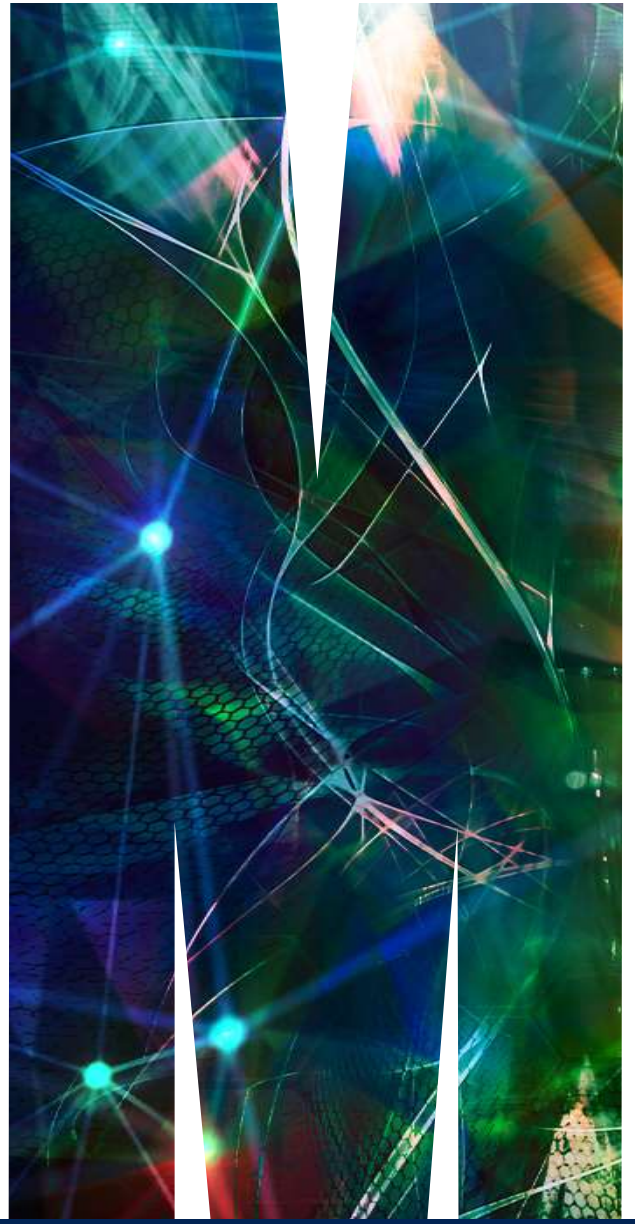
Formamidinium – Caesium Perovskite Solar Cells from Lead Acetate-Based Precursors



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Monash University

06/12/2023

Introduction – Lead Halide Perovskite Solar Cells

Compounds with the general formula: ABX_3

Large cation A:

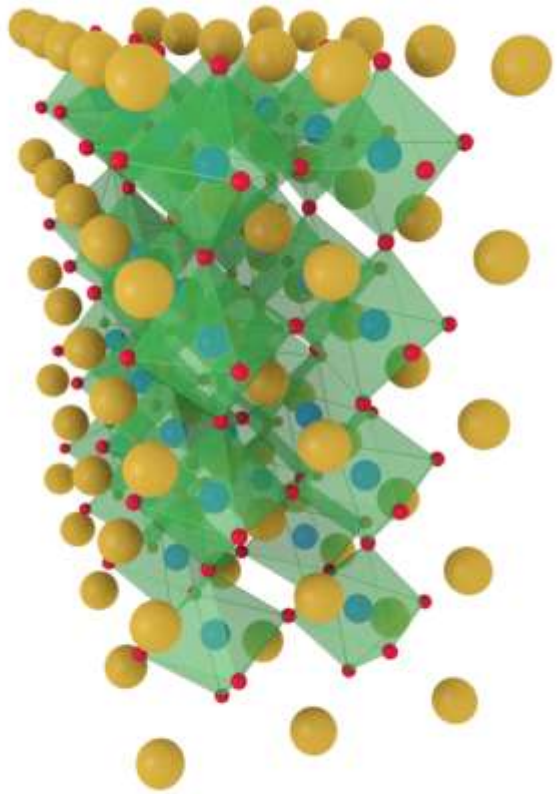
cesium, methylammonium, formamidinium

Metal cation B:

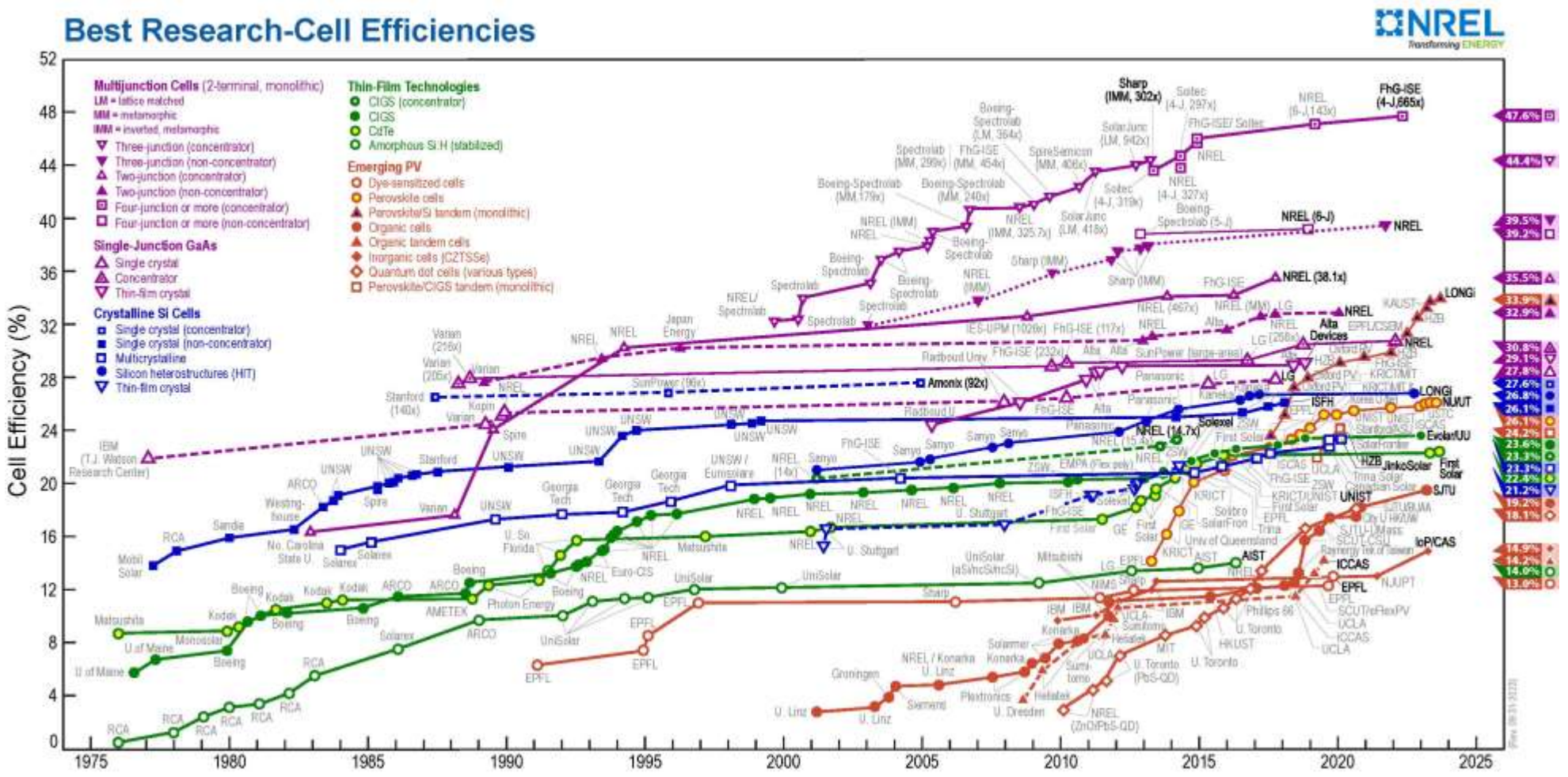
lead, tin

Halide ion X:

iodide, bromide, chloride



Introduction – Lead Halide Perovskite Solar Cells



Silicon/Perovskite Tandem 33.9%

Single Cryst Silicon 26.1%

Perovskite 26.1%

Commercialization?

- Scalability
- Stability

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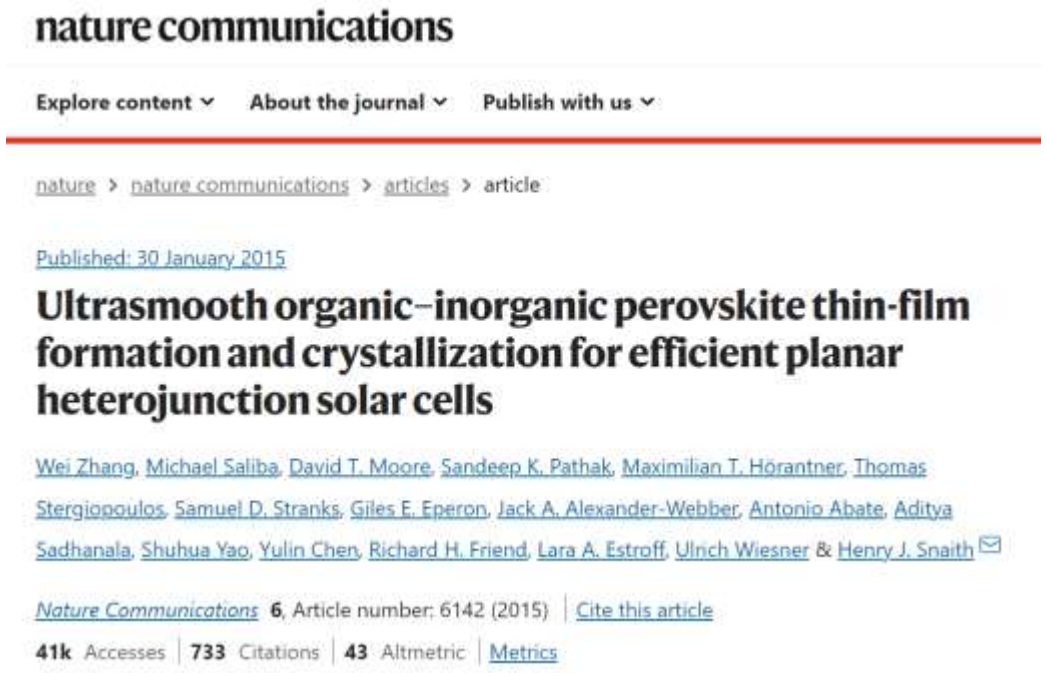
Lead Halide Perovskites: Lead Acetate-Based Precursor

Synthesis route of $MAPbI_3$:

- **For conventional lead Iodide (PbI_2) based precursor : $MAI + PbI_2 \rightarrow MAPbI_3$**
- **For lead acetate ($PbAc_2$) based precursor: $3MAI + PbAc_2 \rightarrow MAPbI_3 + 2MAAc$**



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Published: 30 January 2015

Ultrasmooth organic–inorganic perovskite thin-film formation and crystallization for efficient planar heterojunction solar cells

Wei Zhang, Michael Saliba, David T. Moore, Sandeep K. Pathak, Maximilian T. Hörantner, Thomas Stergiopoulos, Samuel D. Stranks, Giles E. Eperon, Jack A. Alexander-Webber, Antonio Abate, Aditya Sadhanala, Shuhua Yao, Yulin Chen, Richard H. Friend, Lara A. Estroff, Ulrich Wiesner & Henry J. Snaith

Nature Communications **6**, Article number: 6142 (2015) | Cite this article

41k Accesses | **733** Citations | **43** Altmetric | Metrics

Nat Comm. ***2015,*** 6, 6142

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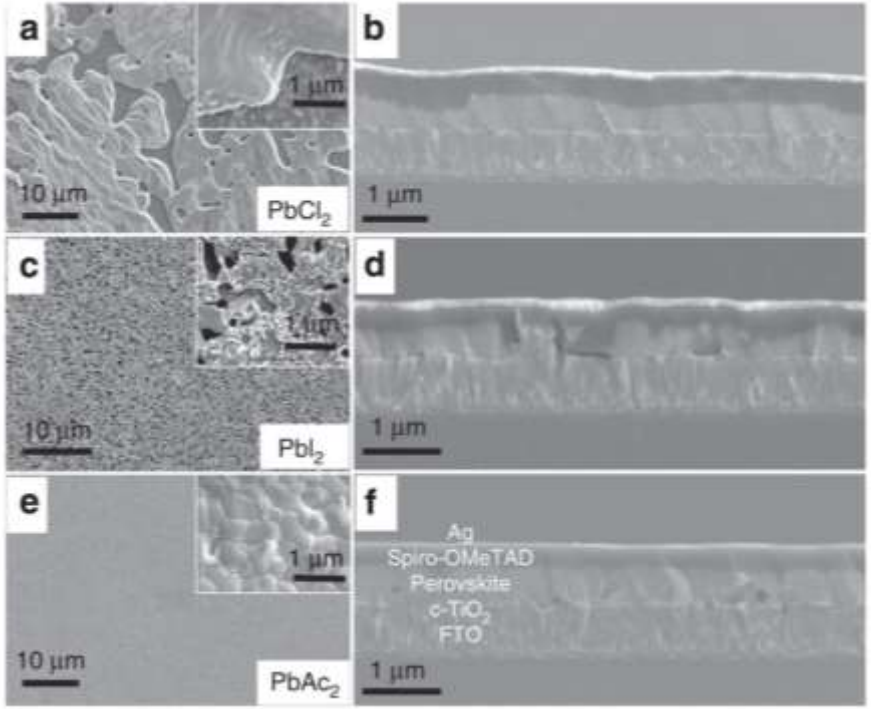
Lead Halide Perovskites: Lead Acetate-Based Precursor

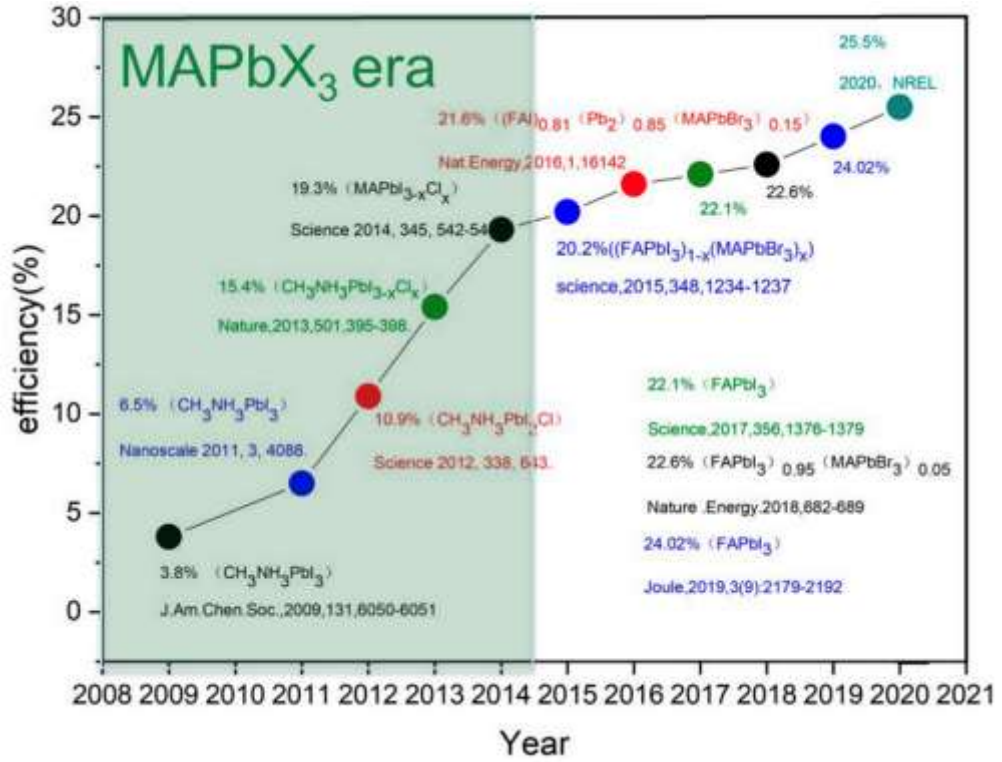
Benefits of the lead acetate route

- Ultrasmooth, pinhole free films
- Very short annealing times
- Better photovoltaic performance
- No need for strongly complexing solvents (DMSO)
- No need for anti-solvent or gas-assisted film formation



Lead acetate only used in MAPI Perovskite

	Lead Source		A-cation Source		Halide Source		Lead Halide Perovskite		Volatile Component
(1)	$PbAc_2$	+	MAX	+	2 MAX	→	$MAPbX_3$	+	2 MAAc ↑



Zhao et al., *Energy & Environmental Science,* ***2023,*** *16, 138-147*

Image source: Tianzhao Dai et al, Crystal 2021, 11, 295

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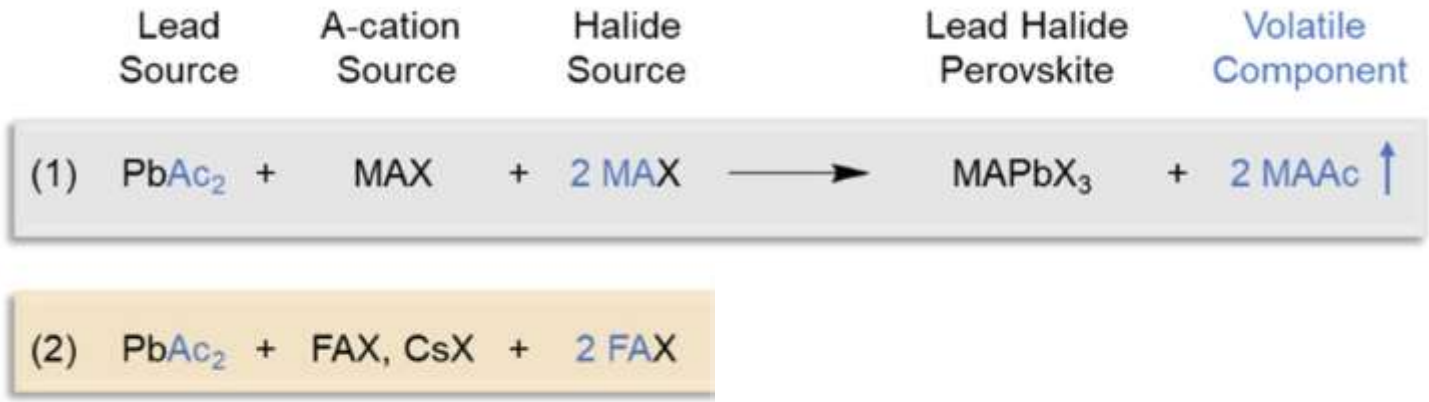
Can we make methylammonium-free perovskite (FACs) from $PbAc_2$?

Synthesis of FACs perovskite from $PbAc_2$



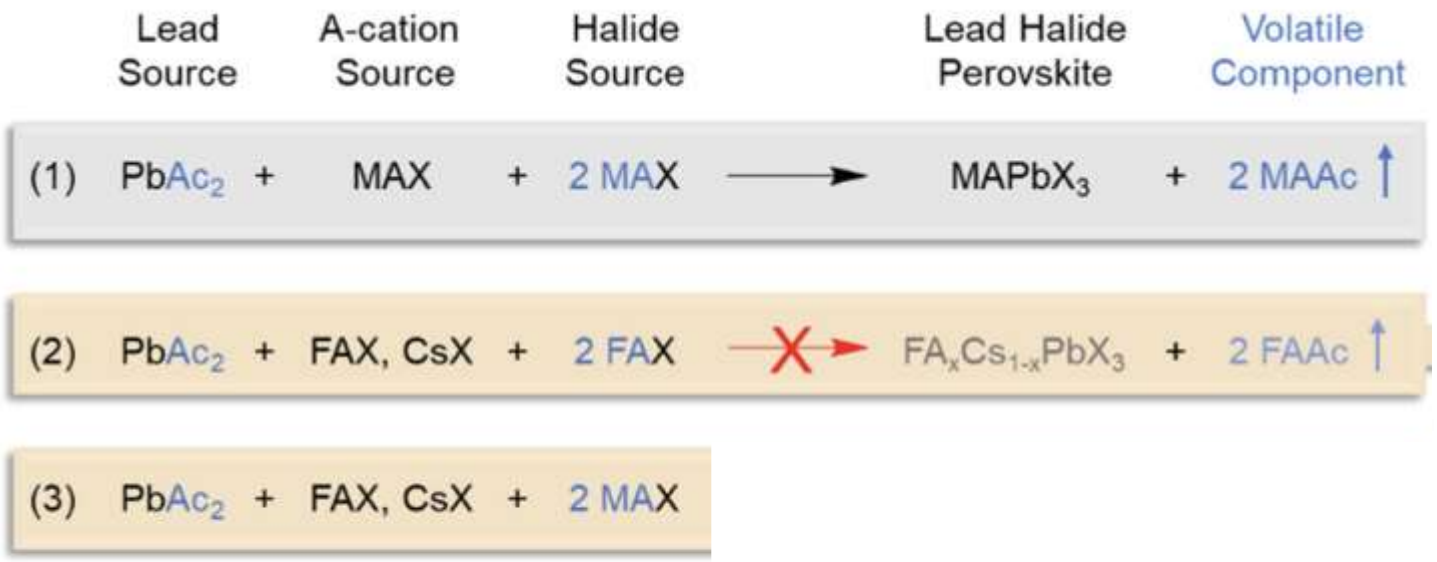
Synthesis of FACs perovskite from $PbAc_2$

	Lead Source		A-cation Source		Halide Source		Lead Halide Perovskite		Volatile Component
(1)	$PbAc_2$	+	MAX	+	2 MAX	→	$MAPbX_3$	+	2 MAAc ↑
(2)	$PbAc_2$	+	FAX, CsX	+	2 FAX	✗→	$FA_xCs_{1-x}PbX_3$	+	2 FAAc ↑

(2b) Side Reaction in Reaction (2):

$$3\,FA^+ + 3\,AcO^- \longrightarrow \text{sym-triazine} + 3\,NH_3\uparrow + 3\,AcOH\uparrow$$

Synthesis of FACs perovskite from $PbAc_2$



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Synthesis of FACs perovskite from $PbAc_2$

	Lead Source		A-cation Source		Halide Source		Lead Halide Perovskite		Volatile Component
(1)	$PbAc_2$	+	MAX	+	2 MAX	→	$MAPbX_3$	+	2 MAAc ↑
(2)	$PbAc_2$	+	FAX, CsX	+	2 FAX	✗→	$FA_xCs_{1-x}PbX_3$	+	2 FAAc ↑
(3)	$PbAc_2$	+	FAX, CsX	+	2 MAX	✗→	$FA_xCs_{1-x}PbX_3$	+	2 MAAc ↑

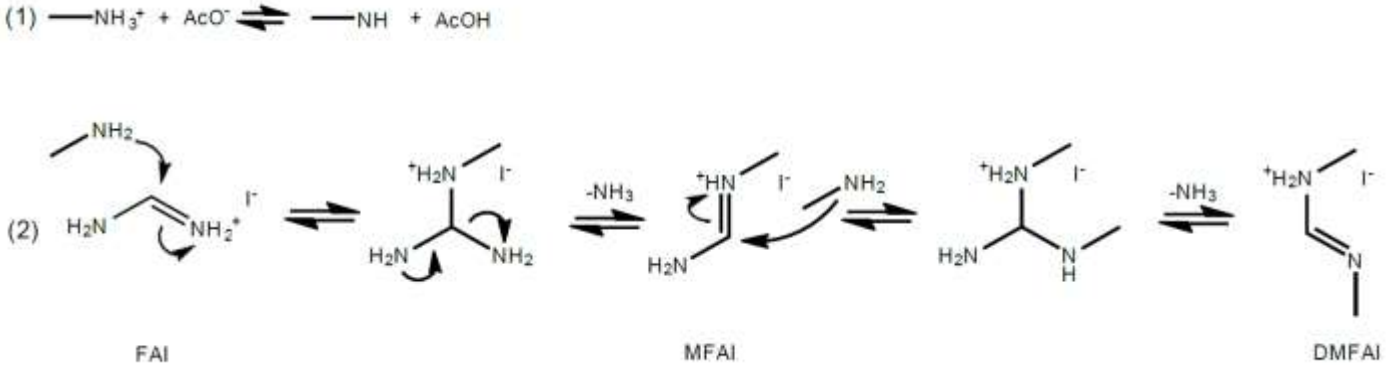
(3b) Side Reaction in Reaction (3):

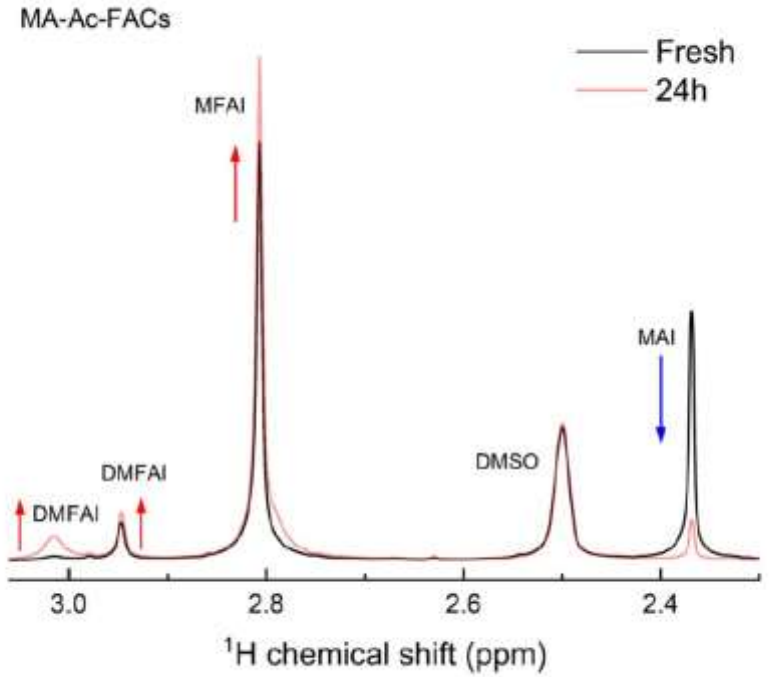
$$FA^+ + MA^+ + AcO^- \rightarrow \text{(N-methylformamidinium)}^+ + NH_3\uparrow + AcOH\uparrow$$

N-methylformamidinium

Synthesis of FACs perovskite from $PbAc_2$

Dr. Sebastian Furer





Zhao et al., *Energy & Environmental Science*, ***2023,*** *16, 138-147*

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Synthesis of FACs perovskite from $PbAc_2$

	Lead Source		A-cation Source		Halide Source		Lead Halide Perovskite		Volatile Component
(1)	$PbAc_2$	+	MAX	+	2 MAX	→	$MAPbX_3$	+	2 MAAc ↑
(2)	$PbAc_2$	+	FAX, CsX	+	2 FAX	✗→	$FA_xCs_{1-x}PbX_3$	+	2 FAAc ↑
(3)	$PbAc_2$	+	FAX, CsX	+	2 MAX	✗→	$FA_xCs_{1-x}PbX_3$	+	2 MAAc ↑
(4)	$PbAc_2$	+	FAX, CsX	+	2 NH_4X	→	$FA_xCs_{1-x}PbX_3$	+	2 NH_4Ac ↑

Zhao et al., *Energy & Environmental Science*, ***2023,*** *16, 138-147*

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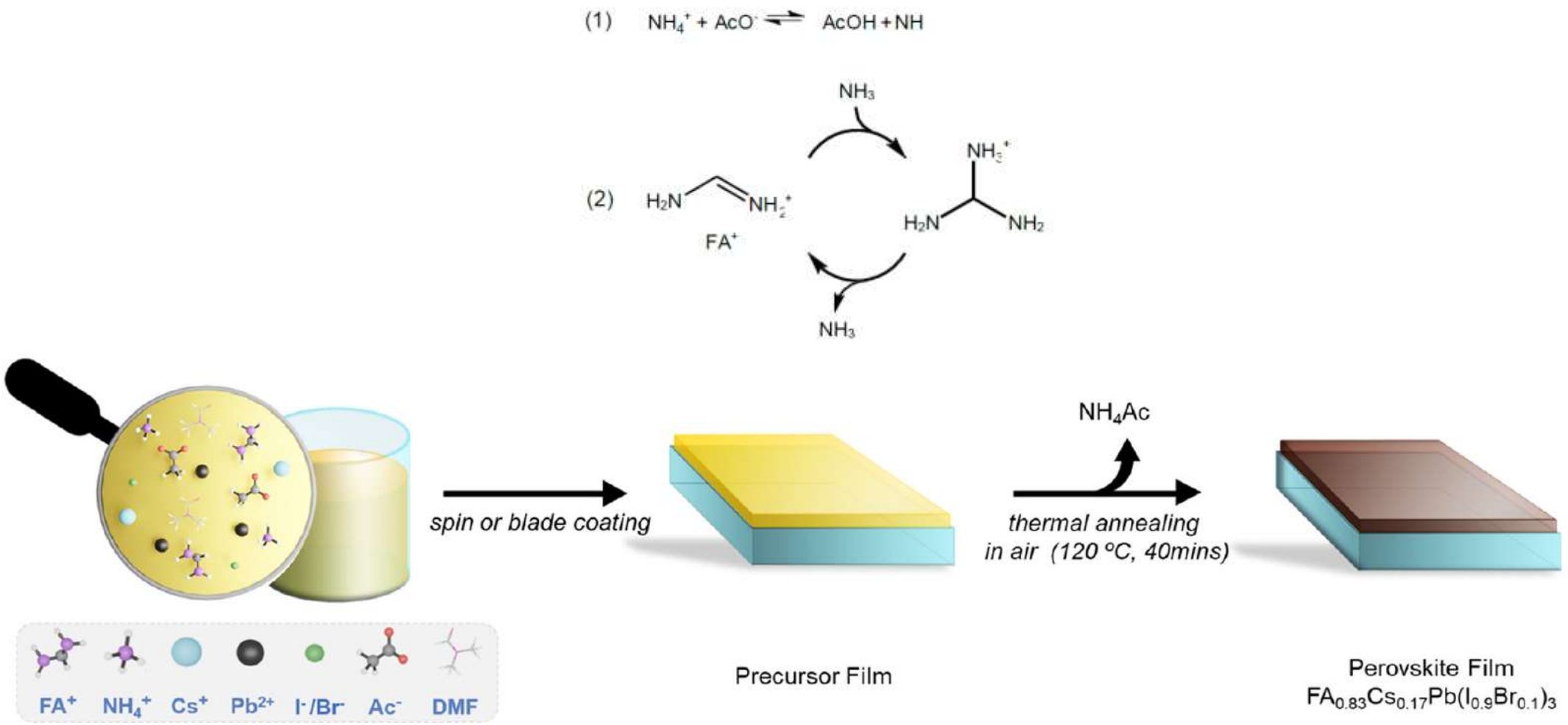
Synthesis of FACs perovskite from $PbAc_2$



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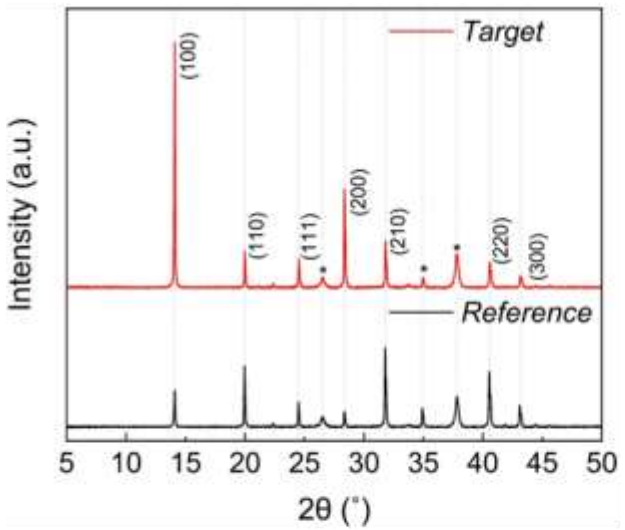
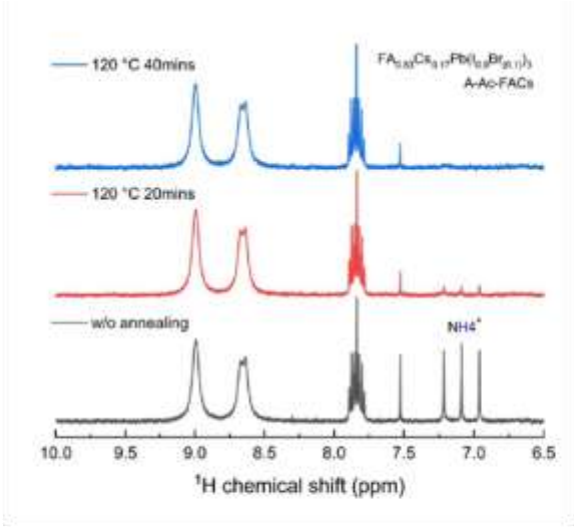
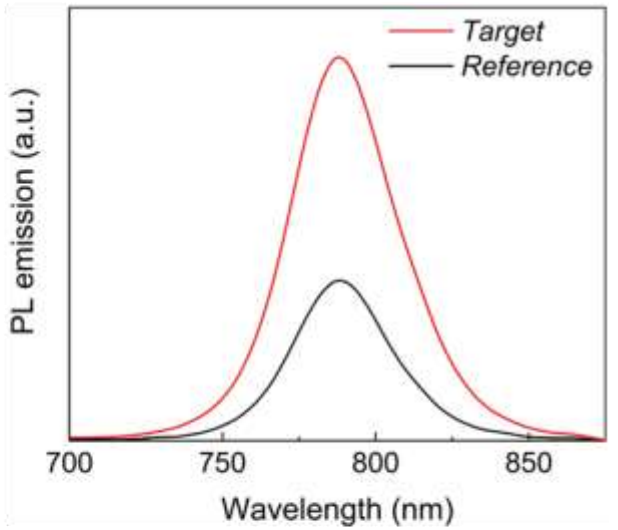
Characterizations of $FA_{0.83}Cs_{0.17}Pb(I_{0.9}Br_{0.1})_3$ made via $PbAc_2$ route

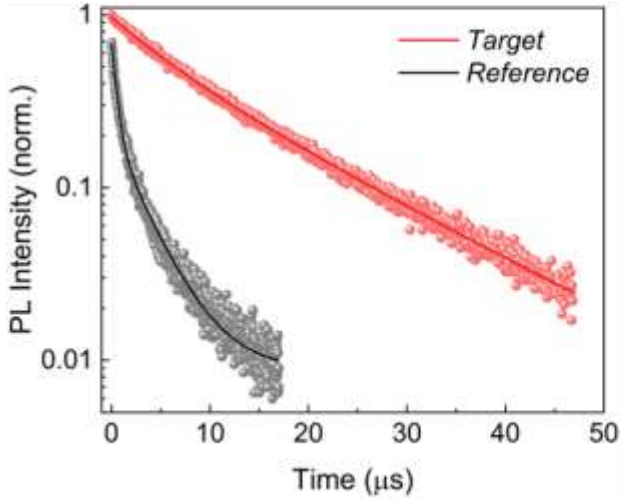
Reference:
Conventional PbI_2 route

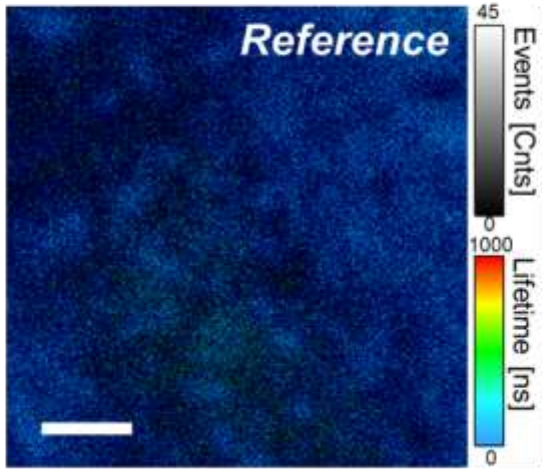
Target:
$PbAc_2$ route

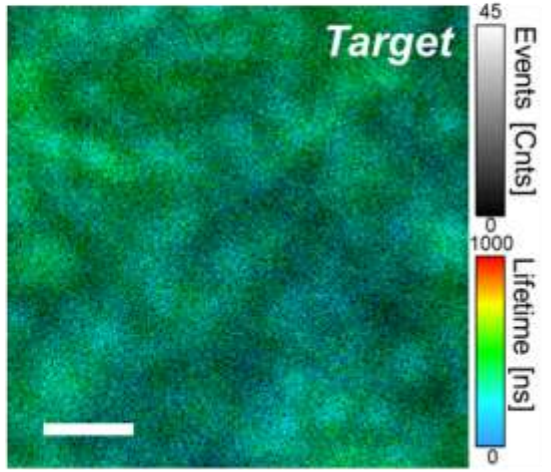












Scale Bar: 2 μm

Zhao et al., *Energy & Environmental Science*, ***2023,*** *16, 138-147*

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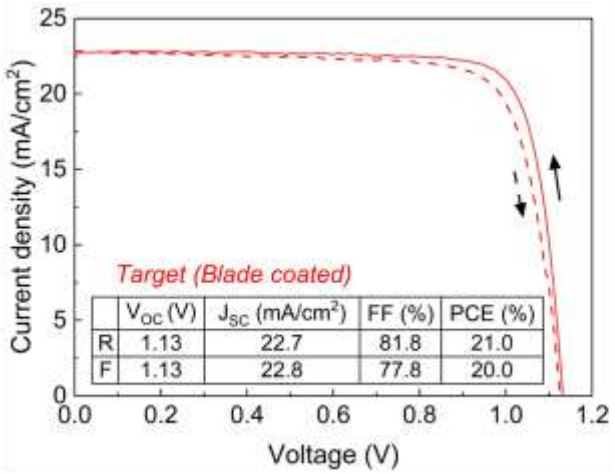
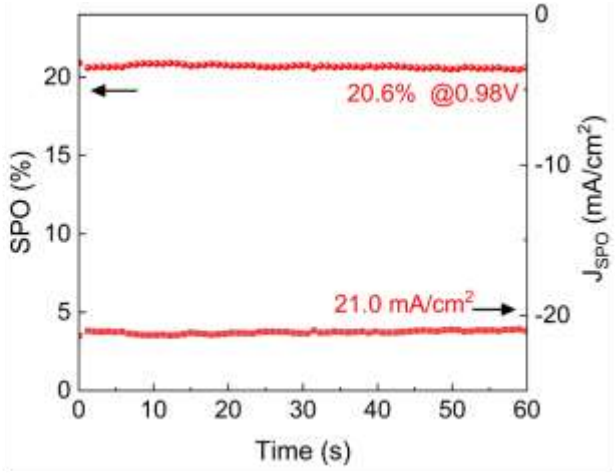
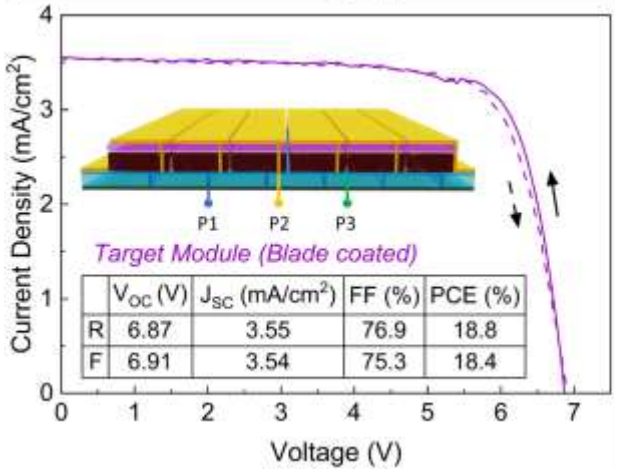
Blade coated PSCs and PSMs from PbAc2

Prof. Jianfeng Lu

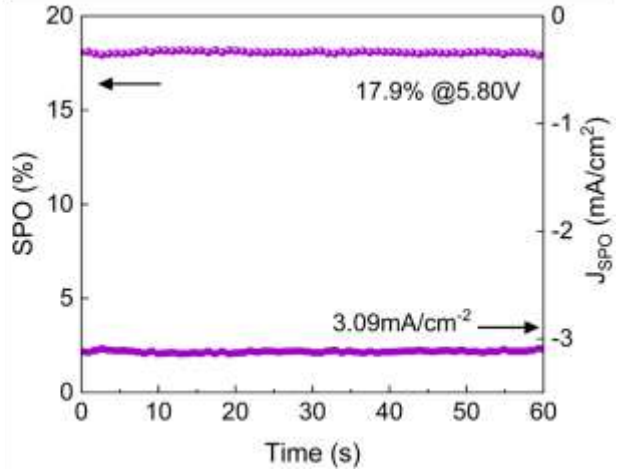


	V_{OC} (V)	J_{SC} (mA/cm²)	FF (%)	PCE (%)
R	1.13	22.7	81.8	21.0
F	1.13	22.8	77.8	20.0





	V_{OC} (V)	J_{SC} (mA/cm²)	FF (%)	PCE (%)
R	6.87	3.55	76.9	18.8
F	6.91	3.54	75.3	18.4



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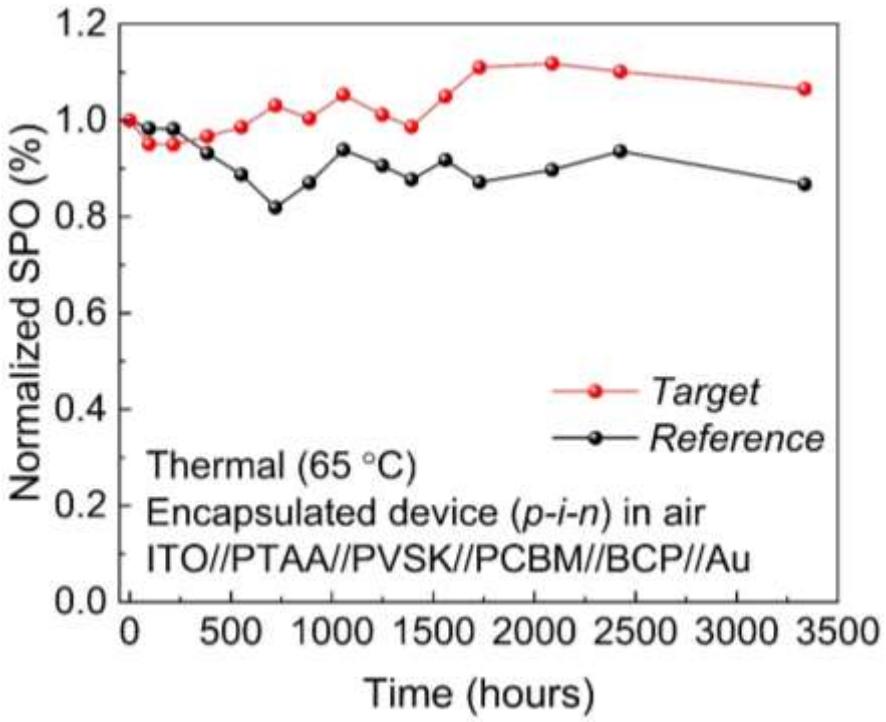
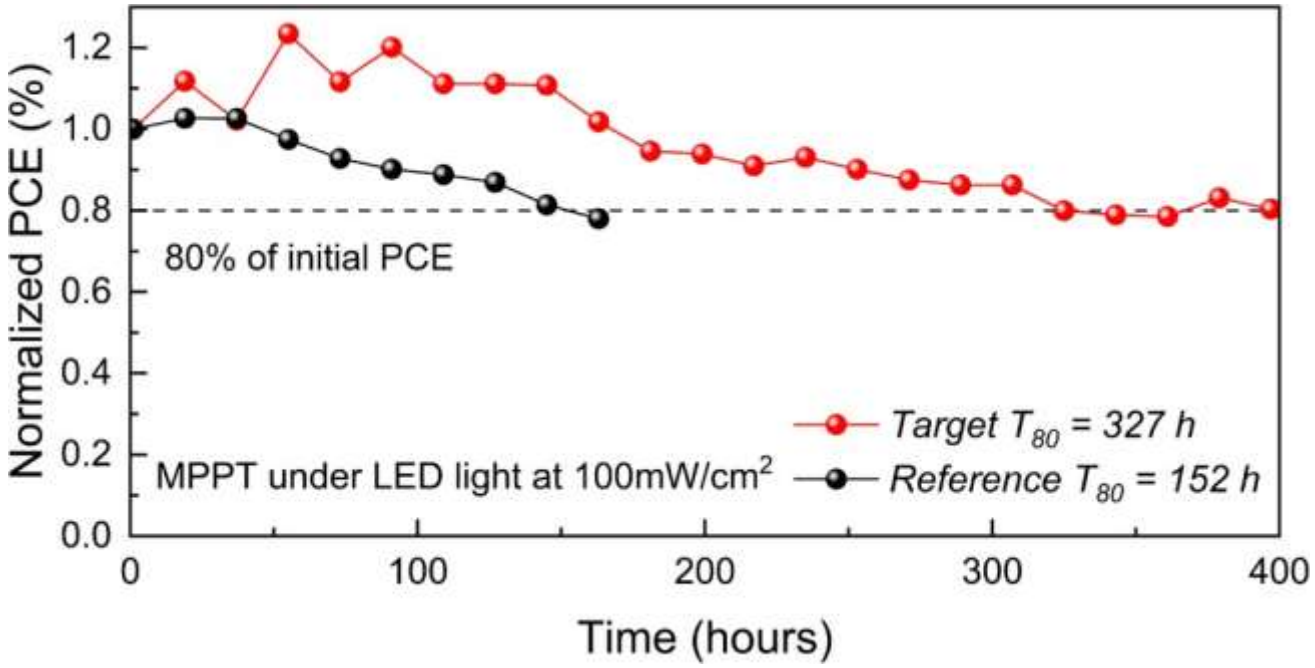
Stability: PSCs

Thermal Stability



MPPT (n-i-p in nitrogen PTAA was used as HTM)



Zhao et al., *Energy & Environmental Science*, ***2023,*** *16, 138-147*

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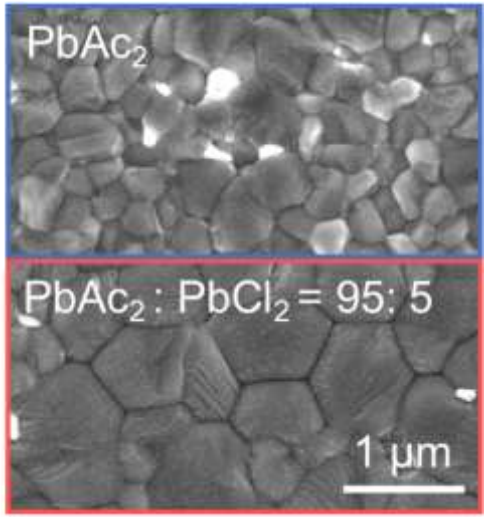
Lead Acetate-Based Precursors for High Open-Circuit Voltage WBG PSCs

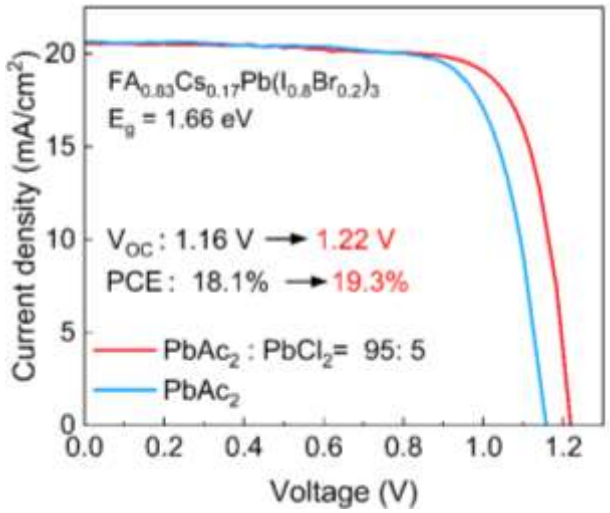
$$FAX, CsX + Pb(Ac/Cl)_2 + NH_4X \rightarrow FA_xCs_{1-x}PbX_3 + 2NH_4(Ac/Cl)$$

Evaporation Rate: $NH_4Cl < NH_4Ac$

$FA_{0.83}Cs_{0.17}Pb(I_{0.8}Br_{0.2})_3$

E_g = 1.66 eV





Zhao et al., *ACS Appl. Mater. Interfaces*, ***2023,*** *15, 18800-18807*

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Prof. Yi-Bing Cheng

CSIRO

Dr. Anthony Chesman

Australian Research Council Centre of Excellence in exciton science

MCN Melbourne Centre for Nanofabrication

Australian Government Australian Research Council

ARENA Australian Government Australian Renewable Energy Agency

ACAP

Thank you for your attention!