device efficiency progress and stability



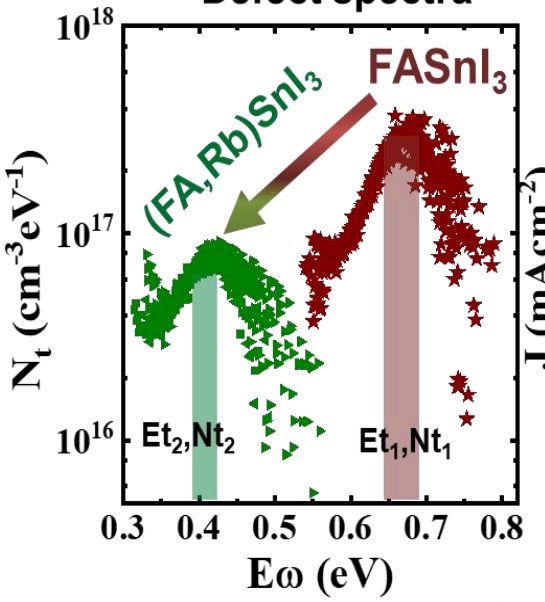
Khadka et al. Sol. RRL 2023, 2300535 (review article)

Our reports on Sn-PSCs

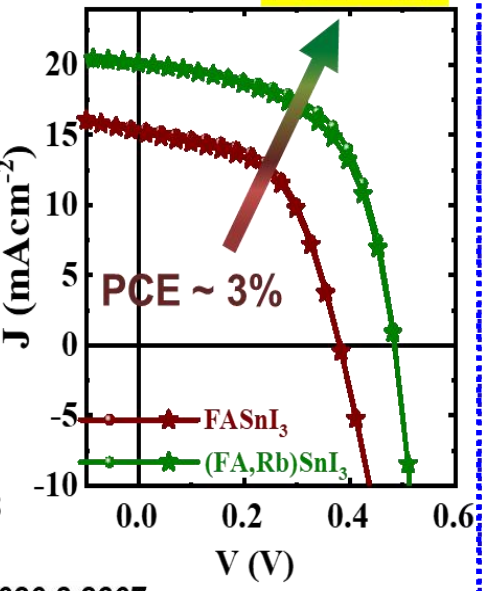
Structural regulation



Defect spectra

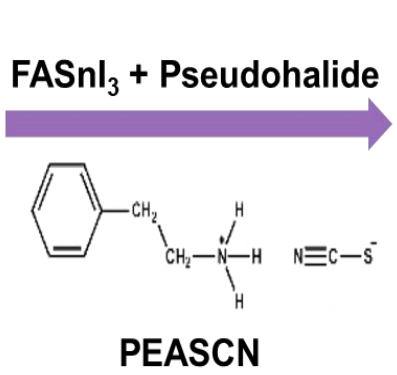


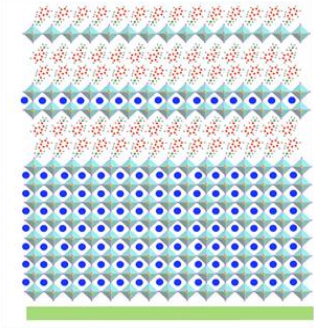
PCE~ 6%



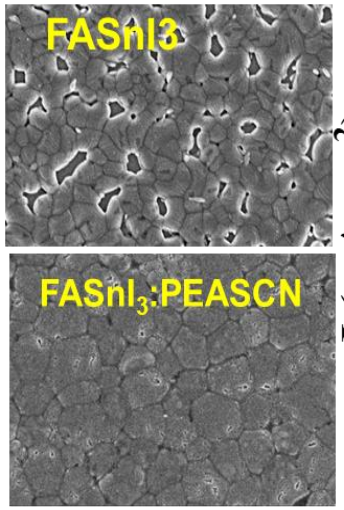
Khadka* et al. Mater. Chem. C,*2020,8,2307*

Pseudohalide additive effect

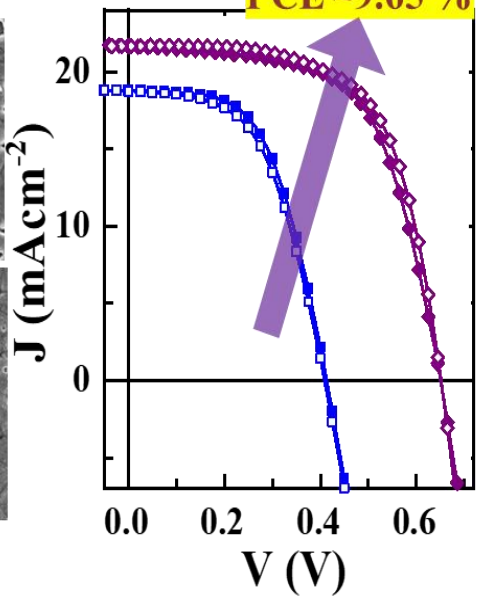




Film growth

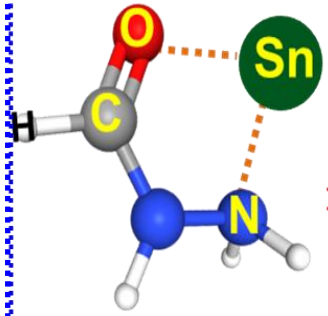


PCE ~9.65 %



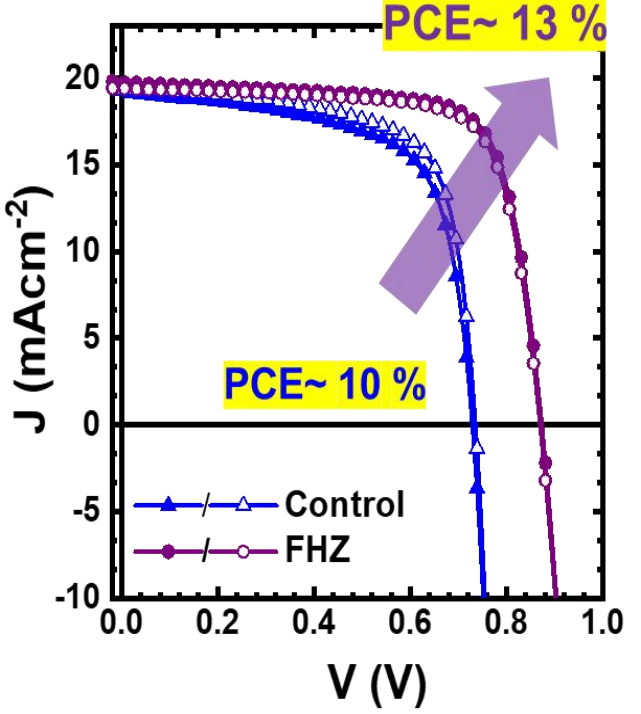
Khadka* et al. *ACS Appl. Energy Mater. 2021, 4, 12819*

Multi-functional ligand-additive



Formohydrazide (FHZ)
>Bidentate ligand

PCE~ 13 %



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

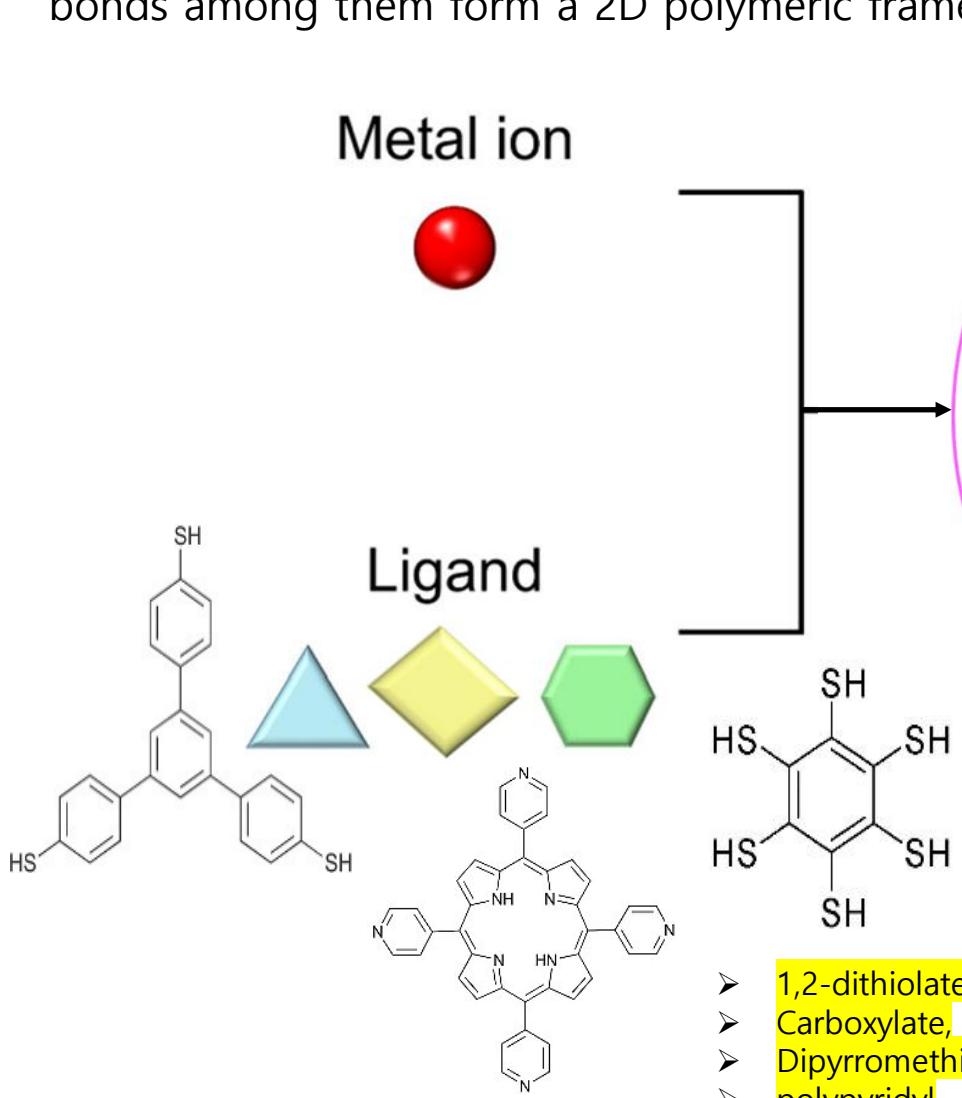
Khadka and co-workers, J. Mater. Chem. A,2025, 13, 23487

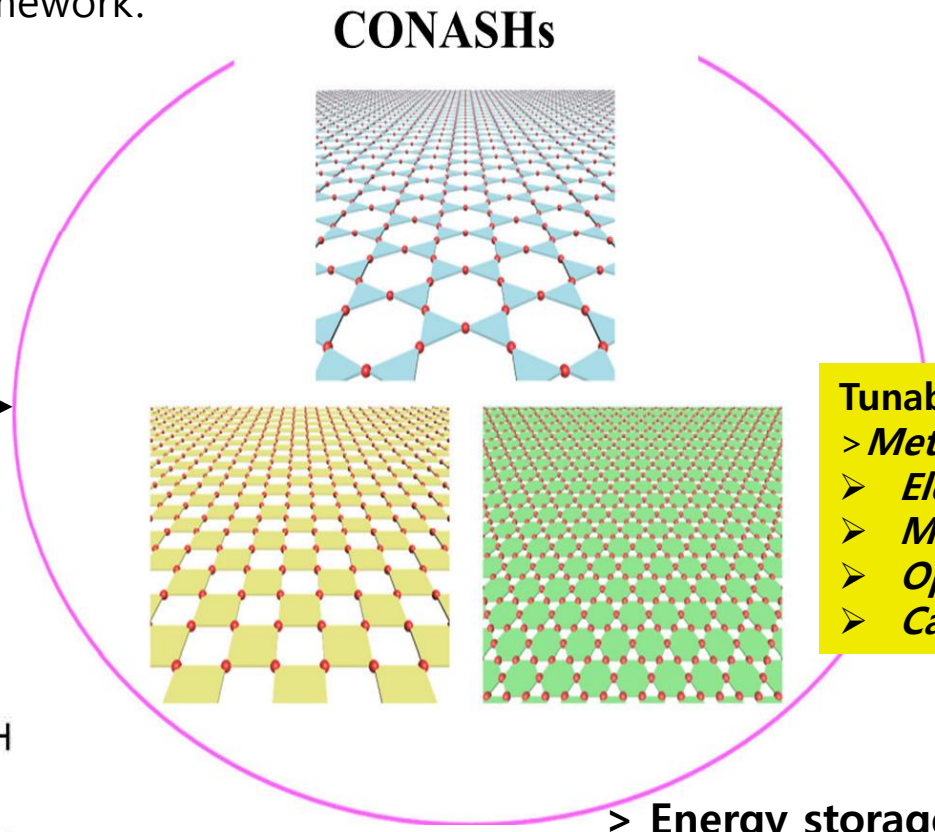
Coordination nanosheets (CONASHs)

Coordination nanosheets (CONASHs)

>Molecule-based nanosheets.

>Organic ligand molecules and metal ions/atoms/clusters, and the coordination bonds among them form a 2D polymeric framework.







Hiroshi Nishihara

Hiroshi Nishihara and coworkers, Chem. Commun.,2017, 53,5781

Tunable chemical and physical properties

>***Metal nodes and organic ligands***

- ***Electronic conductivity***
- ***Magnetic properties***
- ***Optical response***
- ***Catalytic activity***

- 1,2-dithiolate and its derivatives
- Carboxylate,
- Dipyrromethine,
- polypyridyl

> Energy storage and conversion

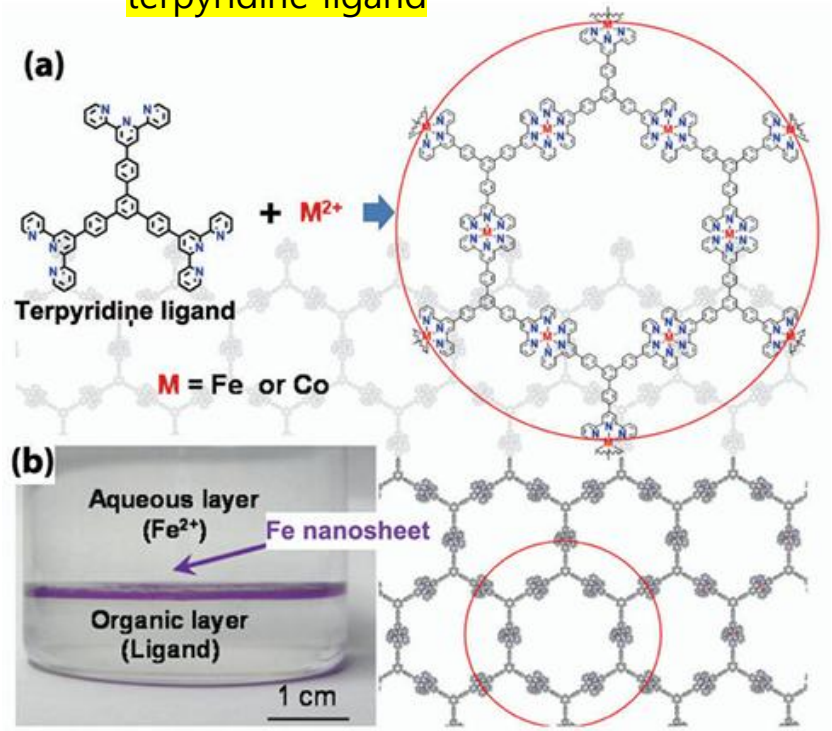
CNSs are used in:

- ***Lithium-/sodium-ion batteries***
- ***Supercapacitors***
- ***Fuel cells***
- ***Solar energy harvesting***

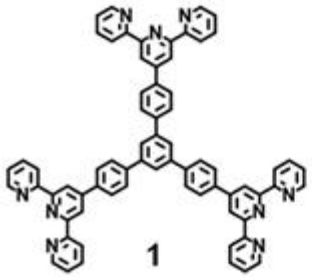
- **2D frameworks facilitate fast ion/electron transport.**

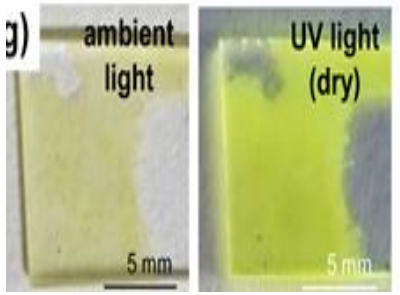
An example of (CONASHs)

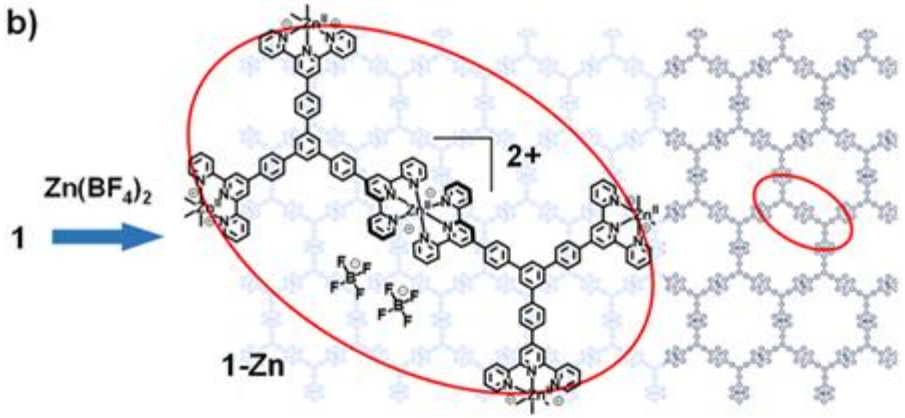
Three armed terpyridine ligand

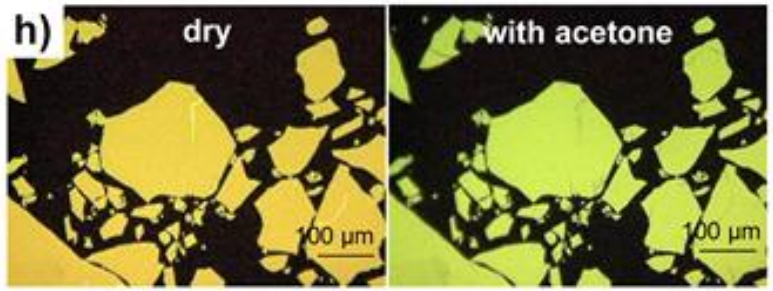












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Article
pubs.acs.org/JACS

Coordination Nanosheets Based on Terpyridine–Zinc(II) Complexes: As Photoactive Host Materials

Takamasa Tsukamoto,[†,‡] Kenji Takada,[†] Ryota Sakamoto,[*,†,§] Ryota Matsuoka,[†] Ryojun Toyoda,[†] Hiroaki Maeda,[†] Toshiki Yagi,[†] Michihiro Nishikawa,[∥] Naoaki Shinjo,[†] Shuntaro Amano,[†] Tadashi Iokawa,[†] Narutaka Ishibashi,[†] Tsugumi Oi,[†] Koshiro Kanayama,[†] Rina Kinugawa,[†] Yoichiro Koda,[†] Toshiyuki Komura,[†] Shuhei Nakajima,[†] Ryota Fukuyama,[†] Nobuyuki Fuse,[†] Makoto Mizui,[†] Masashi Miyasaki,[†] Yutaro Yamashita,[†] Kuni Yamada,[†] Wenxuan Zhang,[†] Ruocheng Han,[†] Wenyu Liu,[†] Taro Tsubomura,[∥] and Hiroshi Nishihara[*,†]

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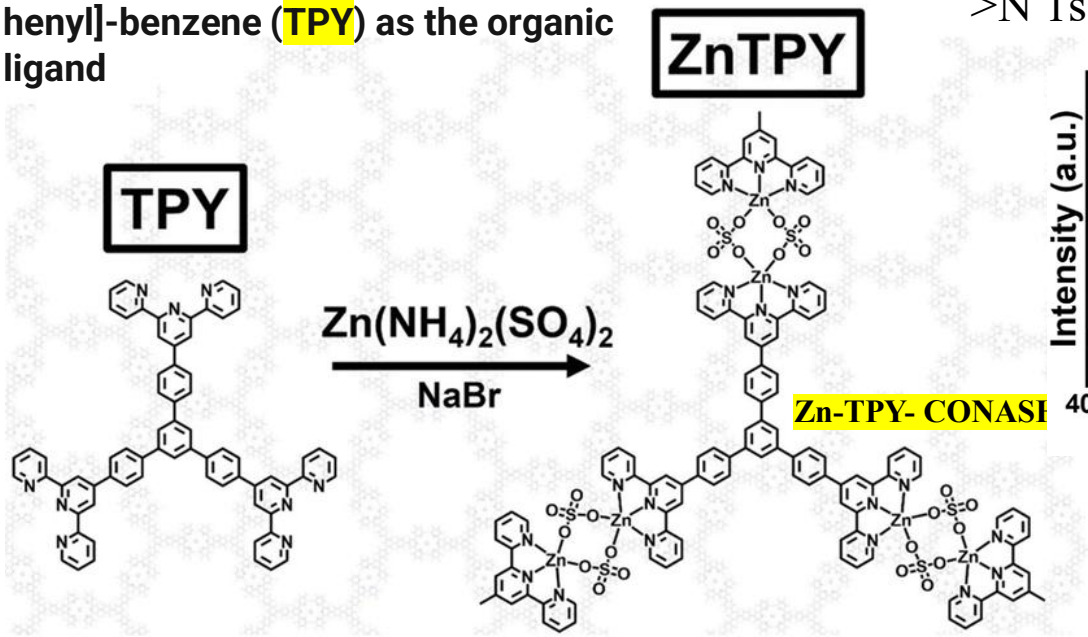
[§]JST-PRESTO, 4-1-8 Honjcho, Kawaguchi, Saitama 332-0012, Japan
[∥]Department of Materials and Life Science, Seikei University, 3-3-1 Kichijoji-kitamachi, Musashino-shi, Tokyo 180-8633, Japan

Supporting Information

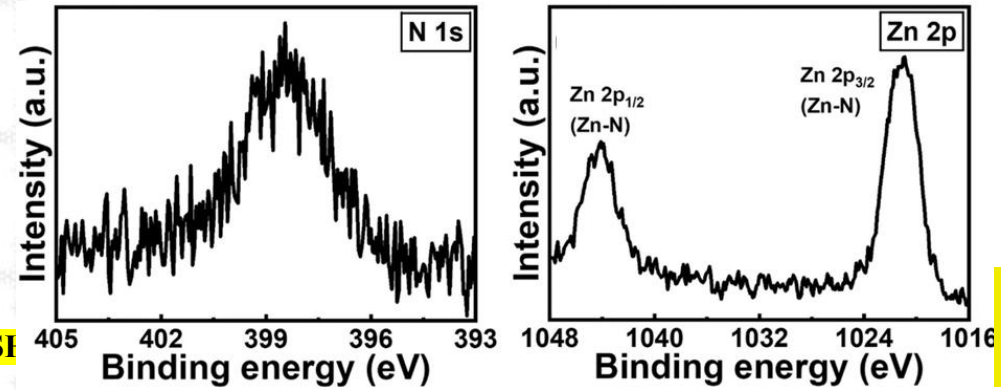
Hiroshi Nishihara and coworkers, J. Am. Chem. Soc. 2017, 139, 15, 5359

Zn-TPY-CONASH-Synthesis

1,3,5-tris[4-(4'-2,2':6',2"-terpyridyl)phenyl]-benzene (TPY) as the organic ligand



XPS spectra of as-synthesized ZnTPY CONASHs
>N 1s and Zn 2p core levels

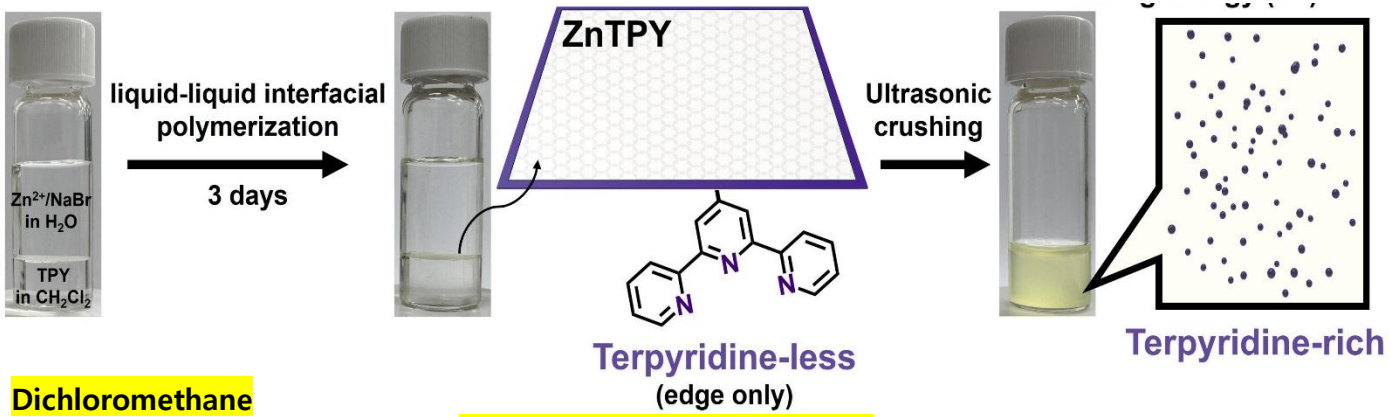




Dr. Ying-Chiao Wang
NIMS Alumni
(National Sun Yat-sen University)

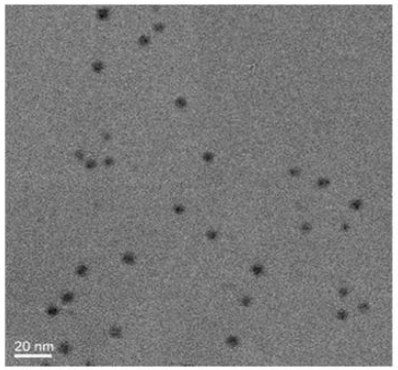
> Successful formation of ZnTPY CONASHs

- Liquid/liquid interfacial synthesis

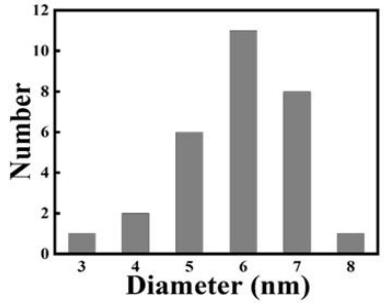


Dichloromethane

Zn-TPY-CONASH/DMF suspension



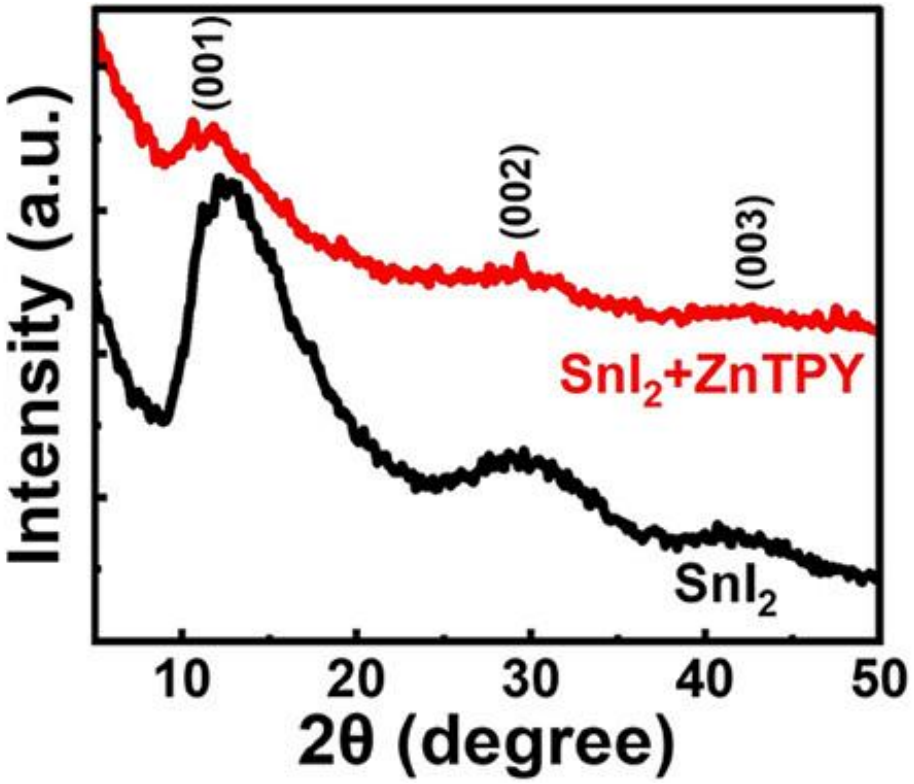
TEM image

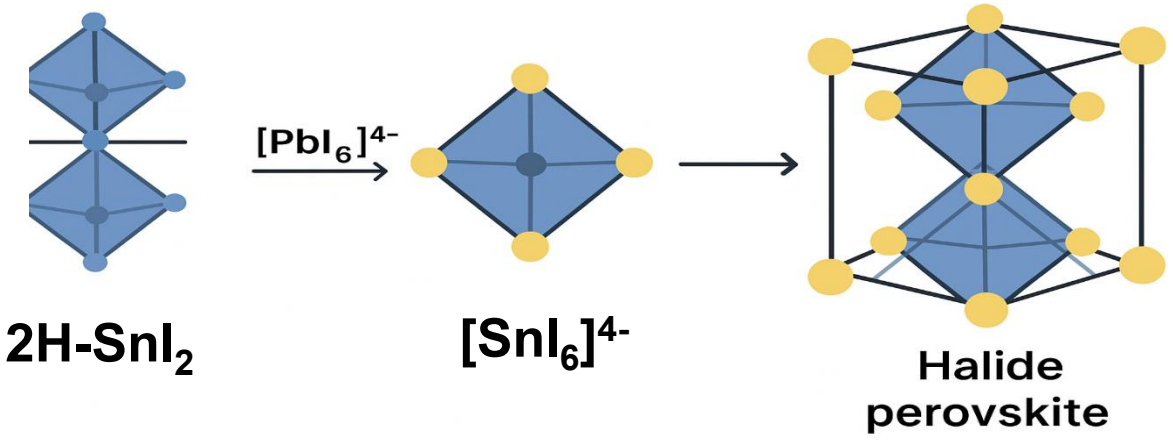


Khadka et al. ACS Appl. Mater. Interfaces 2025, 17, 18, 26813

Growth of CONASH/Halide Perovskite

XRD- SnI_2 and Zn-TPY

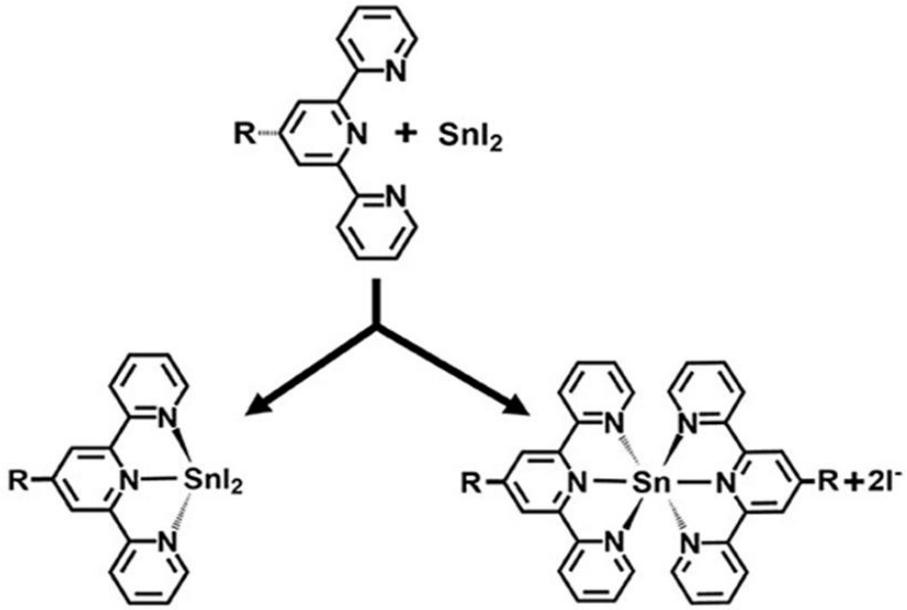




2D-sheet by edge sharing

$[(SnI_{6-x})_4^{-}$–ZnTPY

Two possible routes of the formation of Zn-TPY: SnI_2 adducts



Diffraction peak-(001) – hexagonal 2H polytype SnI_2 Suppressed

>Facile insertion of ZnTPY into SnI_2 aggregates through multidentate chelation.

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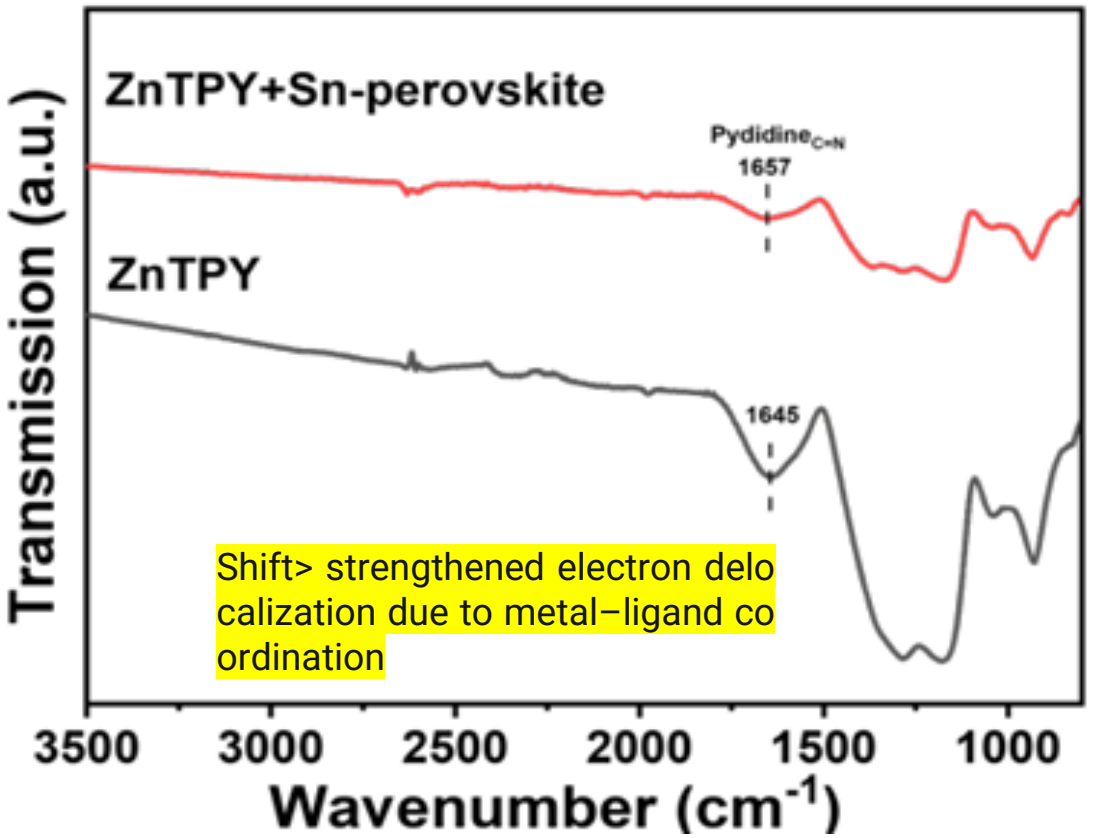
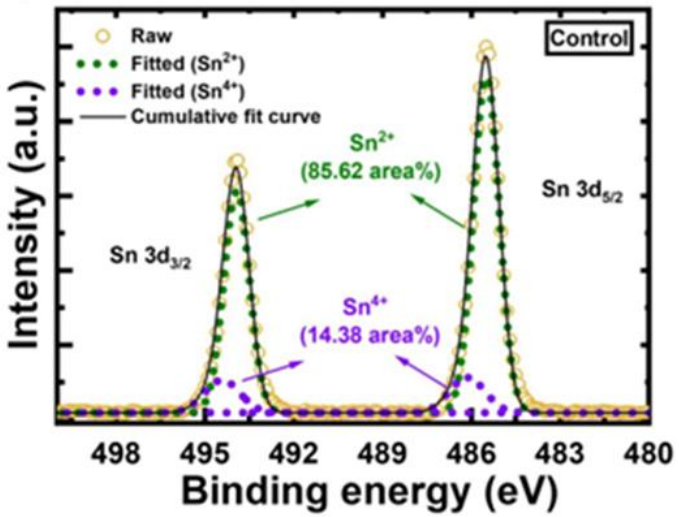
Interaction of CONASH and Sn- Perovskite

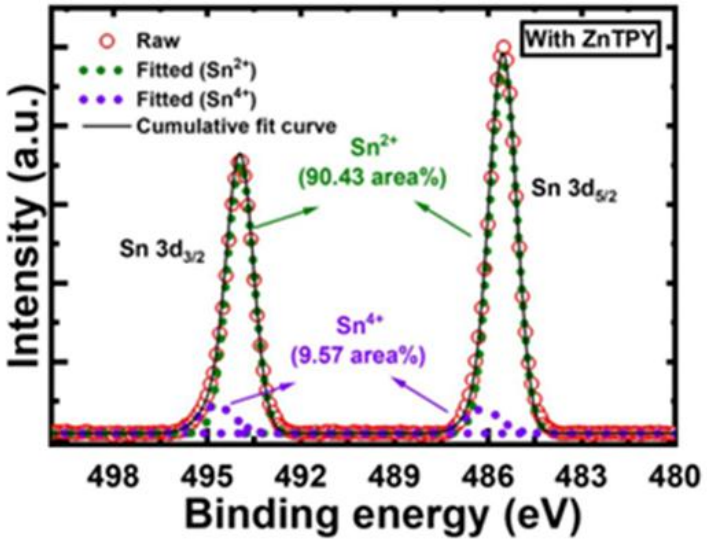
FTIR spectra of ZnTPY and the ZnTPY-Sn perovskite



Shift> strengthened electron delo calization due to metal–ligand co ordination

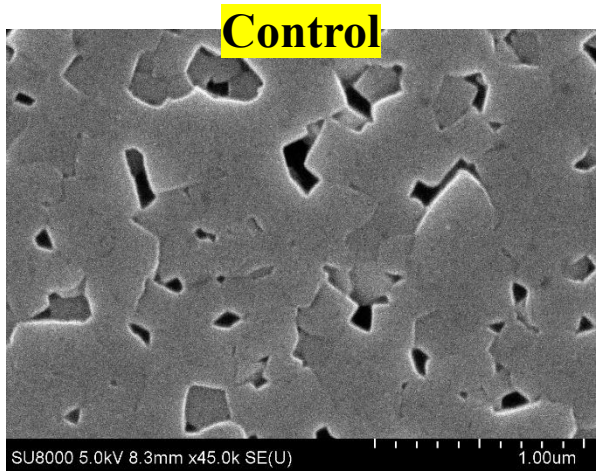
Chemical interaction –XPS Sn-perovskite and Zn-TPY

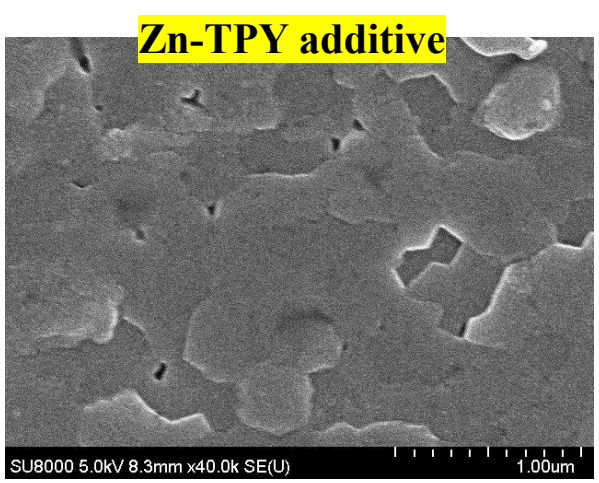




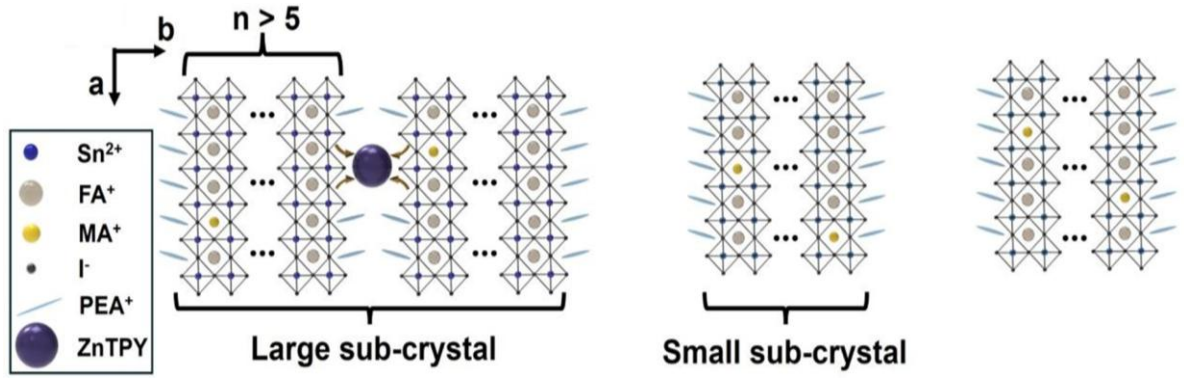
Sn4+ suppressed with Zn-TPY additive

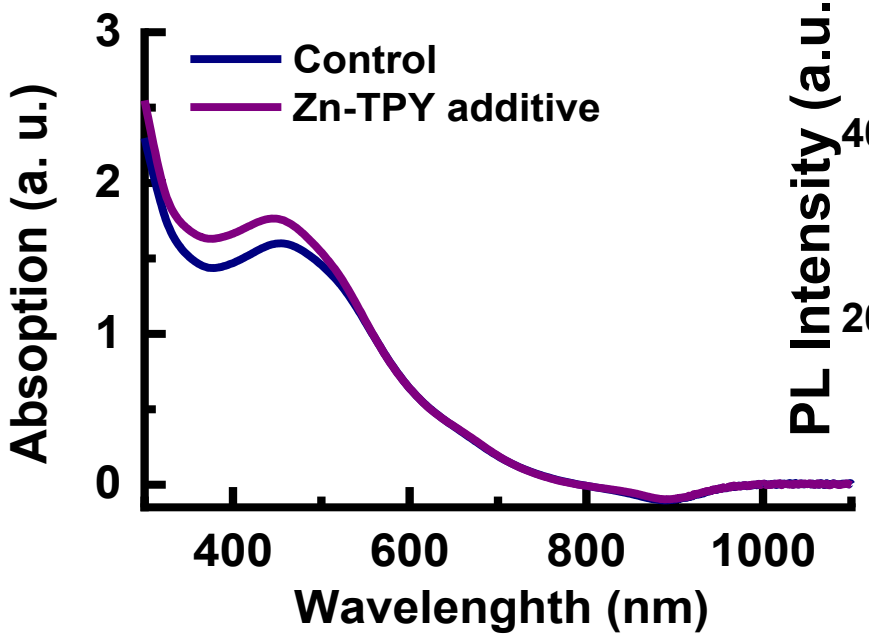
Effect of CONASH- Sn-perovskite film

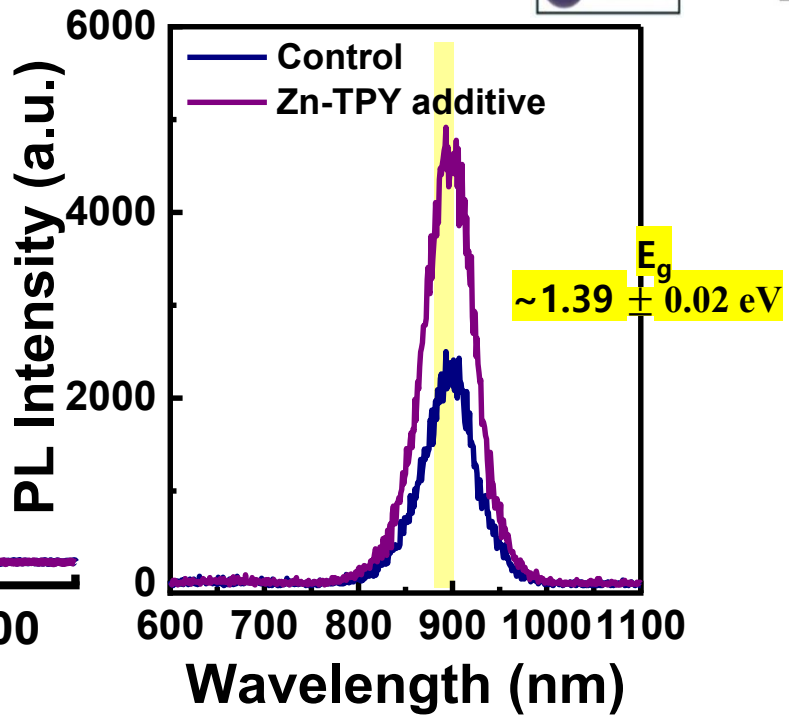


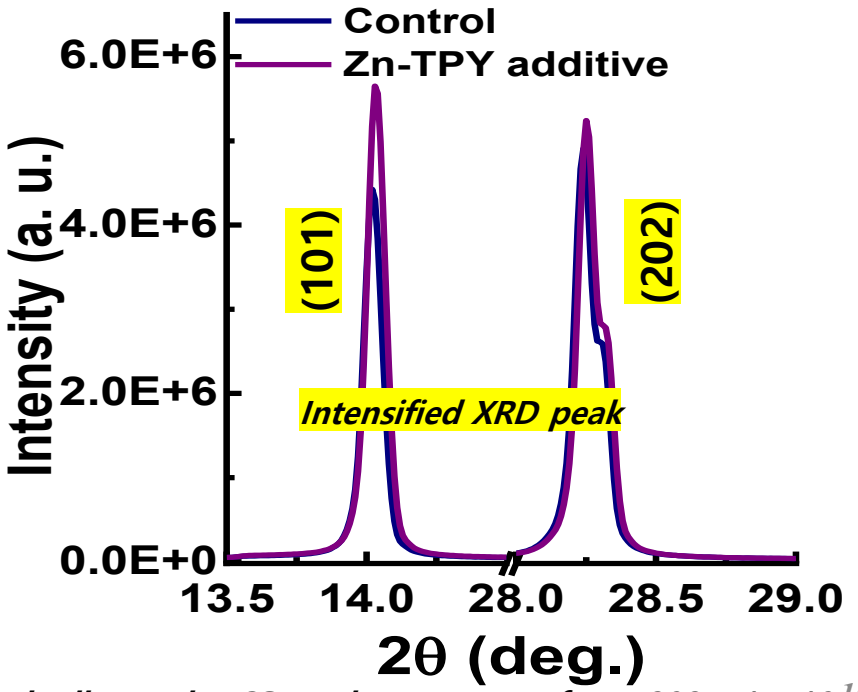


- Stronger intensity for (10$\bar{1}$)' plane-(20$\bar{2}$)' facet> reduction in the periodicity of along the b-axis.
- Introduction of ZnTPY> strong chelation between ZnTPY and Sn-perovskites, effectively preventing PEA^+ from rapidly cleaving crystals.









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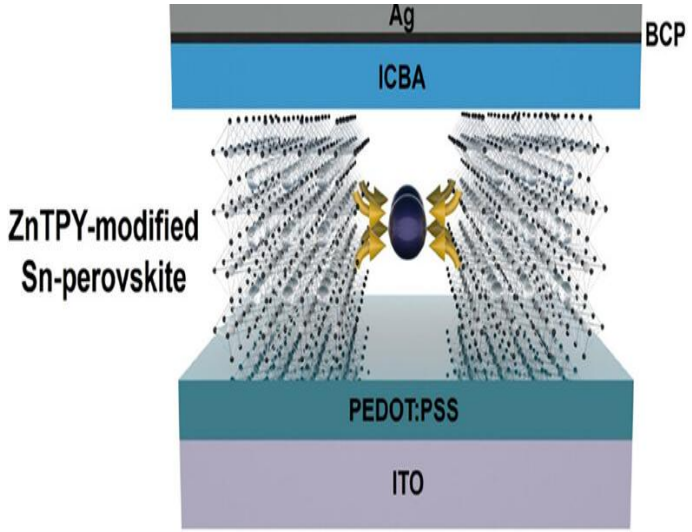
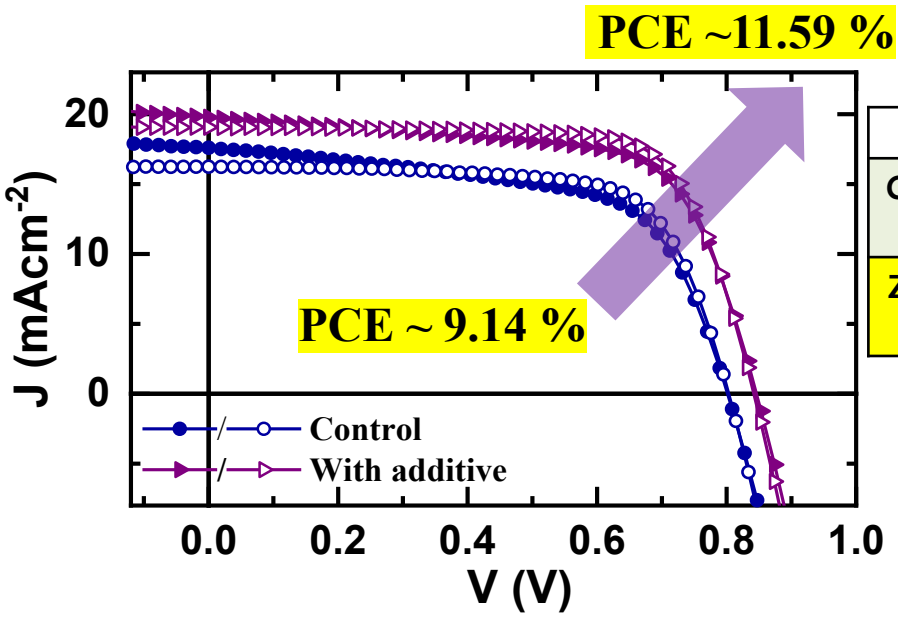
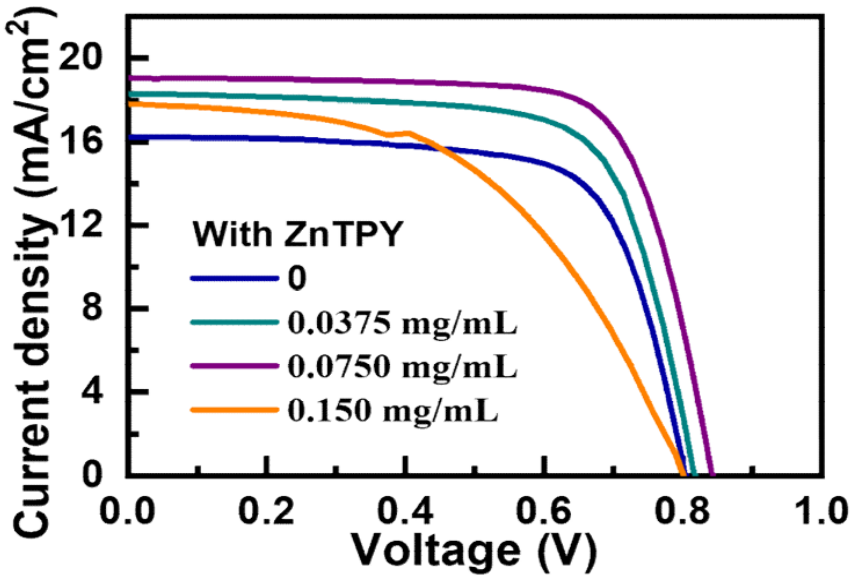
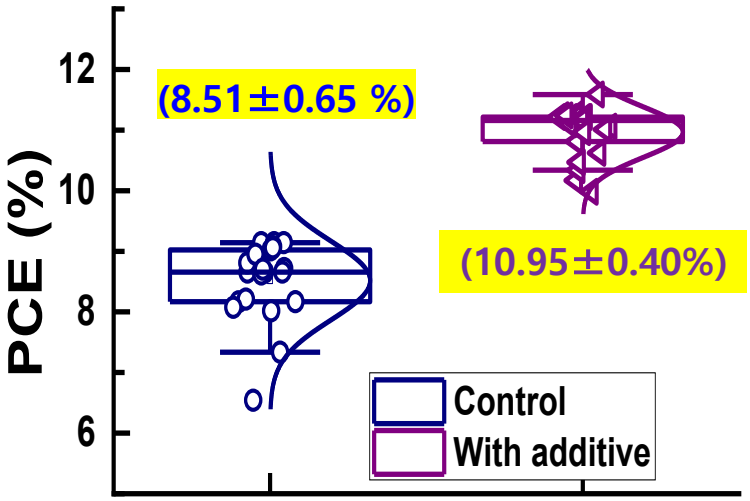
Effect of CONASH- Perovskite Device



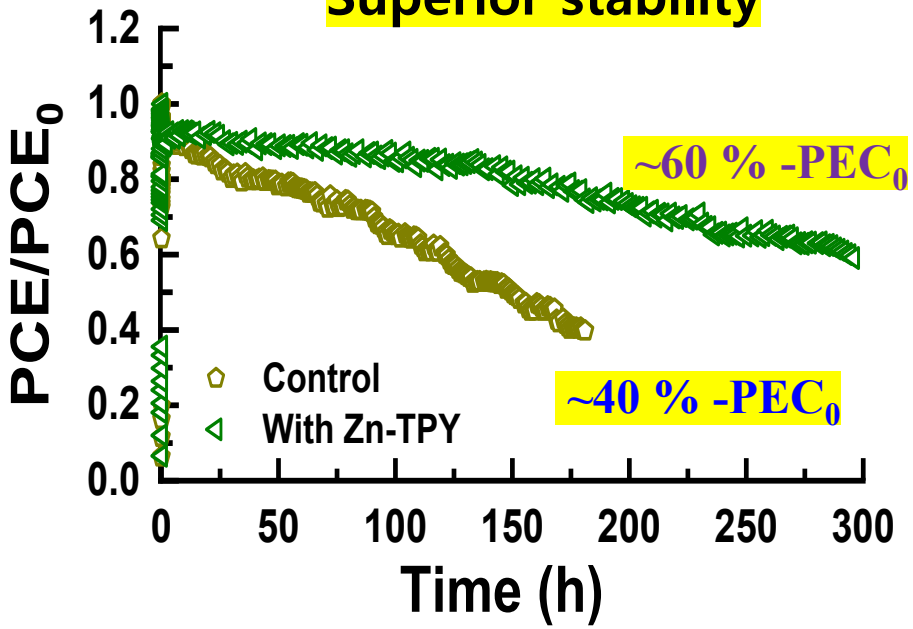


Devices	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF (%)	PCE (%)
Control FS/ RS)	16.25/ 17.68	0.807/ 0.801	69.70/ 61.12	9.14/ 8.66
ZnTPY (FS/ RS)	19.06/ 19.83	0.842/ 0.848	72.19/ 66.70	11.59/ 11.2

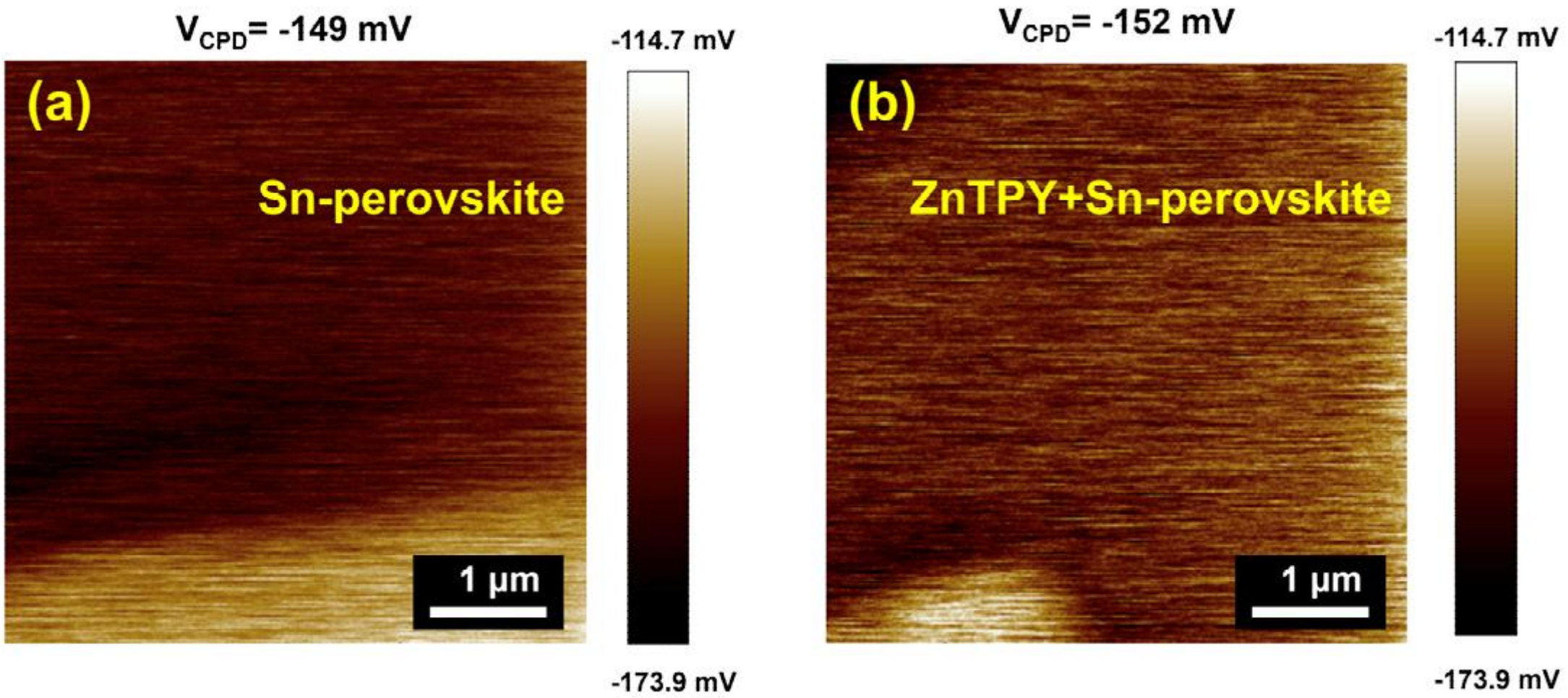




Superior stability

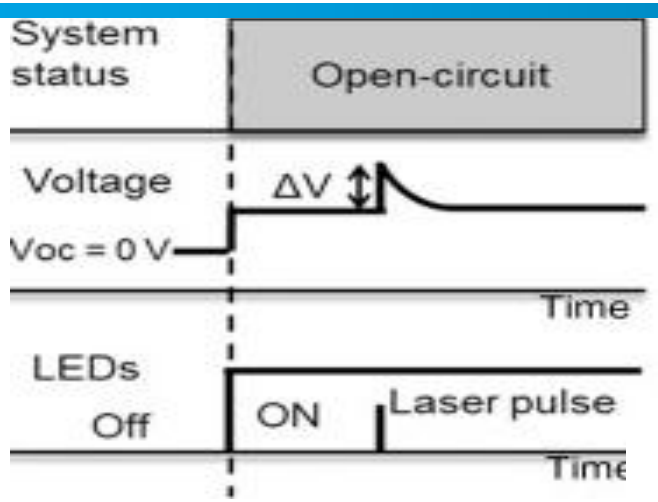


Surface Energy Modulation



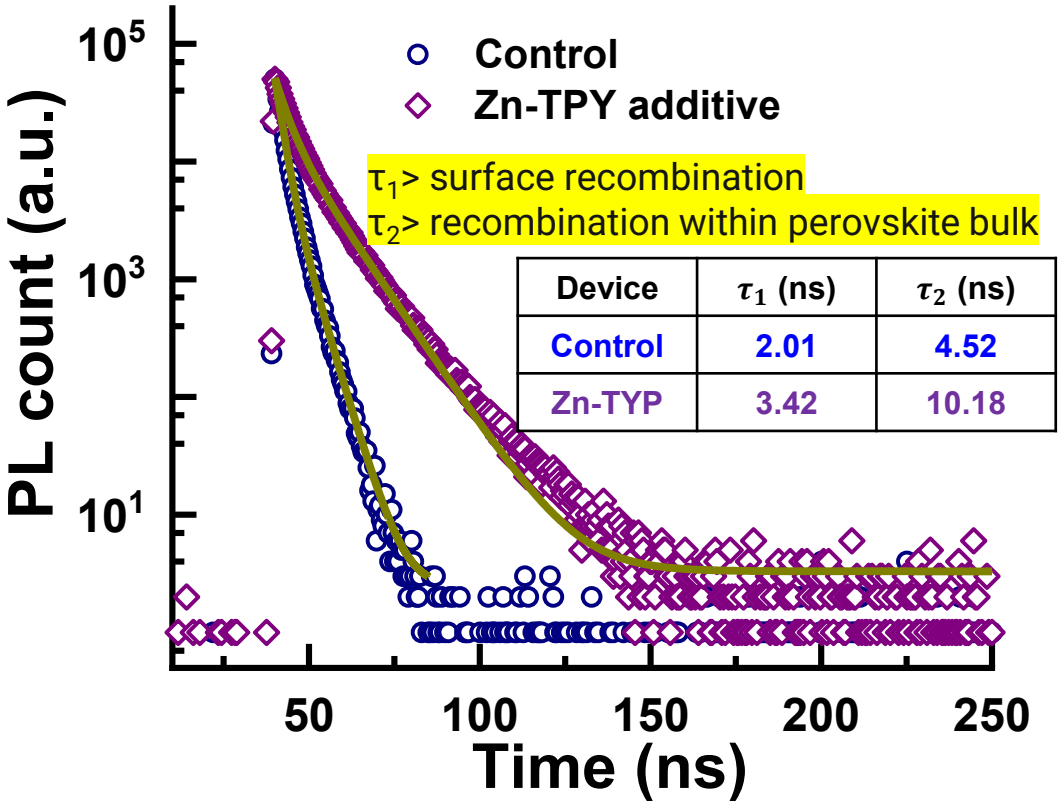
>KPFM images of Sn-perovskite films
> A slight change in contact potential difference (CPD) - indicate surface energy modulation with the incorporation of Zn-TPY

Transient characteristics: Defect passivation



Transient Photovoltage Analysis

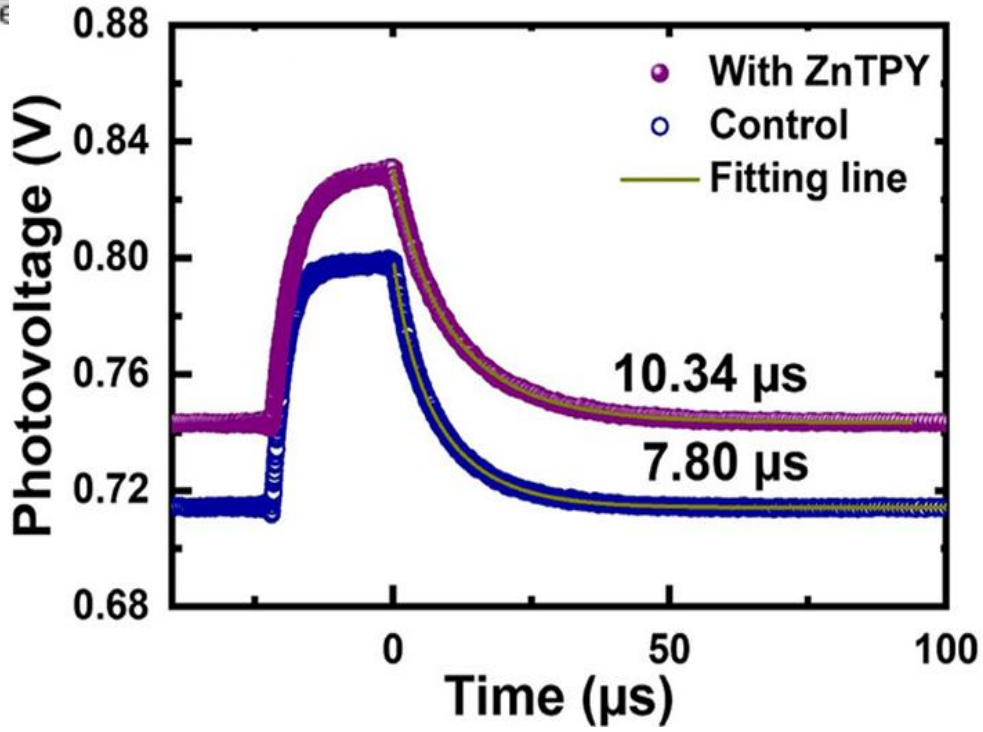
TRPL data



τ_1> surface recombination
τ_2> recombination within perovskite bulk

Device	τ_1 (ns)	τ_2 (ns)
Control	2.01	4.52
Zn-TYP	3.42	10.18

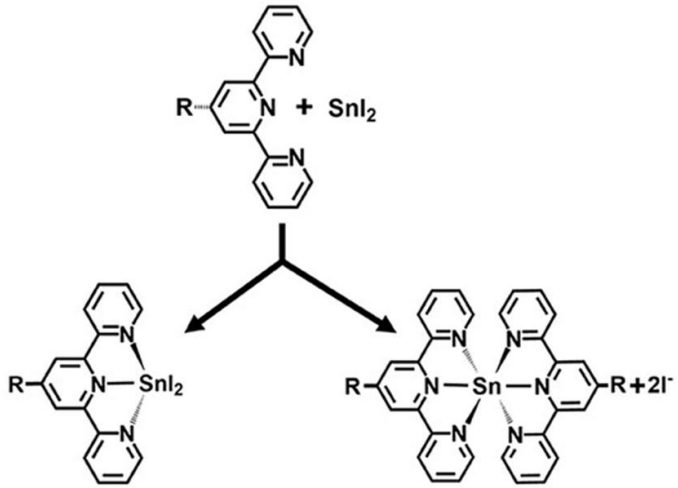
$$V(t) = V_0 e^{-t/\tau}$$



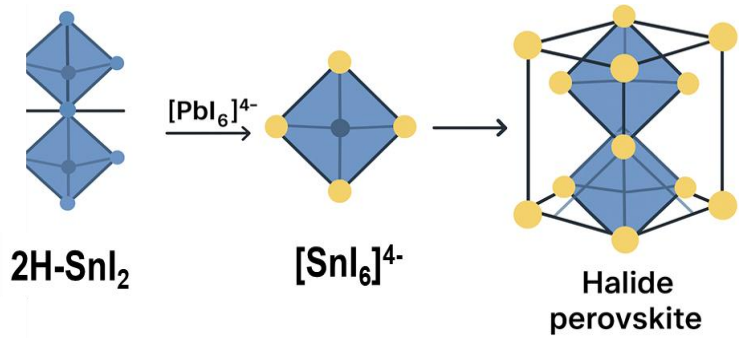
Longer lifetime: Defect mitigation

Report Summary

Effects of CONASH in Sn- Perovskite Solar Cells

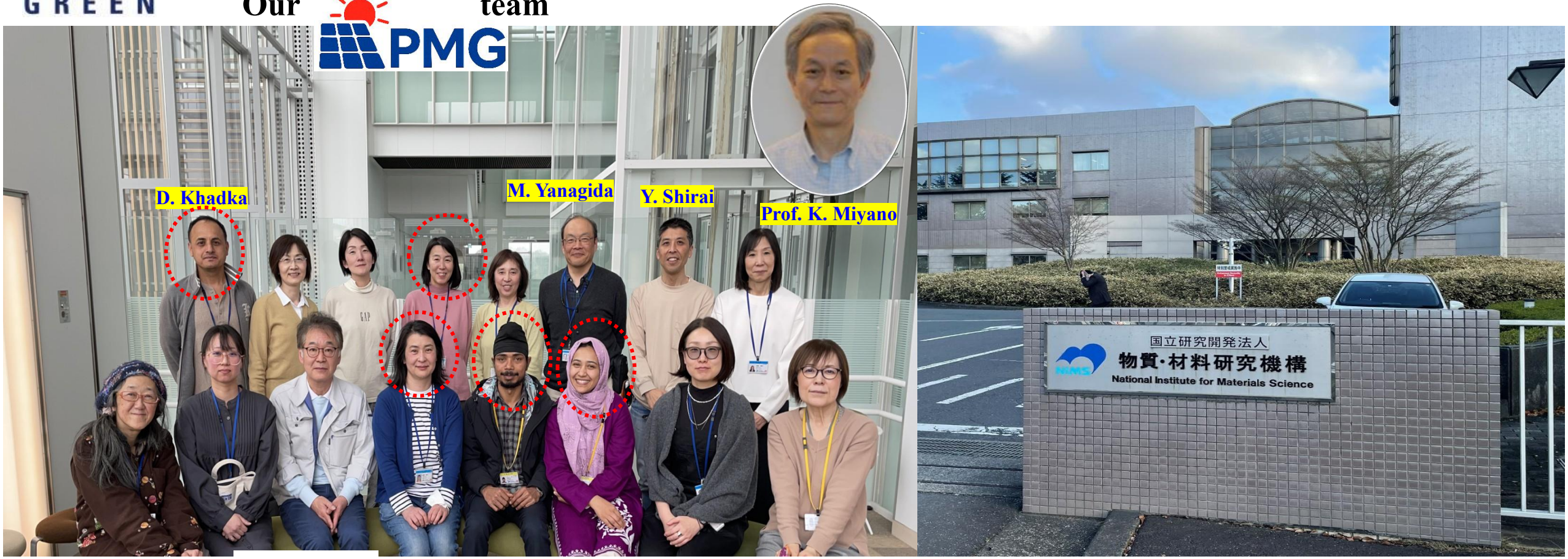


- **Precursor modulation:** Uncoordinated terpyridine moieties that strongly chelate SnI_2, forming a well-dispersed ZnTPY:SnI_2 complex
- **ZnTPY:SnI_2 complexes:** Heterogeneous nucleation ($[SnI_{6-x}]^{4-}$ octahedral) facilitates efficient precursor-to-Sn-perovskite film growth
- ***Defect passivation:*** ***Attenuate defect densities and enhance carrier dynamics***
- ***Device PCE increased-*** ***from 9.1> 11.6% - with improved stability***



Acknowledgement

Our team



Thank you for your attention