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中国科学技术大学

University of Science and Technology of China

$\text{Sb}_2(\text{S,Se})_3$ Solar Cells:

Film Preparation and Device Structure Design

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University of Science and Technology of China

Outline

Contents

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Introduction to $\text{Sb}_2(\text{S,Se})_3$

2

Recent Research

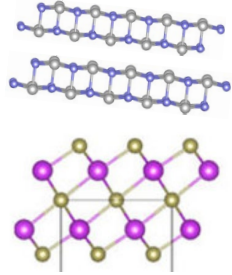
- **Thin Film Fabrication**
- **Defect Engineering**
- **Device Structure Design**

3

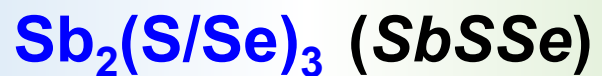
Summary and Outlook

Group V-VI Compounds & Antimony Selenosulfide

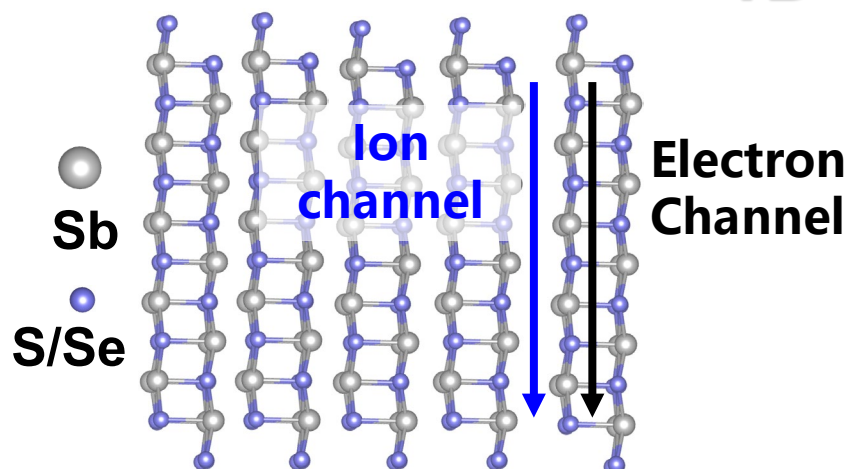
Photovoltaic Materials: Sb_2S_3 , Sb_2Se_3 , $Sb_2(S,Se)_3$, Bi_2S_3

V - VI	Chemical Formulas	Structure & Property
7 N Nitrogen 14.007 8 O Oxygen 15.999 15 P Phosphorus 30.974 16 S Sulfur 32.066 33 As Arsenic 74.922 34 Se Selenium 78.971 51 Sb Antimony 121.760 52 Te Tellurium 127.6 83 Bi Bismuth 208.980 84 Po Polonium [208.982] 115 Mc Moscovium [289] 116 Lv Livermorium [293]	Sb_2S_3 Sb_2Se_3 Sb_2Te_3 Bi_2S_3 Bi_2Se_3 Bi_2Te_3	Quasi-1D crystal structure 2D crystal structure  Photovoltaic materials Thermoelectric, Topological insulator

1D Antimony Selenosulfide

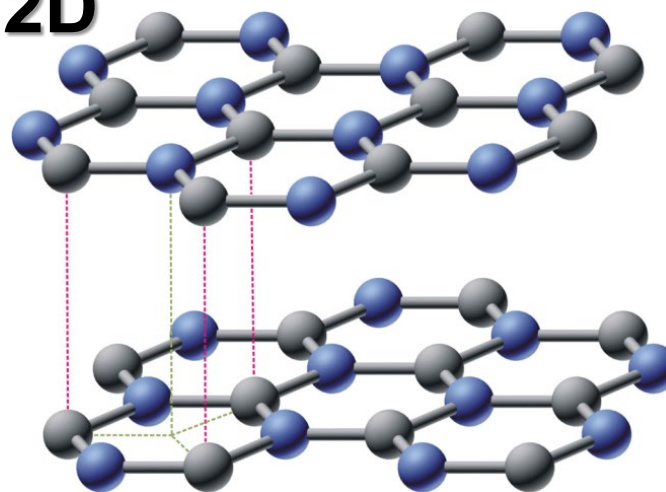


1D

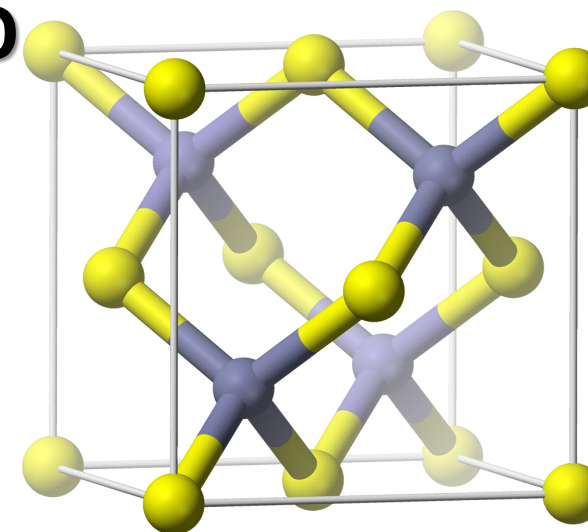


- ✓ High efficiency carrier transport
- ✓ Mechanically flexible
- ✓ High extinction coefficient, tunable band gap (1.1-1.8 eV)
- ✓ Stable, nontoxic, abundant storage

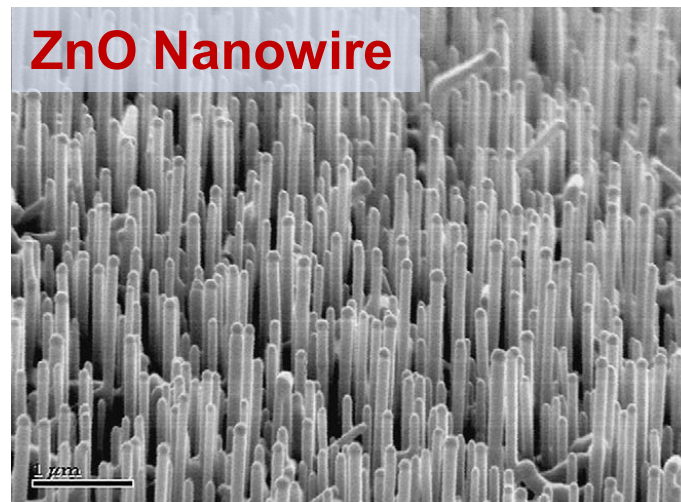
2D



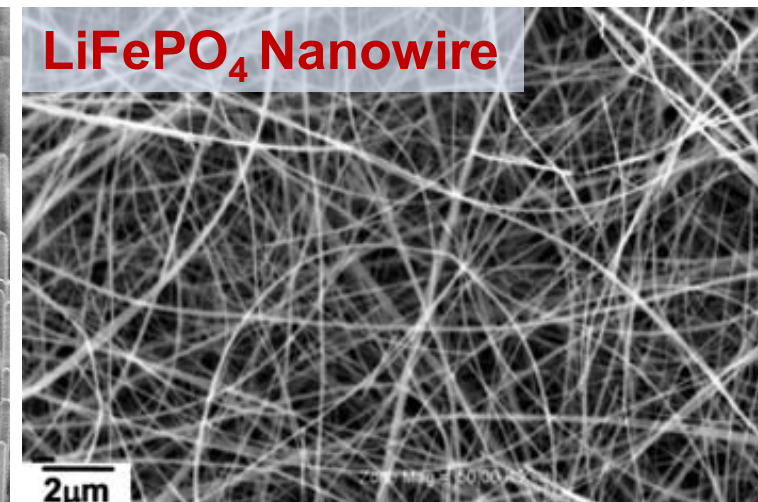
3D



ZnO Nanowire



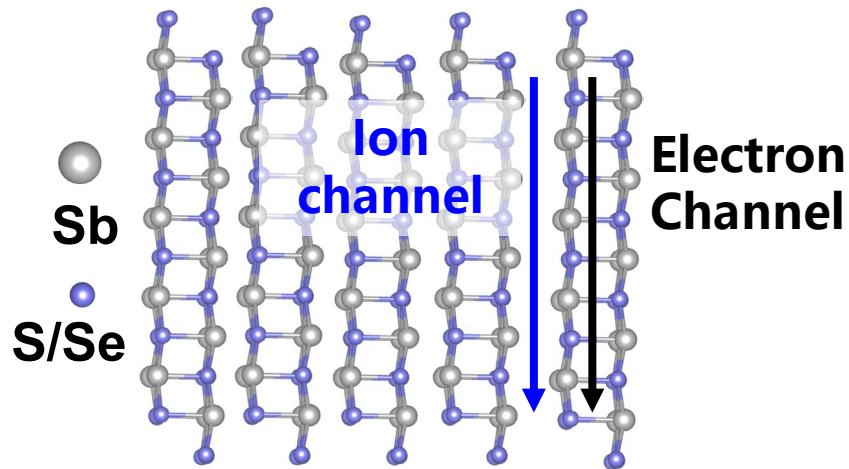
LiFePO₄ Nanowire



$\text{Sb}_2(\text{S},\text{Se})_3$ and One-Dimensional Chain-Like Materials

$\text{Sb}_2(\text{S}/\text{Se})_3$ (SbSSe)

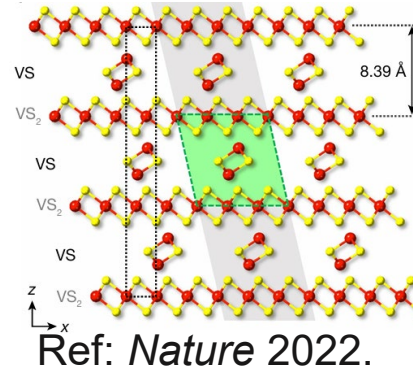
1D



- ✓ High efficiency carrier transport
- ✓ Mechanically flexible
- ✓ High extinction coefficient, tunable band gap (1.1–1.8 eV)
- ✓ Stable, nontoxic, abundant storage

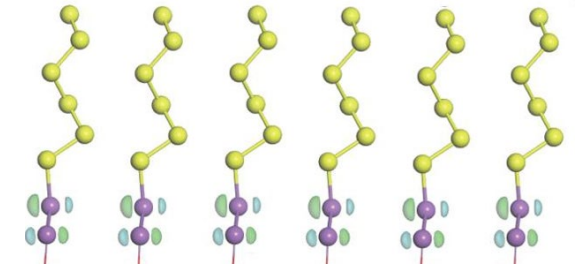
VS (superlattice)

Anomalous Hall effect



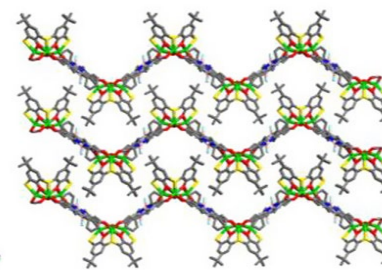
Se, Se-Te

Indoor PV



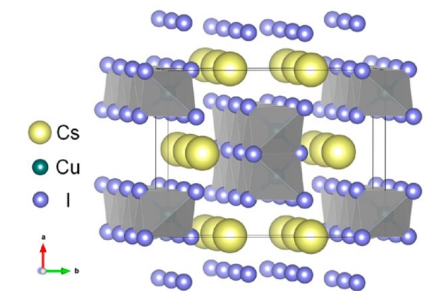
MOF

Photocatalyst



CsCu_2I_3 , $\text{Cs}_5\text{Cu}_3\text{I}_6\text{Cl}_2$

X-ray imaging

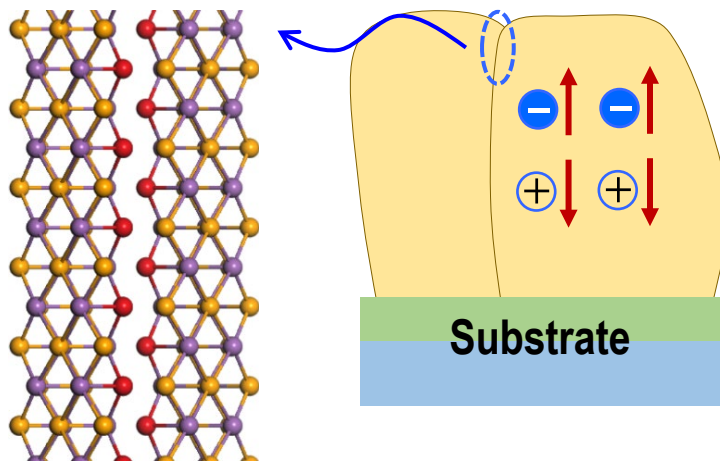


1D PV Materials

Antimony based PV materials: much less dangling bond, high-directional carrier transport, tunable bandgap (1.1-1.8 eV, high absorption coefficient), expecting generating new mechanism and technology in PV applications

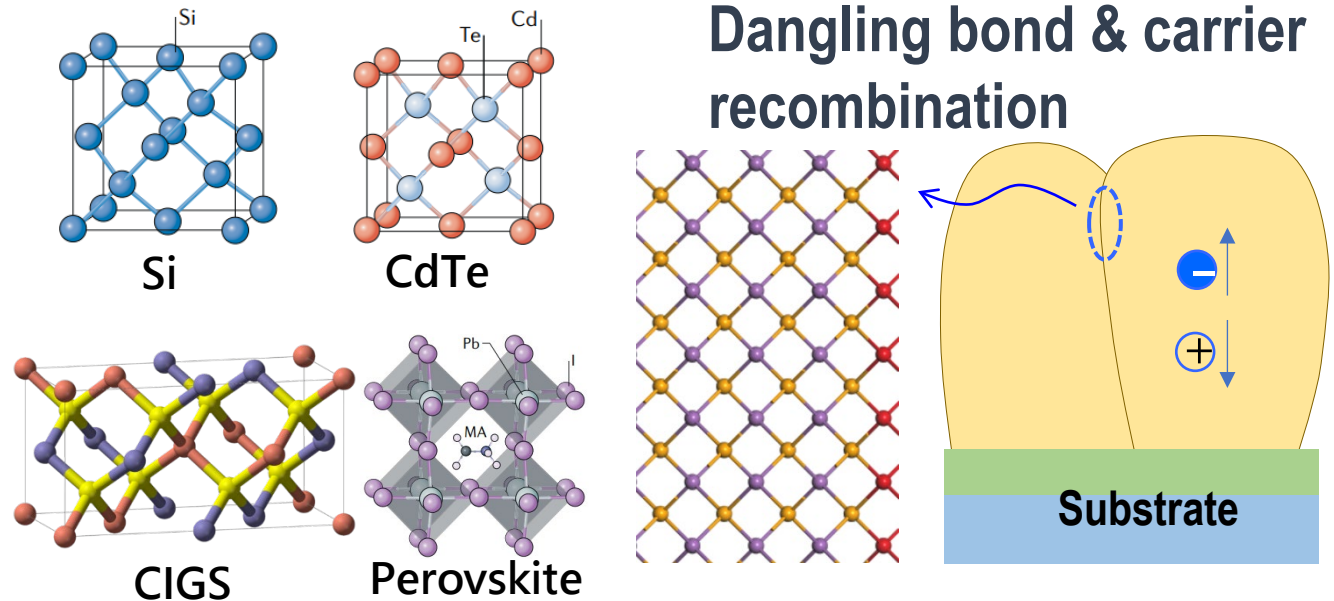
1D PV Materials

Less dangling bond
Highly efficient transport



Conventional 3D PV materials

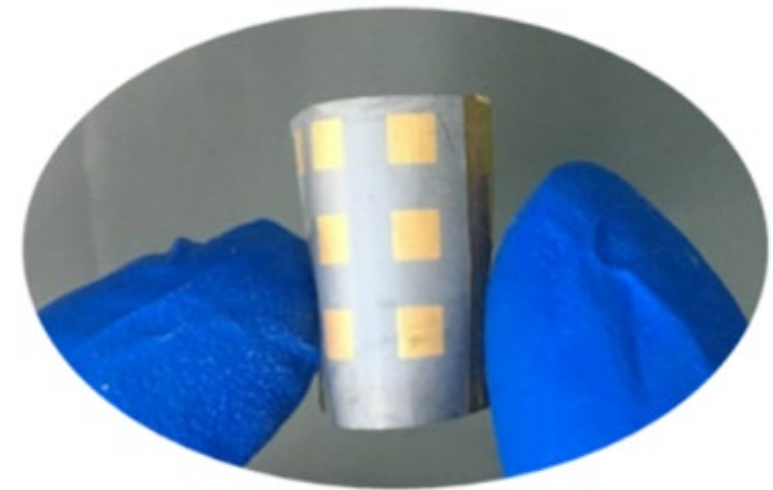
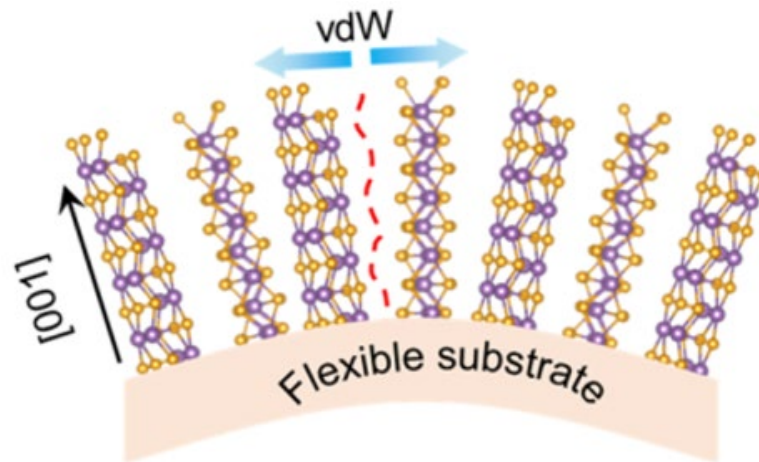
Dangling bond & carrier recombination



Applications of SbSSe Solar Cells

- $\text{Sb}_2(\text{S},\text{Se})_3$: stable, nontoxic, abundance, flexible,..., unique advantages
- Tandem device: E_g of Sb_2S_3 1.8 eV, E_g of Sb_2Se_3 1.1 eV
- Applications: high power to weight ratio, IoT, portable solar cells

High stable
flexible inorganic
solar cells



Ref: *ACS Photonics* 2020, **7**, 352-360.

Efficiency and Challenge

The initial application, 2009

J. Phys. Chem. C **2009**, 113, 4254.

□ 3.37% efficiency

Sb_2S_3 -Sensitized Nanoporous TiO_2 Solar Cells

Yafit Itzhaik, Olivia Nitsso, Miles Page and Gary Hodes*
Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel

J. Phys. Chem. C, 2009, 113 (11), pp 4254–4256

DOI: 10.1021/jp900302b

Publication Date (Web): February 20, 2009

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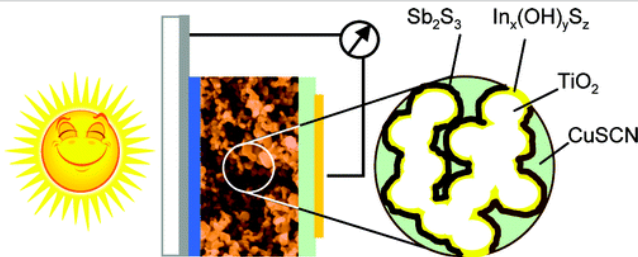
* Corresponding author. E-mail: gary.hodes@weizmann.ac.il.

✓ Cite this: *J. Phys. Chem. C* 2009, 113, 1

Ⓜ RIS Citation GO

Abstract

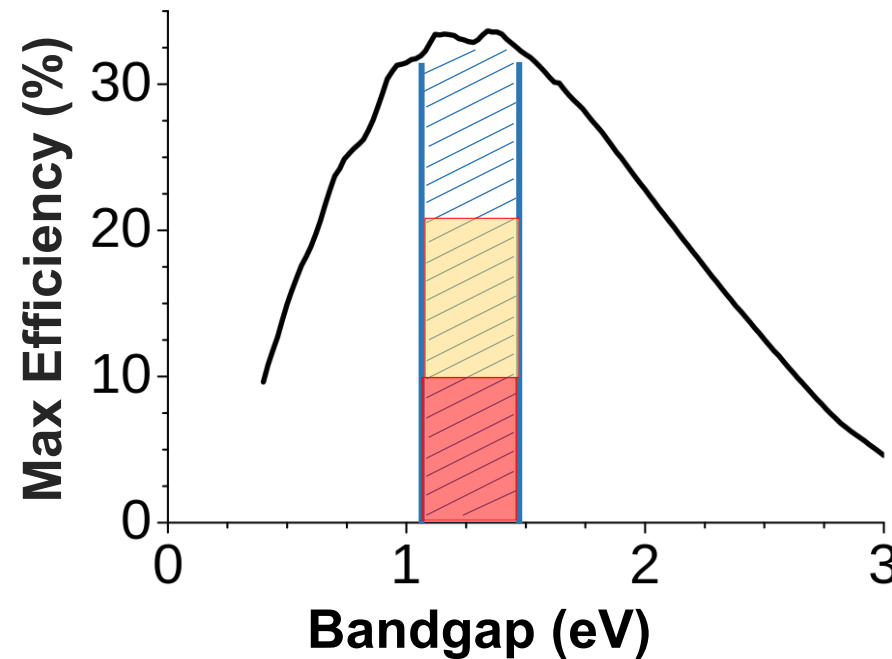
Jump to a section



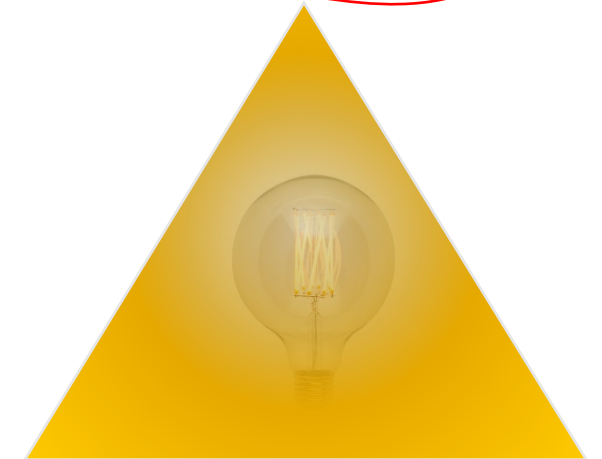
Extremely Thin Absorber (ETA) solar cells were made using chemical-bath-deposited Sb_2S_3 as the absorber and $\text{TiO}_2/\text{CuSCN}$ as the interpenetrating electron/hole conductors. A solar conversion efficiency of 3.37% at 1 sun illumination was obtained. Surface oxidation of the Sb_2S_3 formed a passivation layer on Sb_2S_3 : without this oxidation, much poorer cells were obtained. Preliminary stability measurements showed good stability over 3 days of illumination (at 60 mW/cm^2) under load.



E_g : 1.1–1.8 eV, optimal bandgap



Efficiency



Stability

Survive the stringent test (85% humidity, 80 °C)

Cost

(high abundance, non-toxic, thin film solar cell)

The efficiency requires essential improvement

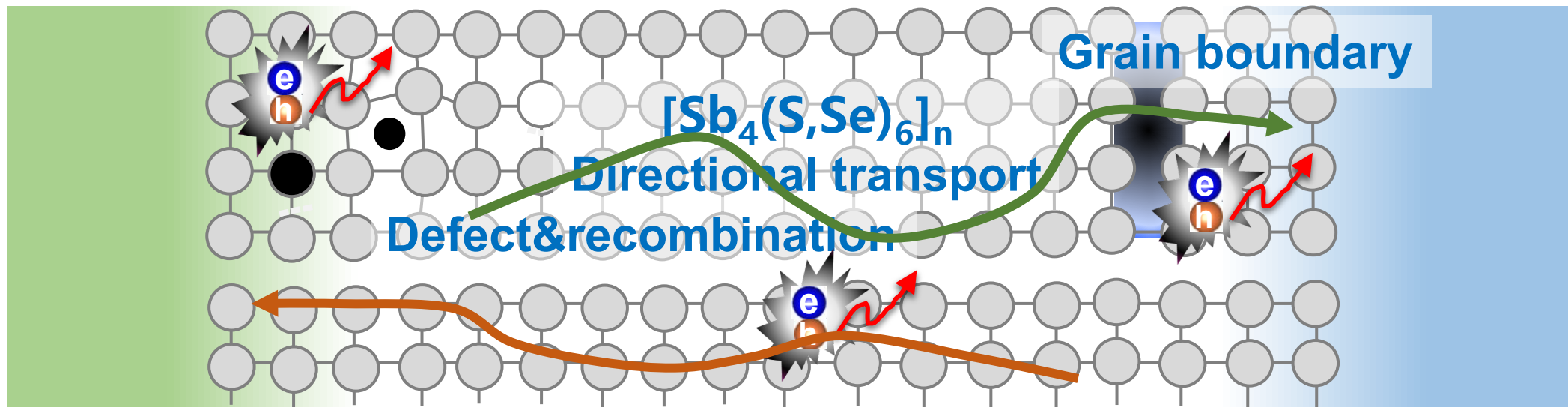
How to improve the efficiency?

High efficient charge transport and collection
——Materials science and device design

Interface

Bulk-Absorber Layer

Interface



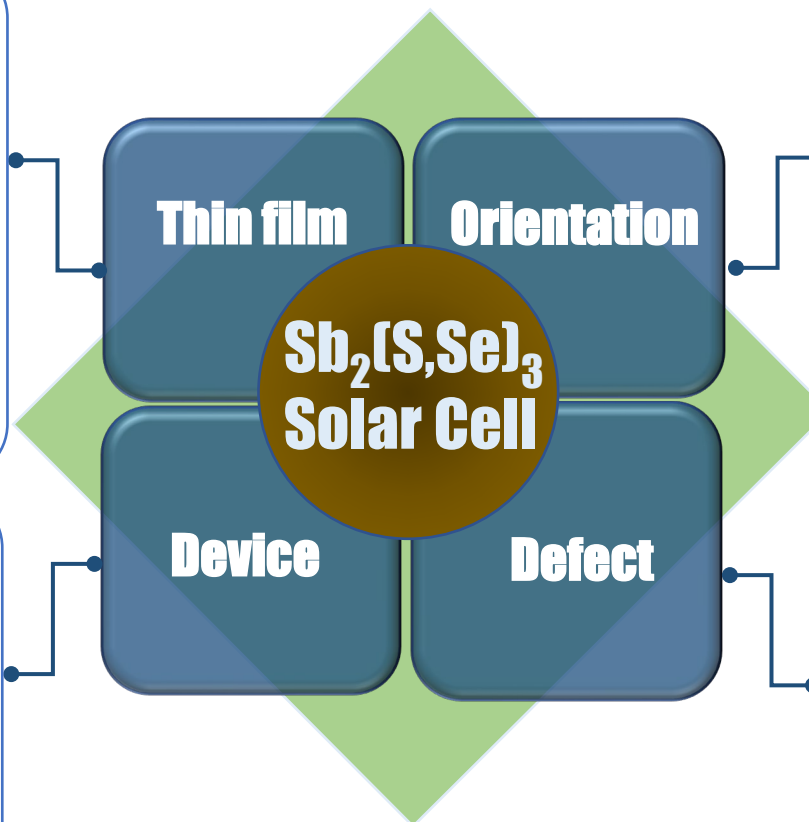
Our Study in This Field (from 2016---)

- **Develop hydrothermal and thermal evaporation methods**

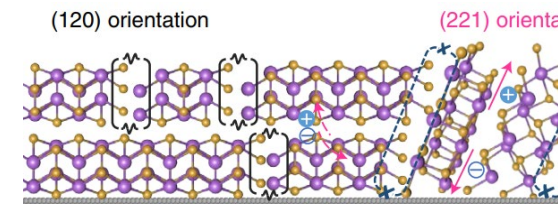
- **Nature Energy** 2020, **5**, 587.
- **Nature Energy** 2025, **10**, 857.
- **Nature Energy** 2026, **11**, 415.
- **Angew. Chem.** 2024, **63**, e202406512.
- **Adv. Mater.** 2026; **38**:e20937.

- **Develop p-SbSSe-n and internal homojunction device structure and efficiency breakthrough**

- **Nature Photonics** 2026, **20**, 644.
- **Nature Commun.** 2019, **10**, 4540.
- **Energy Environ. Sci.** 2025, **18**, 4833.
- **Nanoscale** 2017, **9**, 3386.



- **Preferential orientation**



- **Adv. Mater.** 2021, **33**, 2006689.
- **Adv. Mater.** 2025, **37**, 2414082.
- **Adv. Mater.** 2024, **36**, 2305841.

- **Defect formation, evolution, passivation**

- **Acc. Chem. Res.** 2026, **59**, 1342.
- **Nat. Commun.**, 2021, **12**, 3260.
- **Adv. Mater.**, 2022, **34**, 2208564.
- **Adv. Mater.**, 2024, **36**, 2404826.

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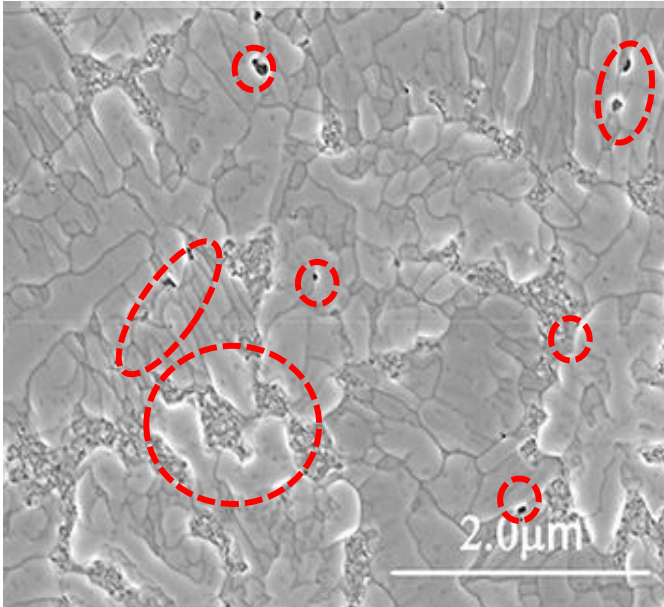
3

Conclusions and Outlook

The Challenge in Film Fabrication

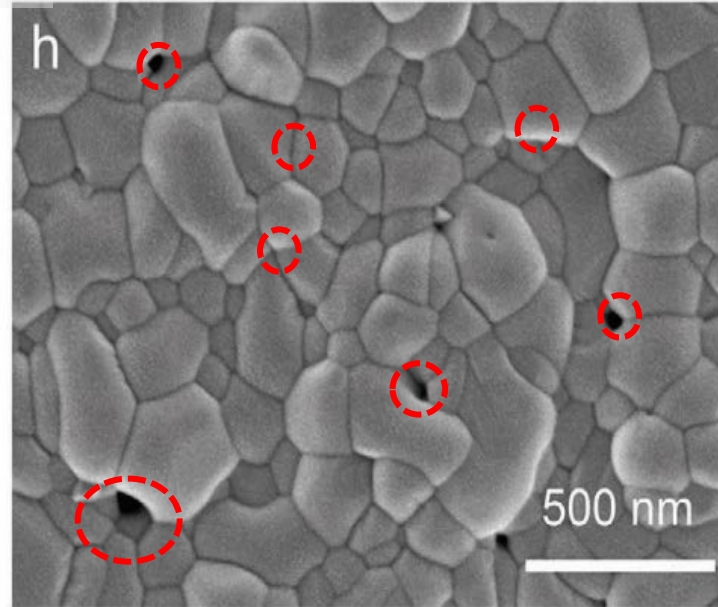
Pinholes in $\text{Sb}_2(\text{S,Se})_3$ film: increase resistance, lead to recombination

Solution processing

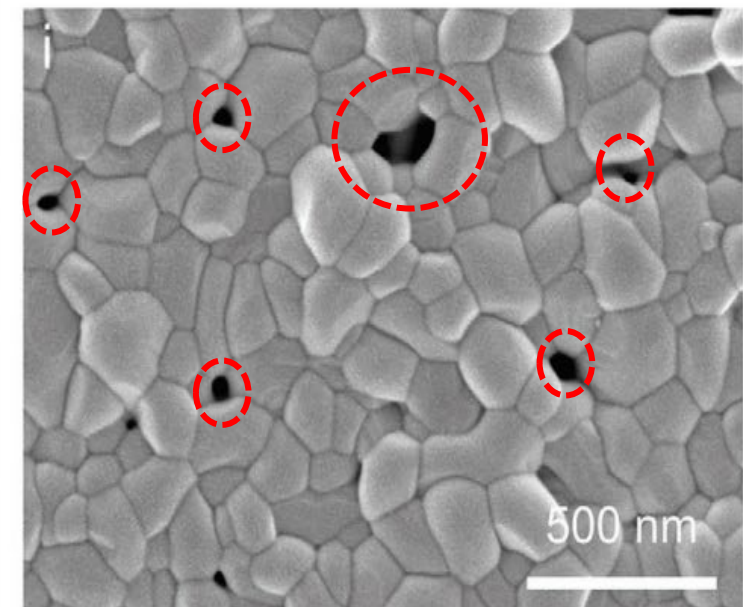


Ref: *ACS AMI* 2019, 11, 3207.

Vapor deposition

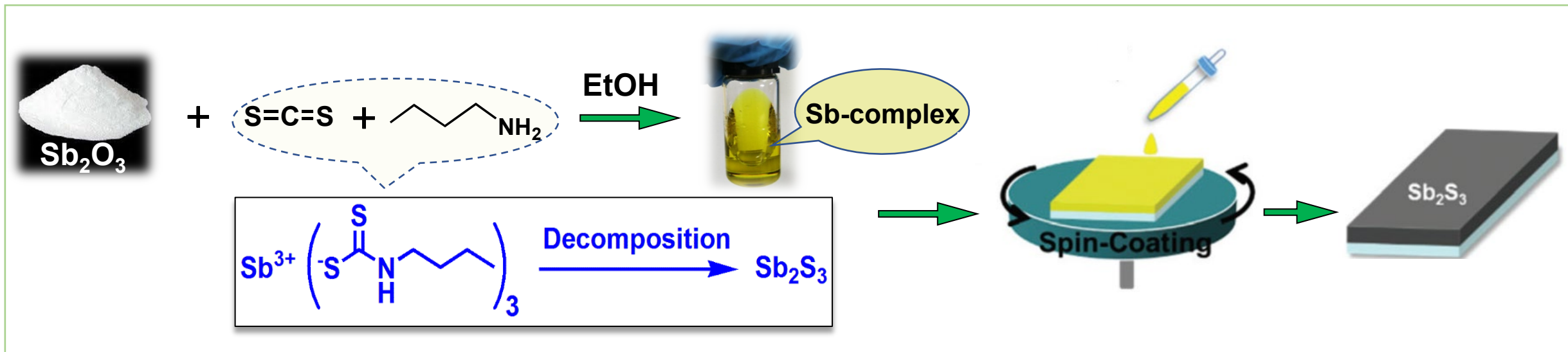
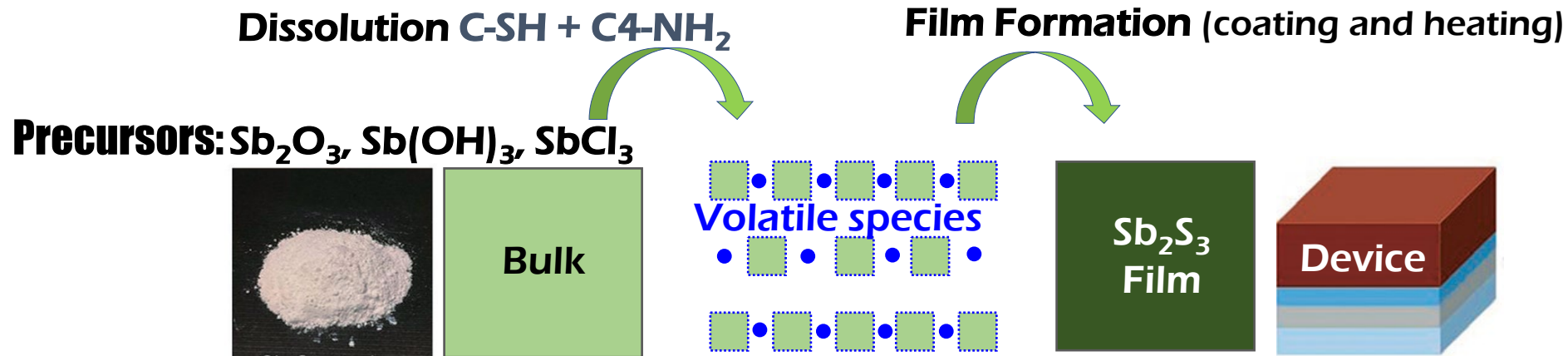


Ref: *Adv. Mater.* 2021, 33, 2006689.



Ref: *Nat. Commun.* 2018, 9, 2179.
Nat. Photon. 2015, 9, 409.

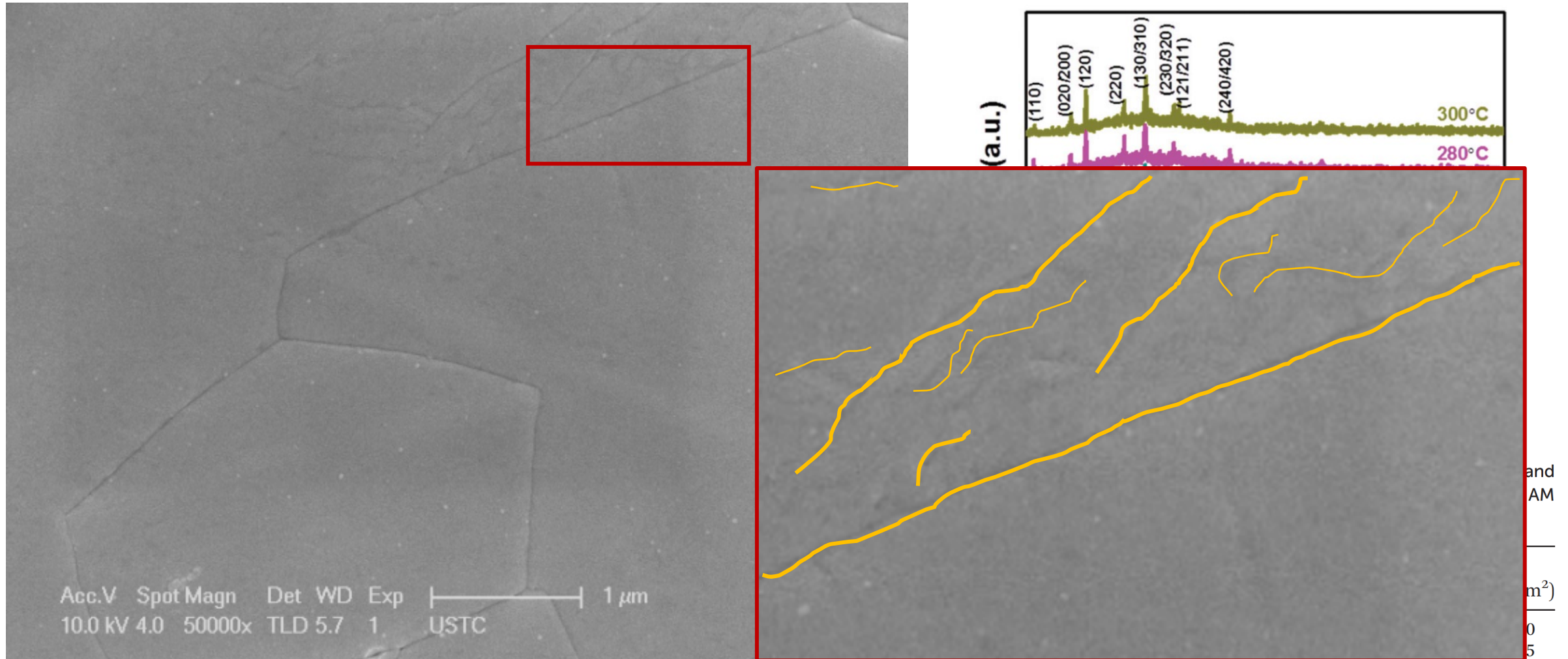
Conventional Spin-Coating Method



Conventional Spin-Coating Method

Sb_2S_3 film

Crystallinity



Improving the Crystallinity and Reducing Bandgap

Selenization can improve the crystallinity and reduce the band gap.

Selenization in
 $\text{Cu}_2(\text{Zn,Sn})\text{Se}_4$ solar cell

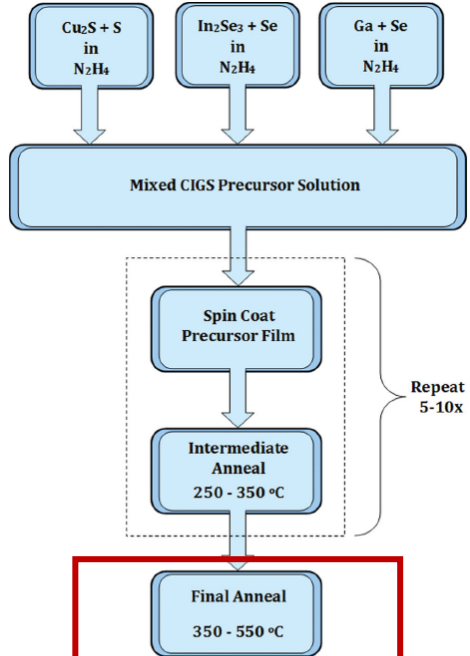
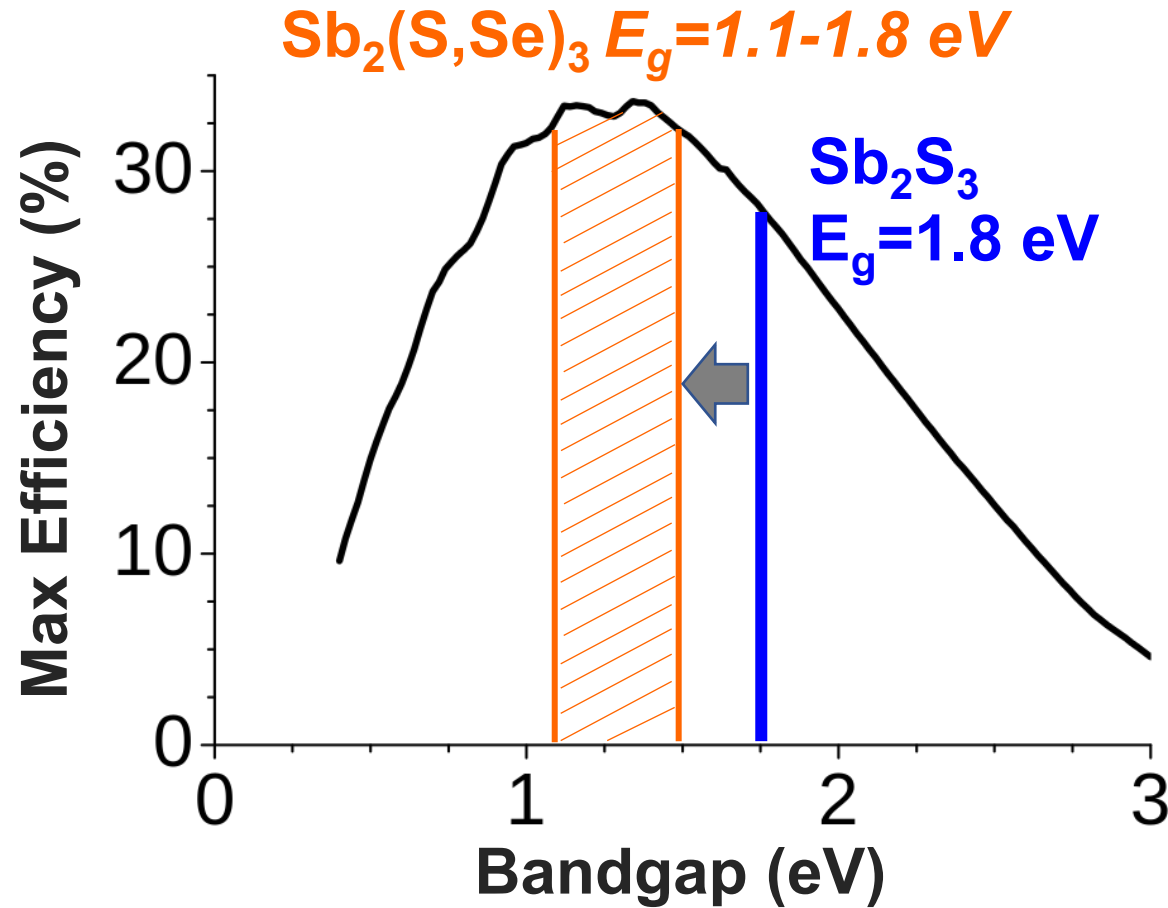


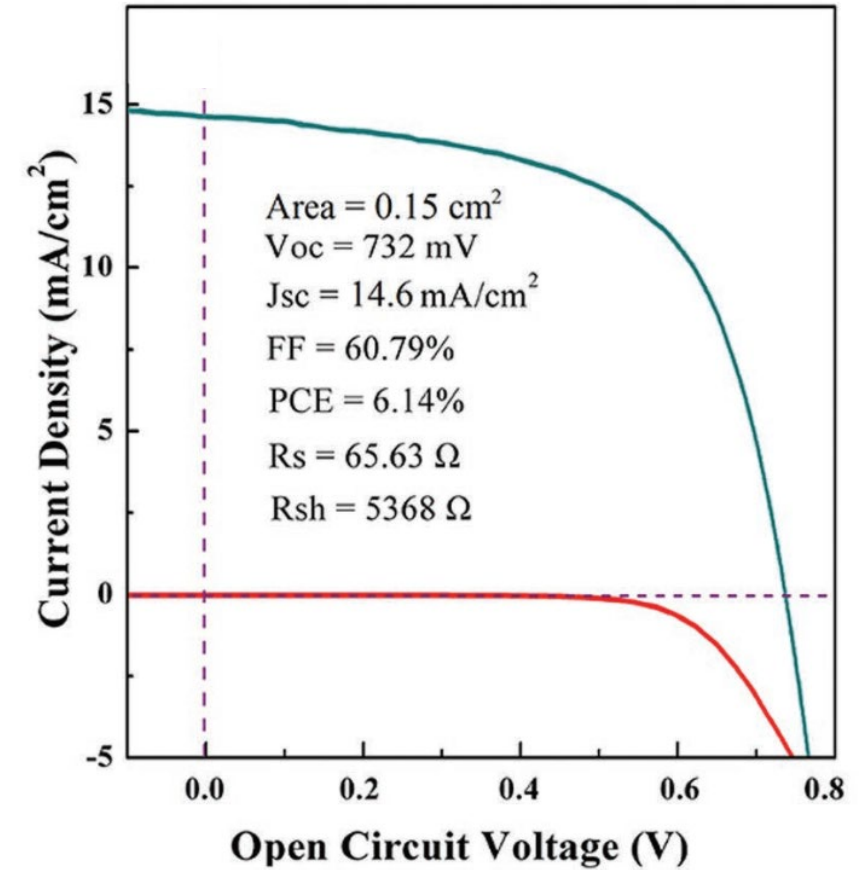
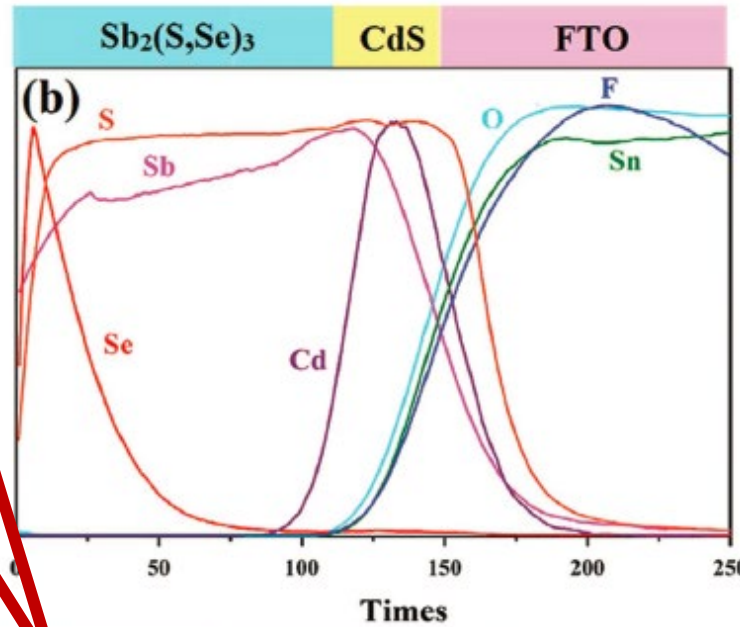
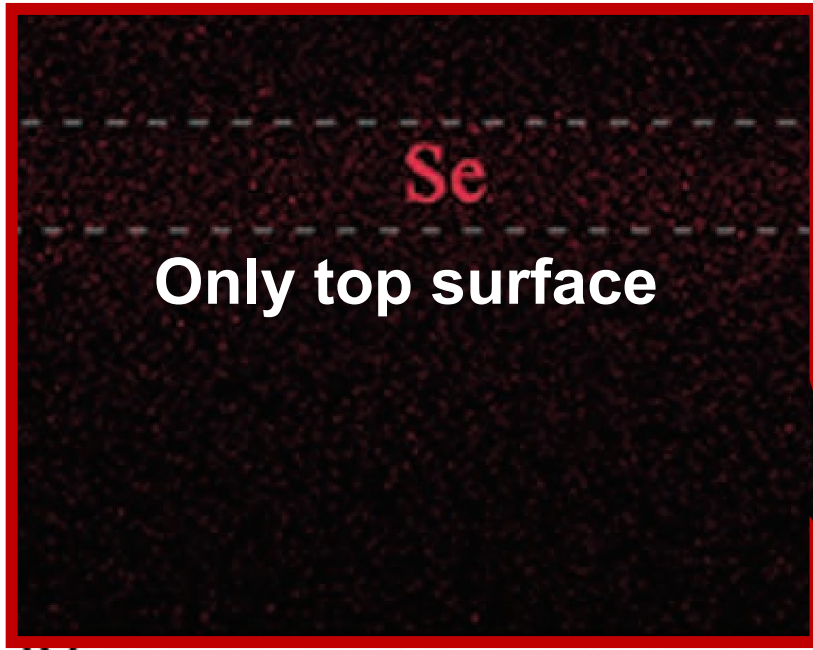
Figure 1. Schematic diagram of the selenization process for $\text{Cu}_2(\text{Zn,Sn})\text{Se}_4$ solar cells.



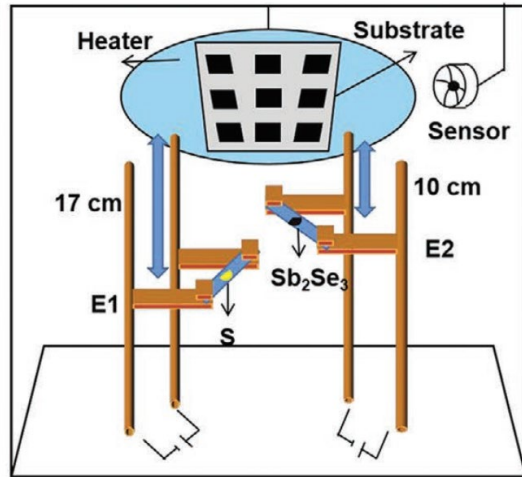
Ref: Adv. Energy Mater. 2012, 2, 504.

From Sb_2S_3 to $\text{Sb}_2(\text{S,Se})_3$

$\text{Se} + \text{Sb}_2\text{S}_3 \rightarrow \text{Sb}_2(\text{S,Se})_3$ solar cell

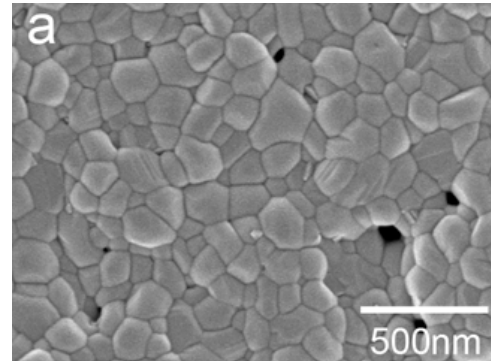


How About Conventional Vapor Deposition Method?

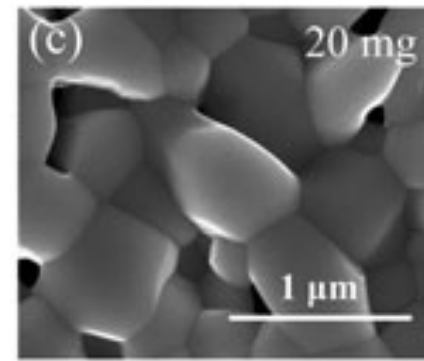


Thermal Evaporation

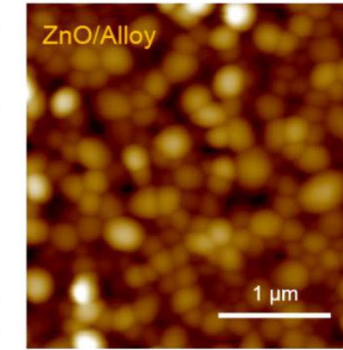
The appearance of pin holes resulting in resistance and recombination



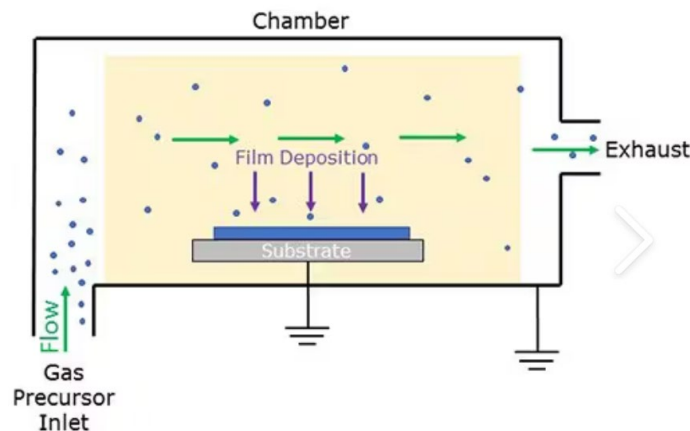
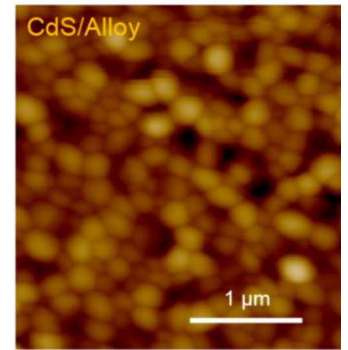
Vapor deposition,
PCE = 8.0%,
Adv. Mater. 2021, 2006689.



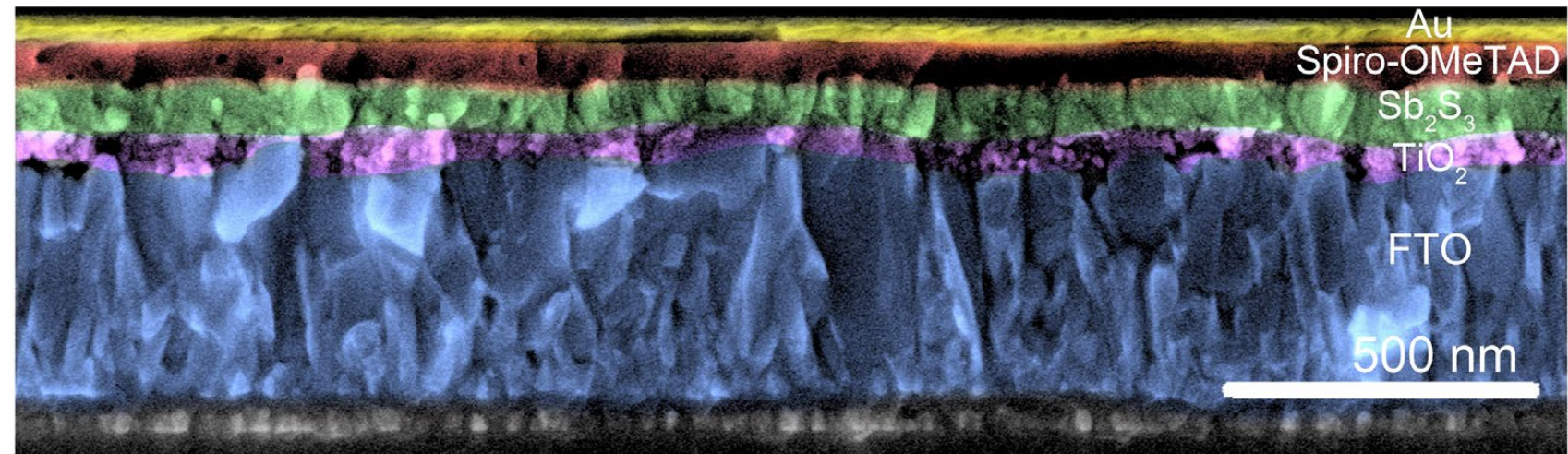
Ref:
Vapor deposition, J. Tang (HUST)
PCE = 5.79%,
Prog. Photovolt: Res. Appl. 2017.



Ref:
Vapor deposition, J. Tang (HUST)
PCE = 5.73%
Solar RRL. 2018.

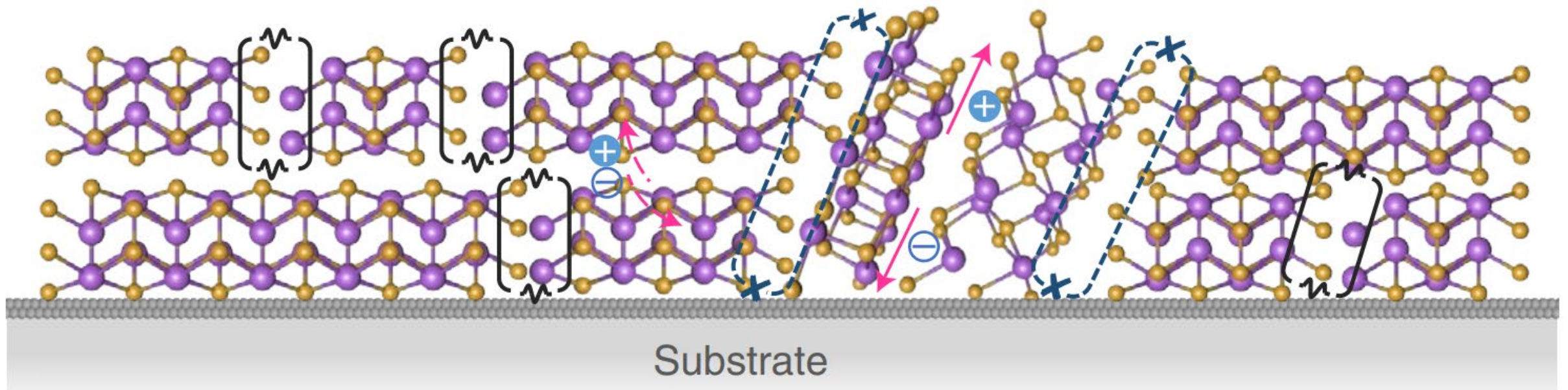


Vapor Transport Deposition



Why is the formation of large grains difficult?

Inert grain boundary, difficult to melt together

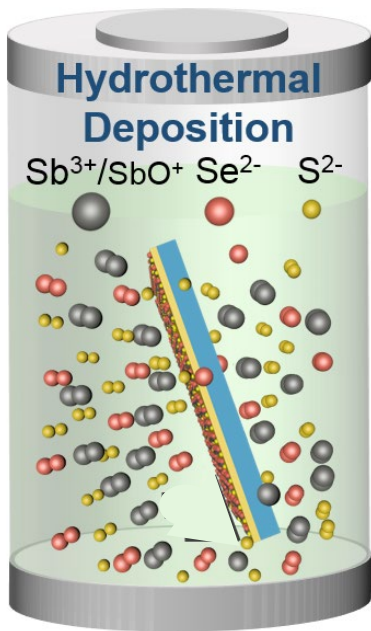


The one-dimensional structure enables fewer dangling bonds and highly efficient directional carrier transport, yet it poses challenges for fabricating large grain sizes.

New Method: Hydrothermal Deposition Method

Developed **hydrothermal deposition** method for the fabrication of $\text{Sb}_2(\text{S},\text{Se})_3$ film, the deposition condition: 135 °C, 2-3 hrs, post-annealing: 300 °C in N_2

Chemical reaction: $2\text{K}[\text{SbO}(\text{C}_4\text{H}_4\text{O}_6)] + 3\text{Na}_2\text{S}_2\text{O}_3 + 3\text{CSe}(\text{NH}_2)_2 + \text{H}_2\text{O} \rightarrow \text{Sb}_2(\text{S}_x\text{Se}_{1-x})_3$



Precursors

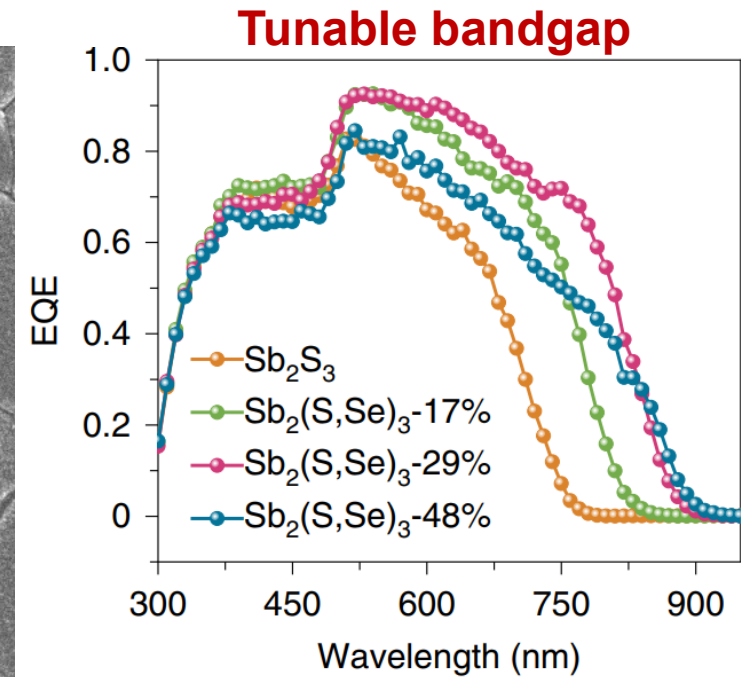
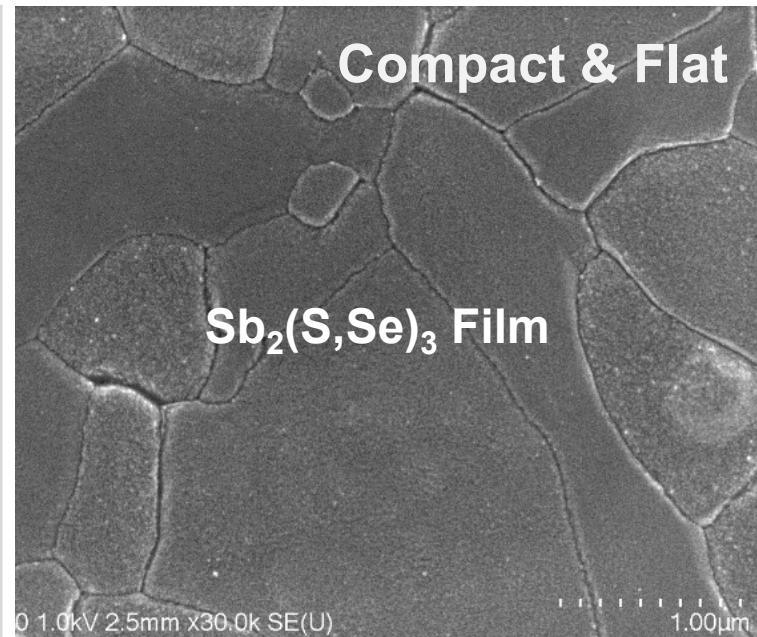
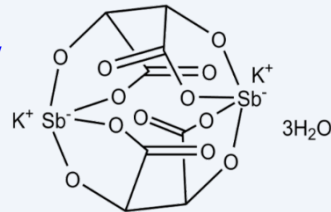
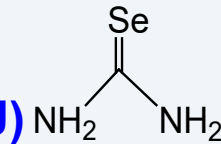
Antimony Source (APT)



Sulfur Source (SSS)



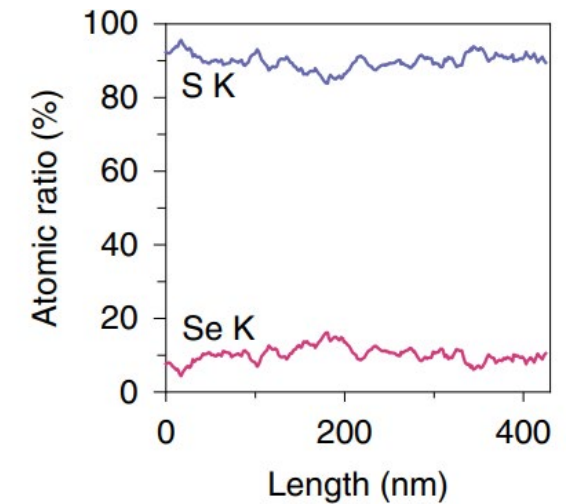
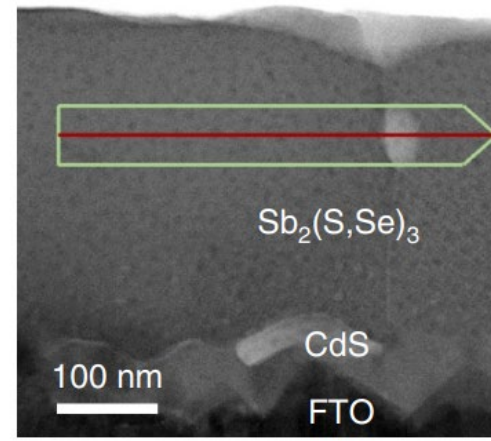
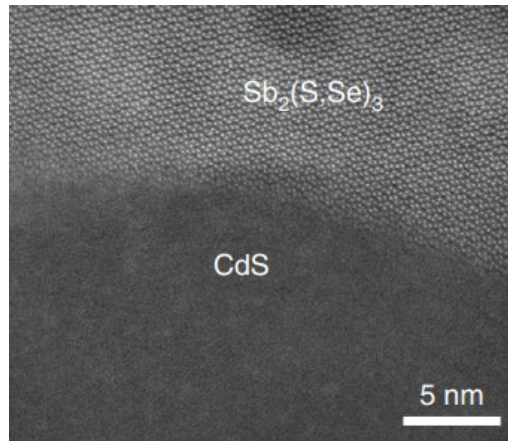
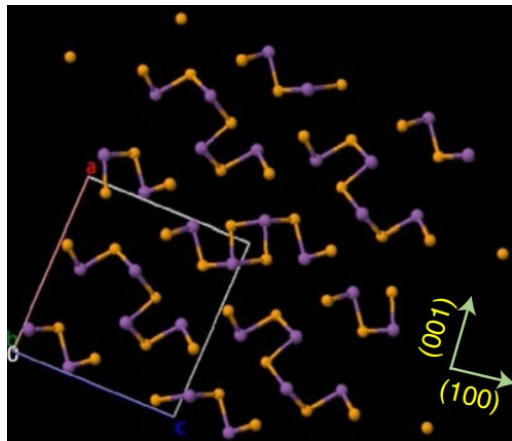
Selenium Source (SU)



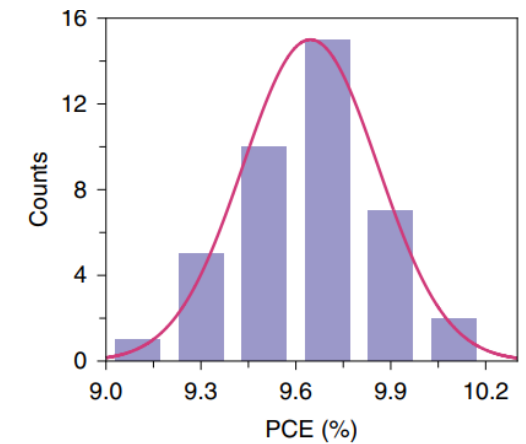
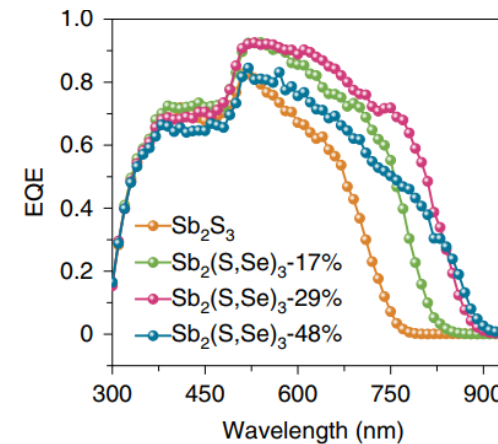
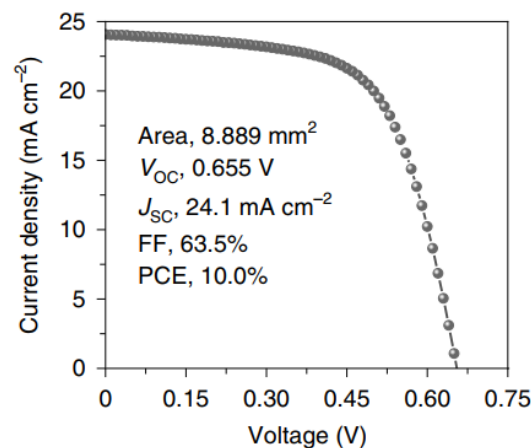
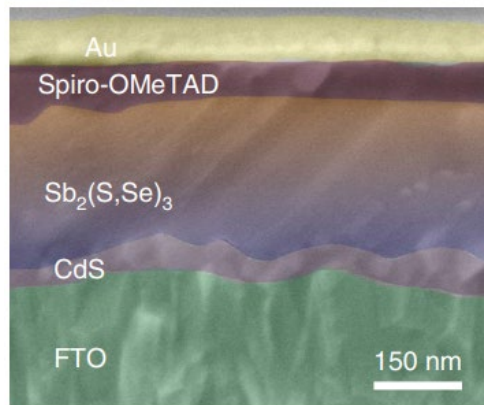
Tang, ..., Zhu,* Hao,* Chen,* *Nature Energy* 2020, **5**, 587.

New Method: Hydrothermal Deposition Method

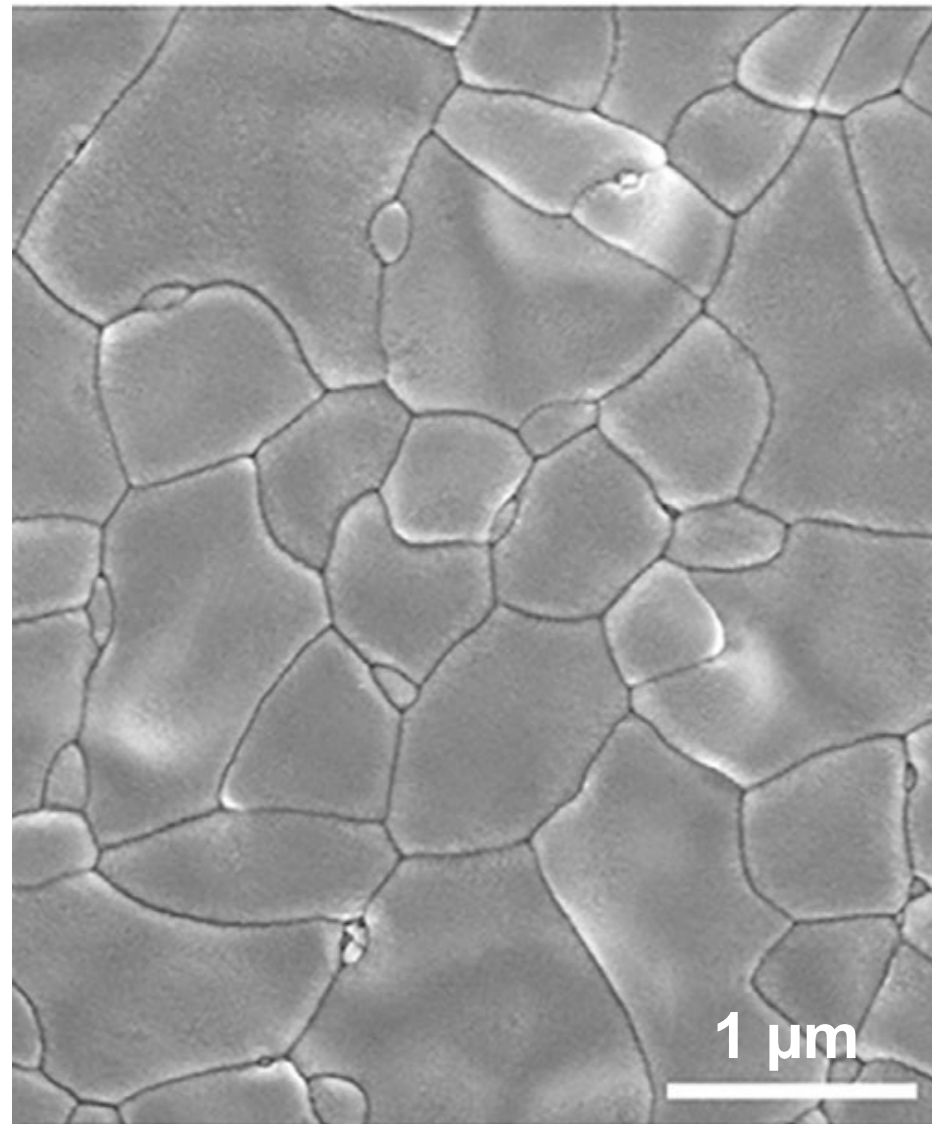
Clear interface between CdS and SbSSe, no interfacial diffusion



10% efficiency breakthrough

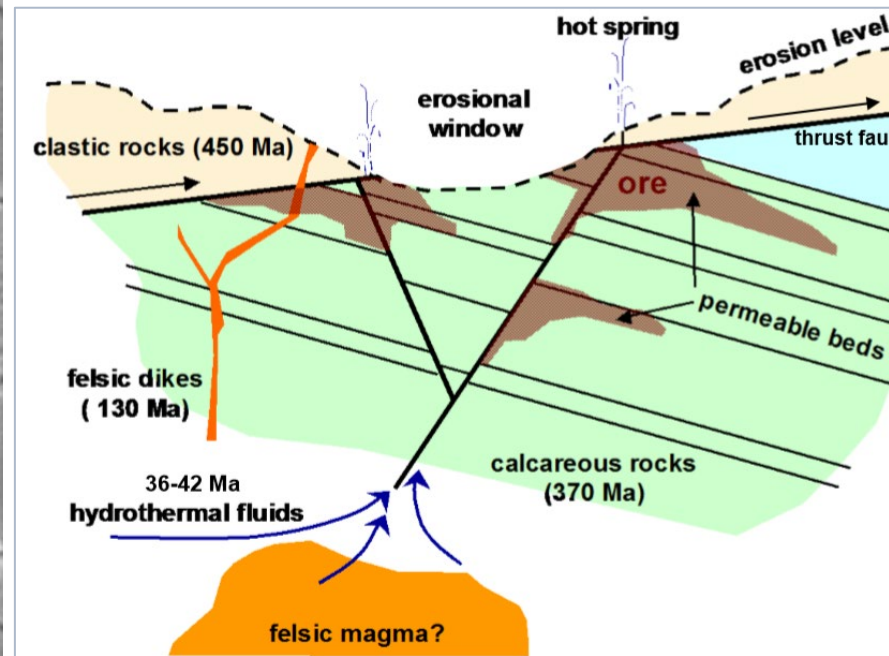


Why Hydrothermal Deposition Can Generate Compact Film?



Hydrothermal Deposition

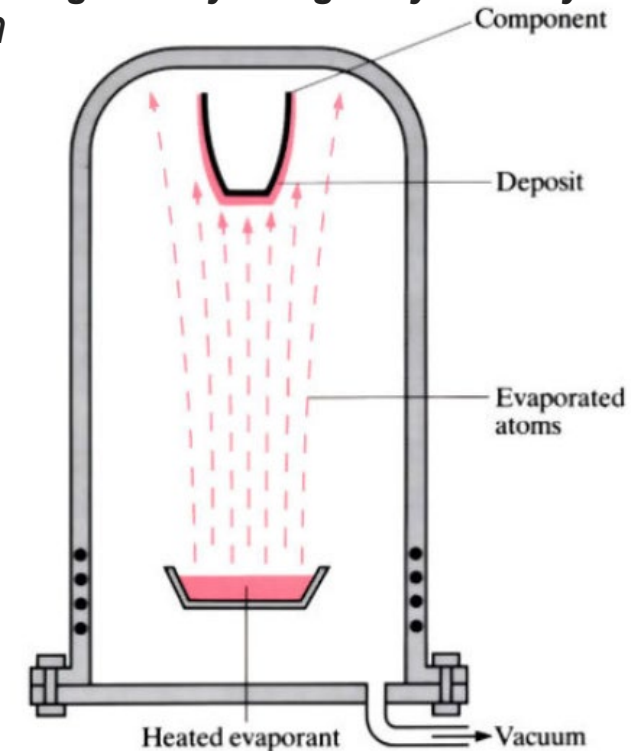
*Hydrothermal mineral deposits are accumulations of valuable minerals which formed from **hot water circulating** in Earth's crust through fractures.*



High concentration precursor ions

Vapor Deposition

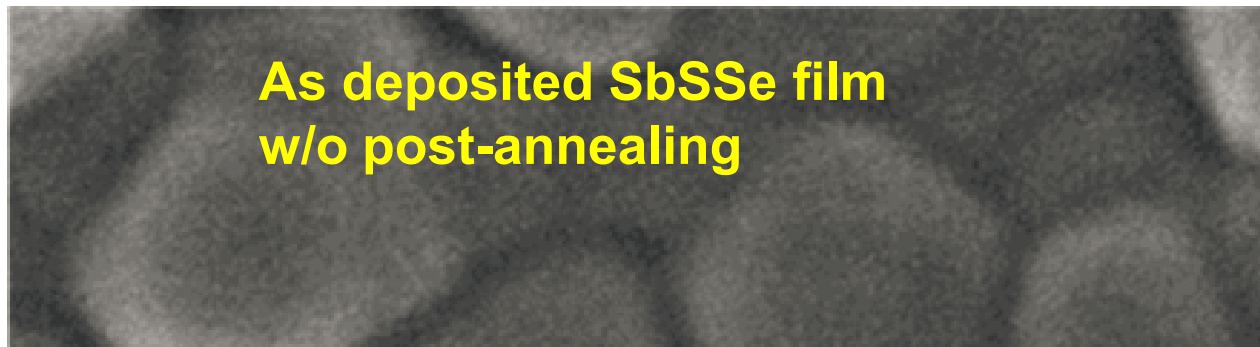
High Purity & High Crystallinity



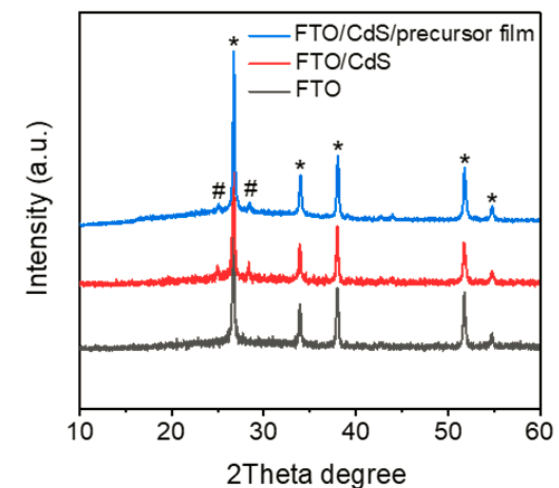
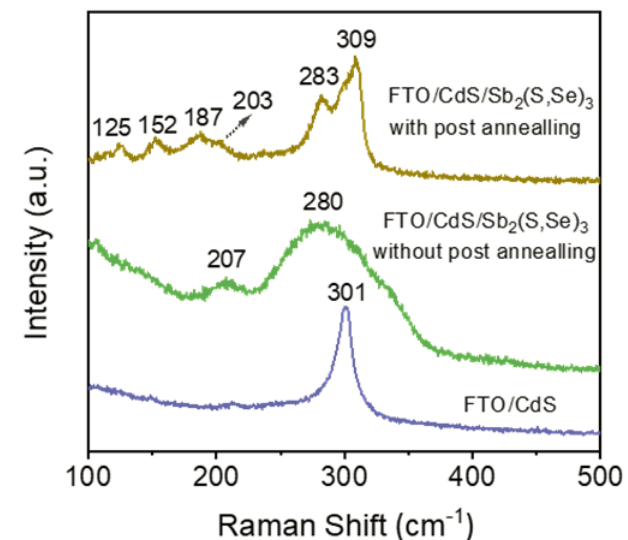
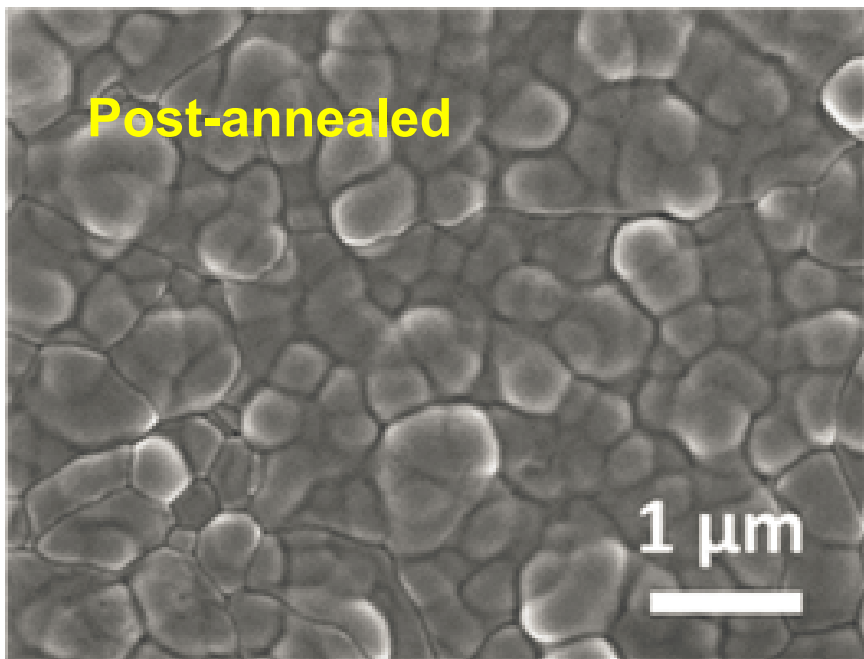
Low concentration Sb_2X_3 , SbX , SbX_2 ...

As Deposited $\text{Sb}_2(\text{S,Se})_3$ Film

As deposited SbSSe film
w/o post-annealing



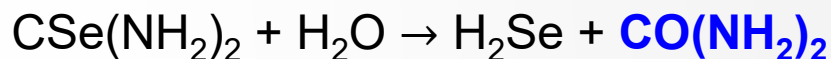
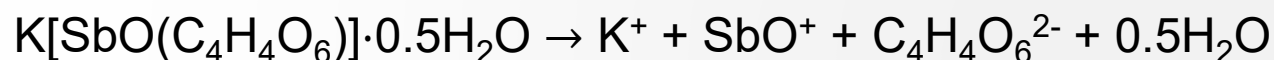
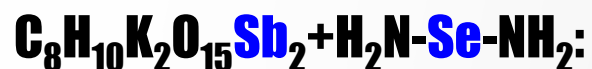
Post-annealed



- ◆ Formation of compact amorphous film with Sb-S and Sb-Se bonds
- ◆ Post-annealing leads to crystallized $\text{Sb}_2(\text{S,Se})_3$ with flat and uniform morphology.

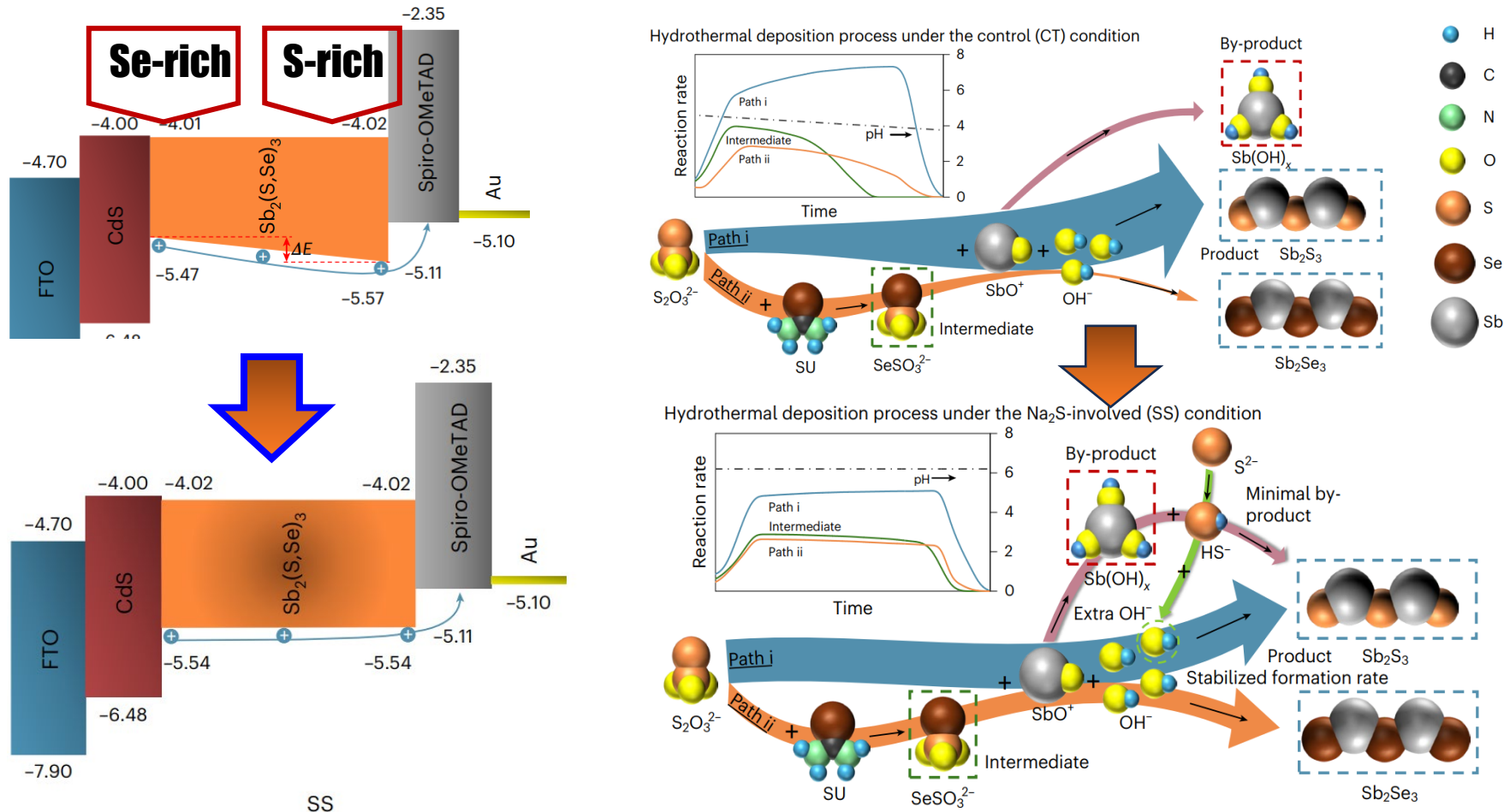
Chemical Reaction Path

Competitive reactions: a slower reaction pathway for sulfide generation and a faster pathway for selenide generation.



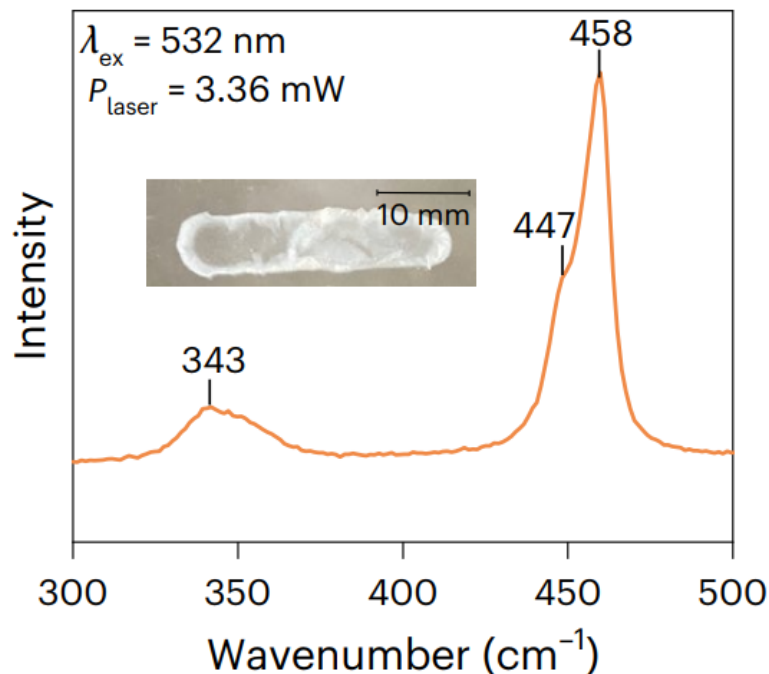
Band Structure Engineering

Introducing Na_2S in the hydrothermal deposition can manipulate reaction path and kinetics and tailoring the band structure



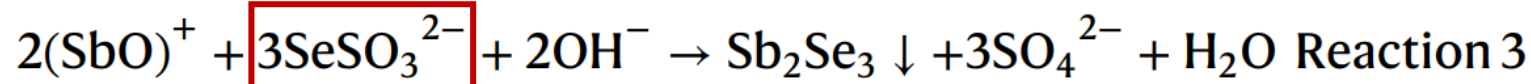
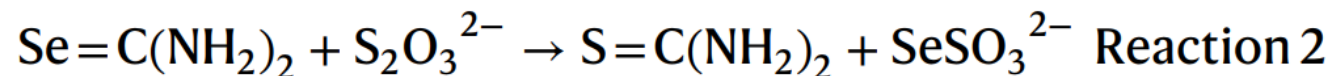
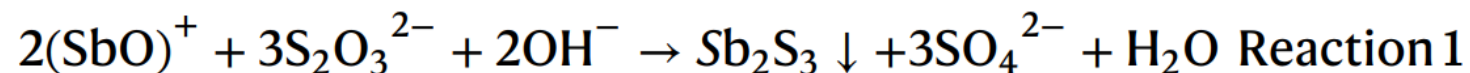
Chen Qian & Me
@ USTC-May 2022

Reaction Mechanism



Se–S stretching vibration of SeSO_3^{2-} and **S–S** stretching vibration of $\text{S}_2\text{O}_3^{2-}$ at 343 and 447 cm^{-1}

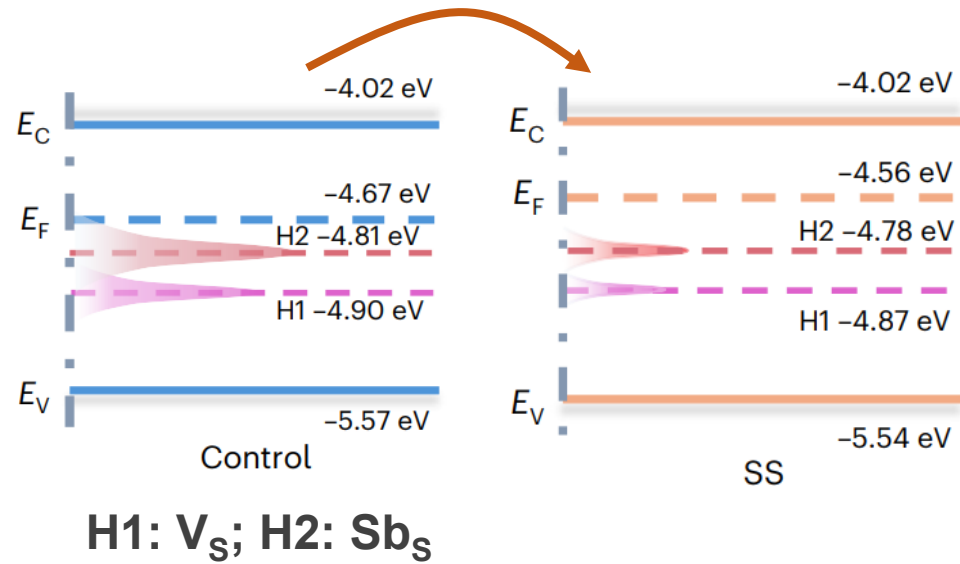
Path i (Reaction 1): direct formation of Sb_2S_3 from SbO^+ and $\text{S}_2\text{O}_3^{2-}$.
 Path ii (Reactions 2–3): SU reacts with $\text{S}_2\text{O}_3^{2-}$ to form SeSO_3^{2-} , which then reacts with SbO^+ to yield Sb_2Se_3 .



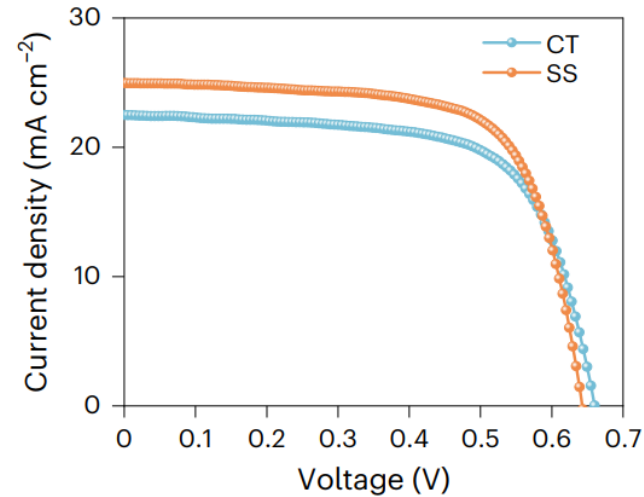
1. **Suppress the formation of Sb_2O_3**
2. **Facilitate the formation of intermediate SeSO_3^{2-}**
3. **Stabilize reaction rate towards Sb_2Se_3**

Device Performance

Suppressed Defect



Device Efficiency



EQE

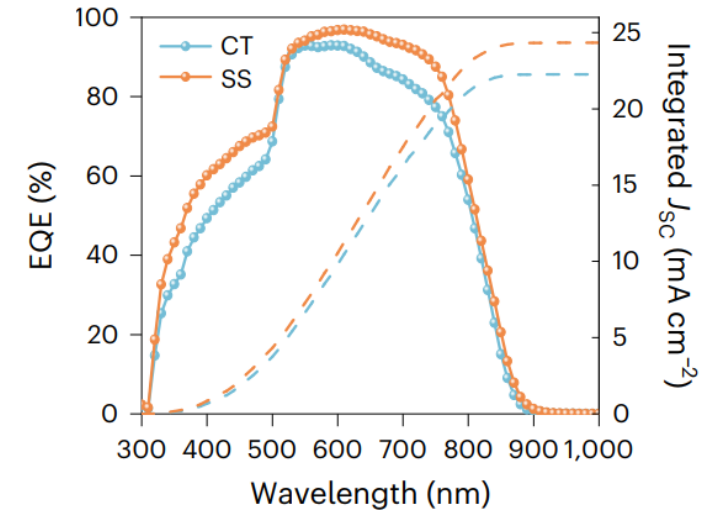
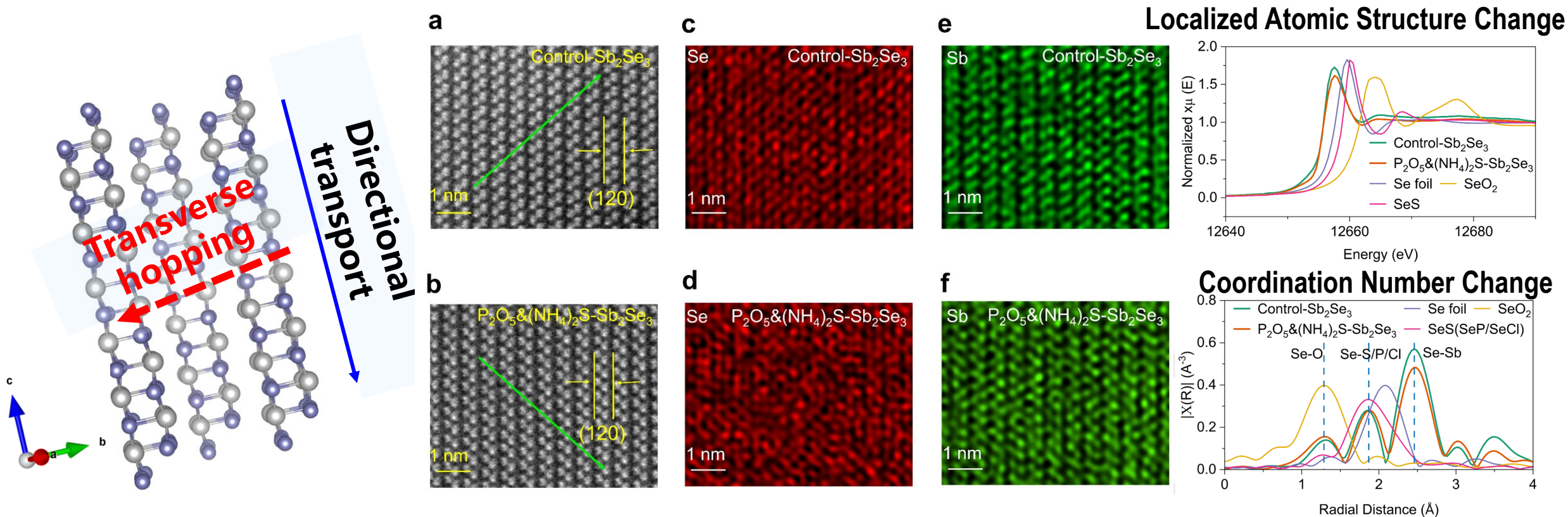


Table 1 | Optoelectronic parameters of the CT and SS devices

Sample	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
CT	660.94 (660.18 $\pm$ 3.48)	22.71 (22.44 $\pm$ 0.43)	66.09 (65.36 $\pm$ 2.02)	9.92 (9.68 $\pm$ 0.33)
SS	639.41 (634.02 $\pm$ 10.39)	24.96 (24.92 $\pm$ 0.69)	69.02 (67.36 $\pm$ 2.50)	11.02 (10.64 $\pm$ 0.48)

Beyond Crystallinity: Cross Bonding Between $(\text{Sb}_4\text{Se}_6)_n$ Ribbons

The introduction of P_2O_5 leads to contraction of crystal lattice, enables cross-link of the ribbons by P-Se chemical bond, finally resulting additional carrier transporting efficiency



Che,..., Zheng,* Tang,* Chen,* **Angew. Chem. Int. Ed.** 2025, e202425639.

Device Performance of P₂O₅-doped Sb₂Se₃ Solar Cell

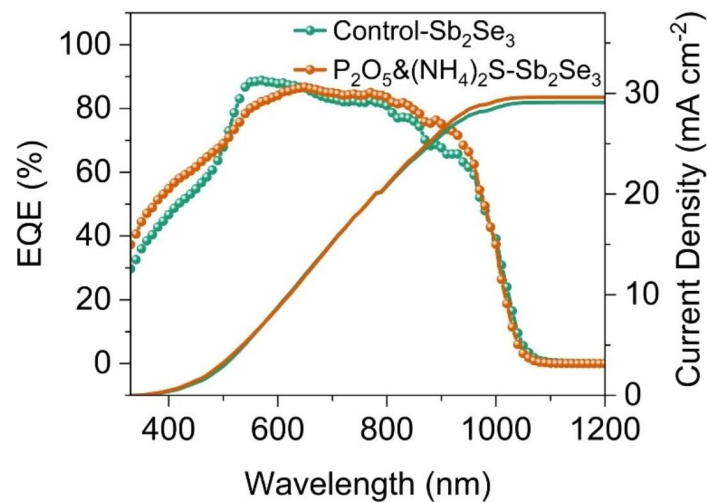
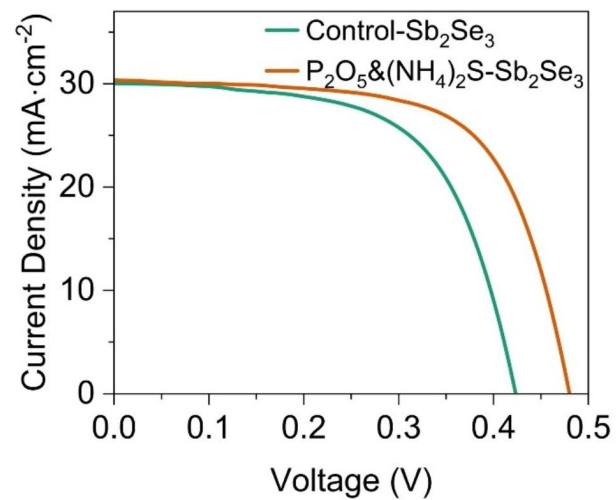
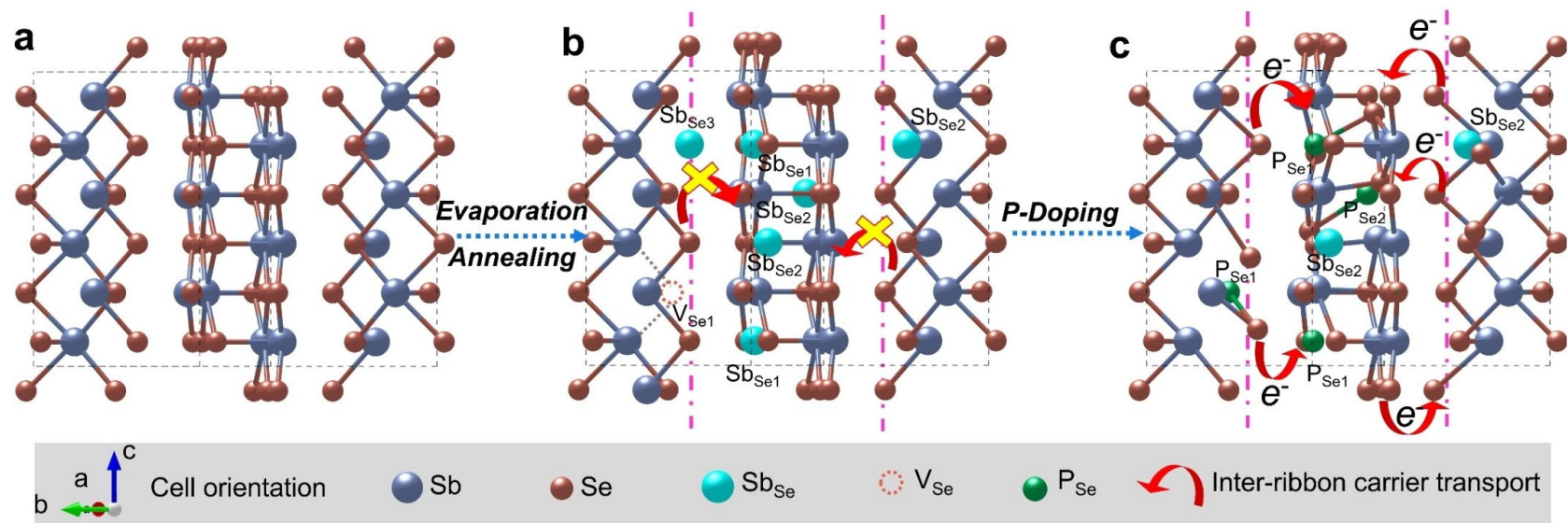


Table 3: Photovoltaic performance parameters of the devices.

Films	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
Control-Sb ₂ Se ₃	423	30.02	61.32	7.79
(NH ₄) ₂ S-Sb ₂ Se ₃	438	29.33	63.47	8.16
P ₂ O ₅ -Sb ₂ Se ₃	454	28.34	62.81	8.08
P ₂ O ₅ &(NH ₄) ₂ S-Sb ₂ Se ₃	469	30.33	66.72	9.50

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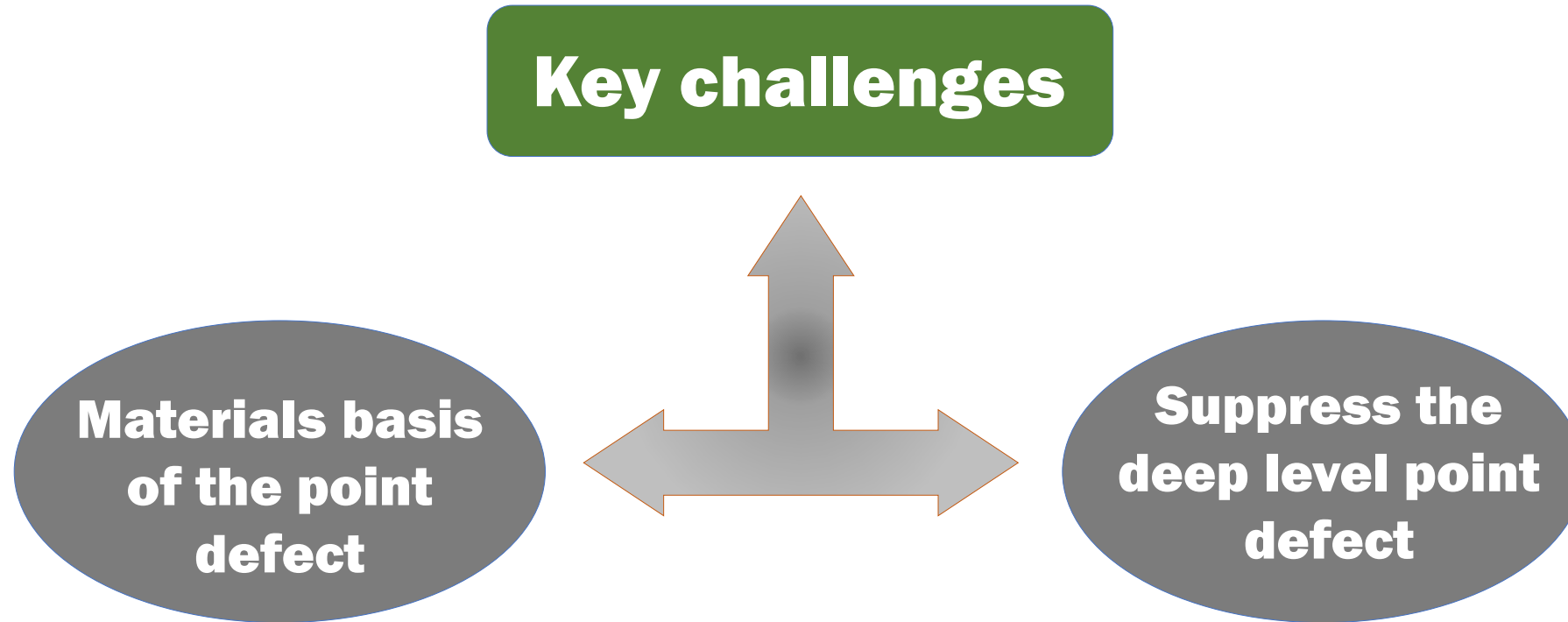
Recent Research

- Thin Film Fabrication
- **Defect Engineering**
- Device Structure Design

3

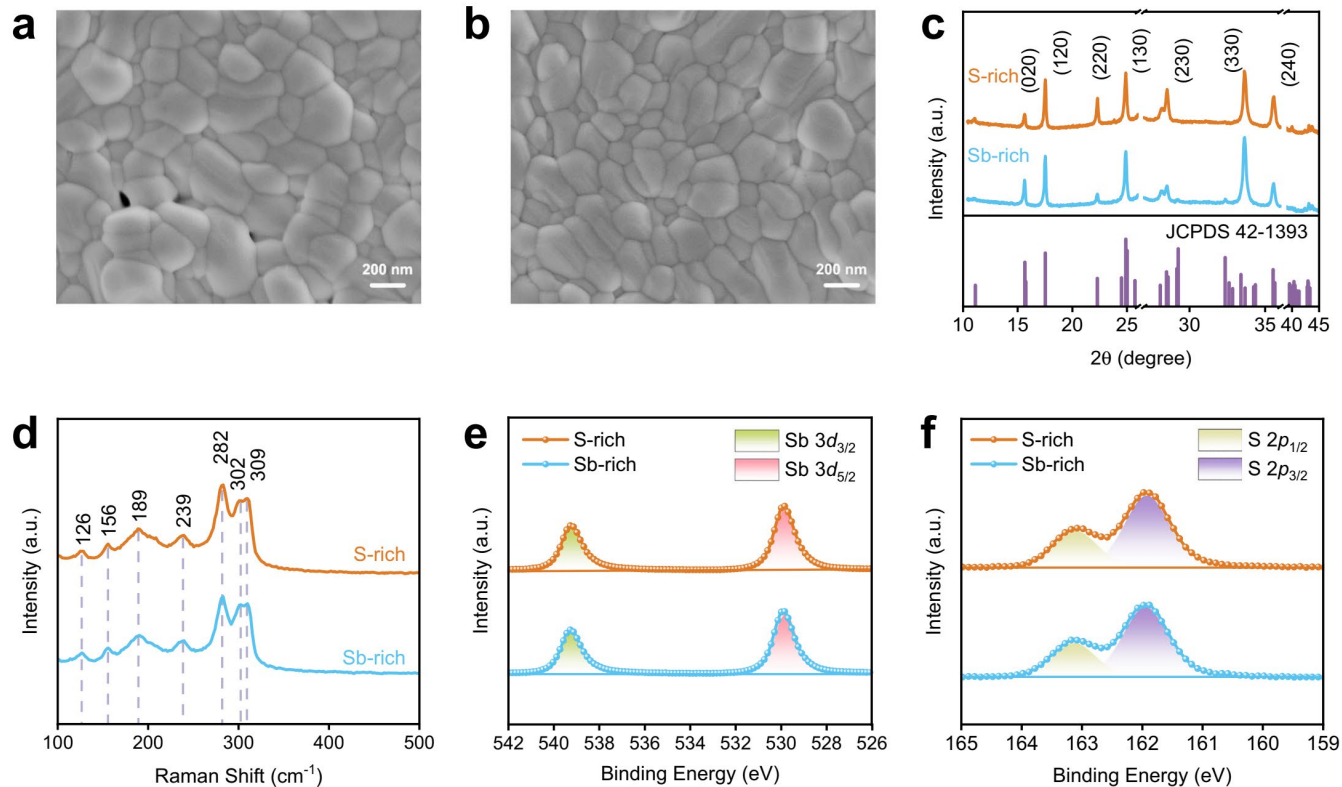
Conclusions and Outlook

Key Challenges in Defect Investigations

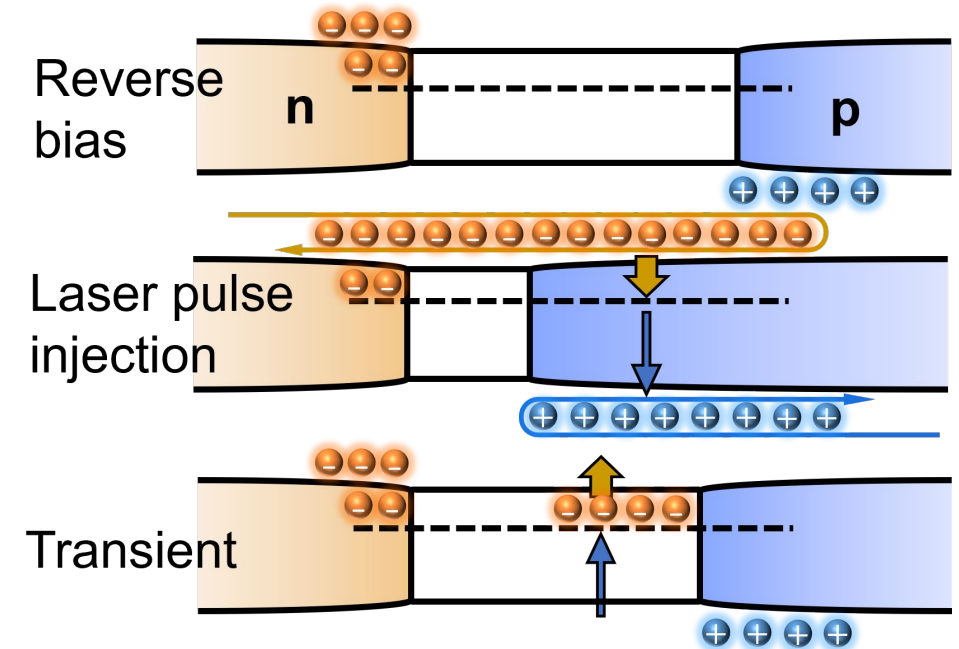


Preparation of High-Purity Sb_2S_3

Using Sb_2S_3 , S, and Sb as the reaction precursor, vapor deposition method



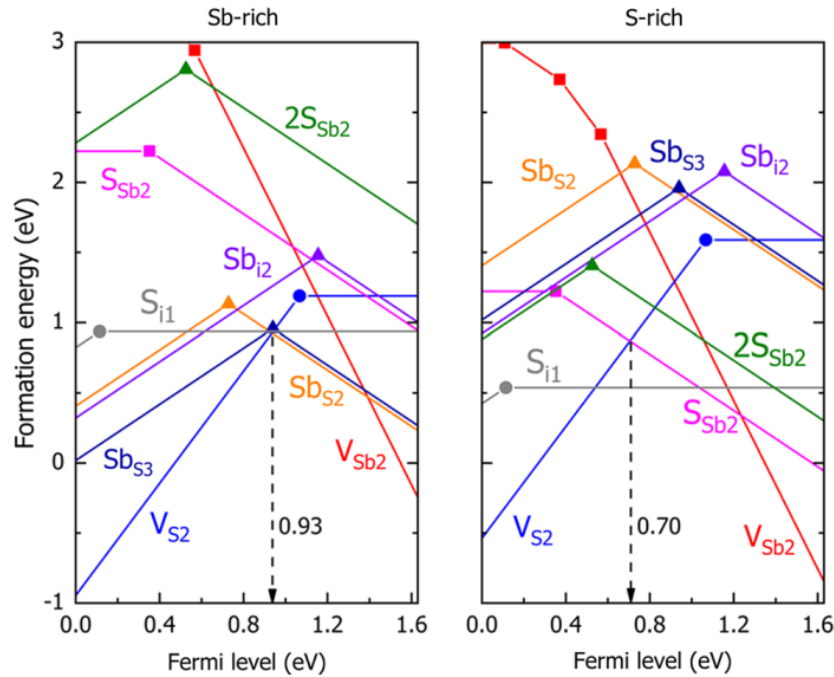
Defect Level Transient Spectroscopy



W. T. Lian,..., T. Chen,* *Nat. Commun.*, 2021, **12**, 3260.

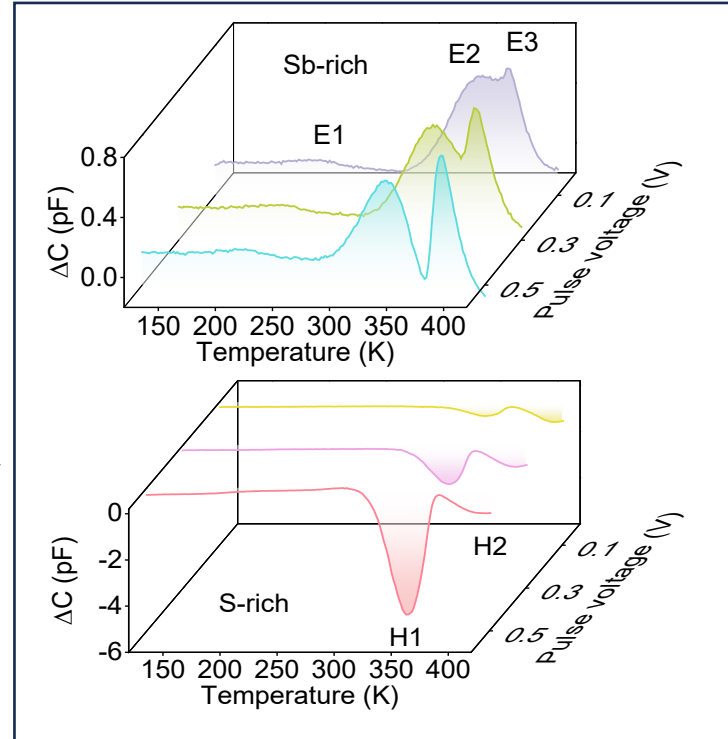
Defect Identification

The correlation between cation/anion ratio and defect characteristics in Sb_2S_3 film



Theoretical
calculation

Experimental
Results

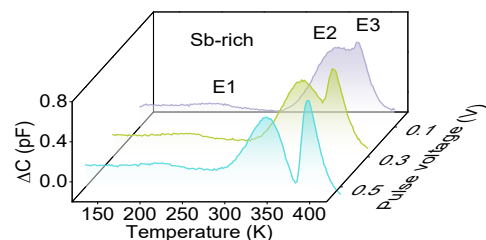


Ref: (Shiyu Chen, FDU) *Solar RRL*, 2019, 1900503.

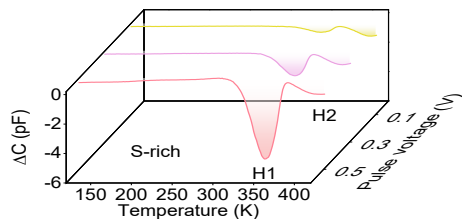
1. **Sb-rich Sb_2S_3** : Sb_{S} antisite, Sb-interstitial (Sb_{i}), S-vacancy (V_{S})
2. **S-rich Sb_2S_3** : V_{Sb} , S_{Sb} (only two kinds of defects)

The Unique Defect Property

Sb rich-Sb₂S₃: Sb_S, Sb_i, V_S



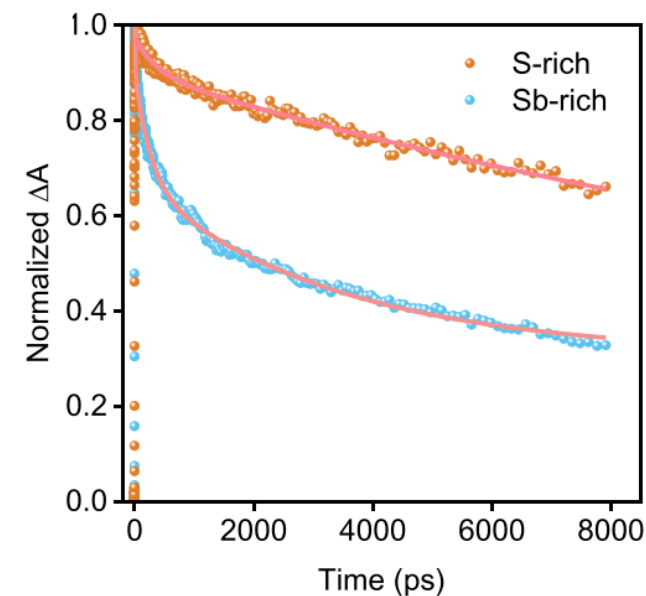
S rich-Sb₂S₃: V_{Sb}, S_{Sb}



Defect tolerance

$$\tau = (v_{th} \sigma N_T)^{-1}$$

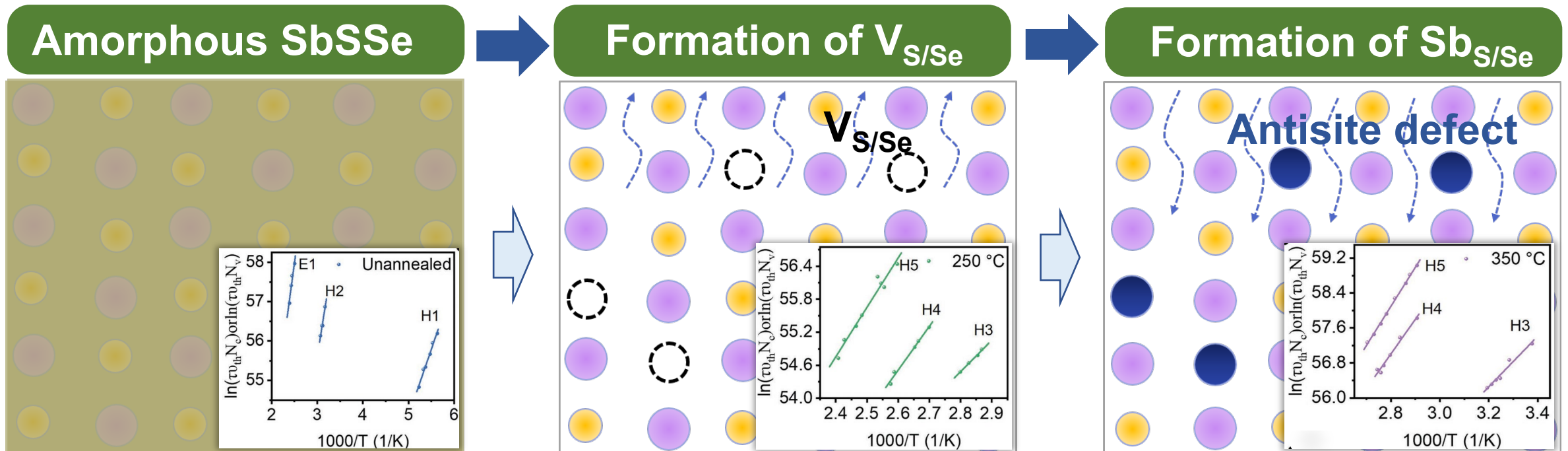
Materials	Point defect	Carrier lifetime (ns)
Sb-rich Sb ₂ S ₃	V _S	64.6
	Sb _S	28.4
	Sb_i	2180
S-rich Sb ₂ S ₃	V _{Sb}	48.3
	S _{Sb}	997



Different from 3D materials, the 1D chain-like materials show **tolerance to interstitial defect**, providing unique opportunity for tailoring optical and electrical properties

Defect Evolution

Annealing temperature-dependent defect study method, discovering the formation mechanism of anti-site defect $\text{Sb}_{\text{S/Se}}$ (**vacancy defect**→**anti-site defect**)

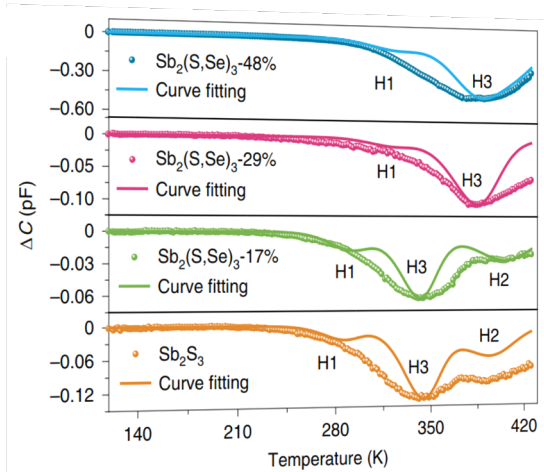


B. Che,..., T. Chen,* *Adv. Mater.*, 2022, **34**, 2208564.

Defect Passivation

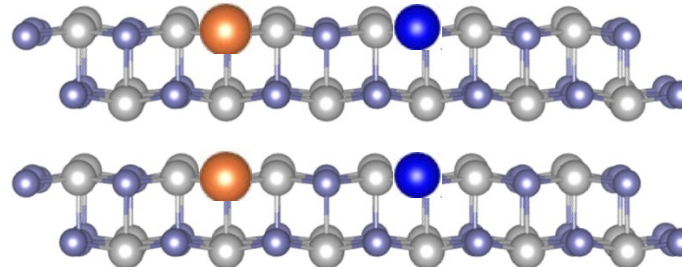
Taking advantage of radius and reaction activity of chalcogens

• Ion-replacement (Se/S)

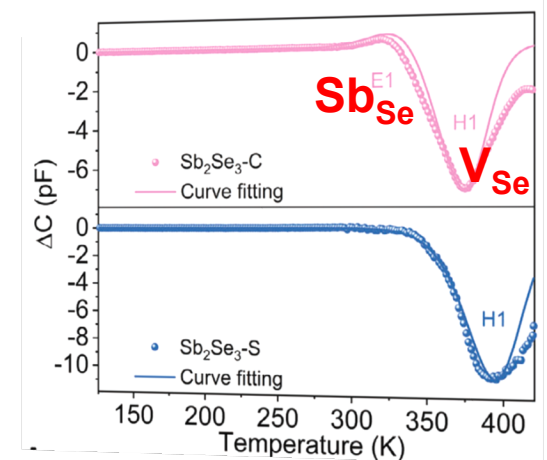


Reduce Sb_S

Reduce V_Se



• S, O passivation



Z. Y. Cai,..., T. Chen,* *Adv. Mater.*, 2024, **36**, 2404826.

Defect Formation and Passivation

ACCOUNTS

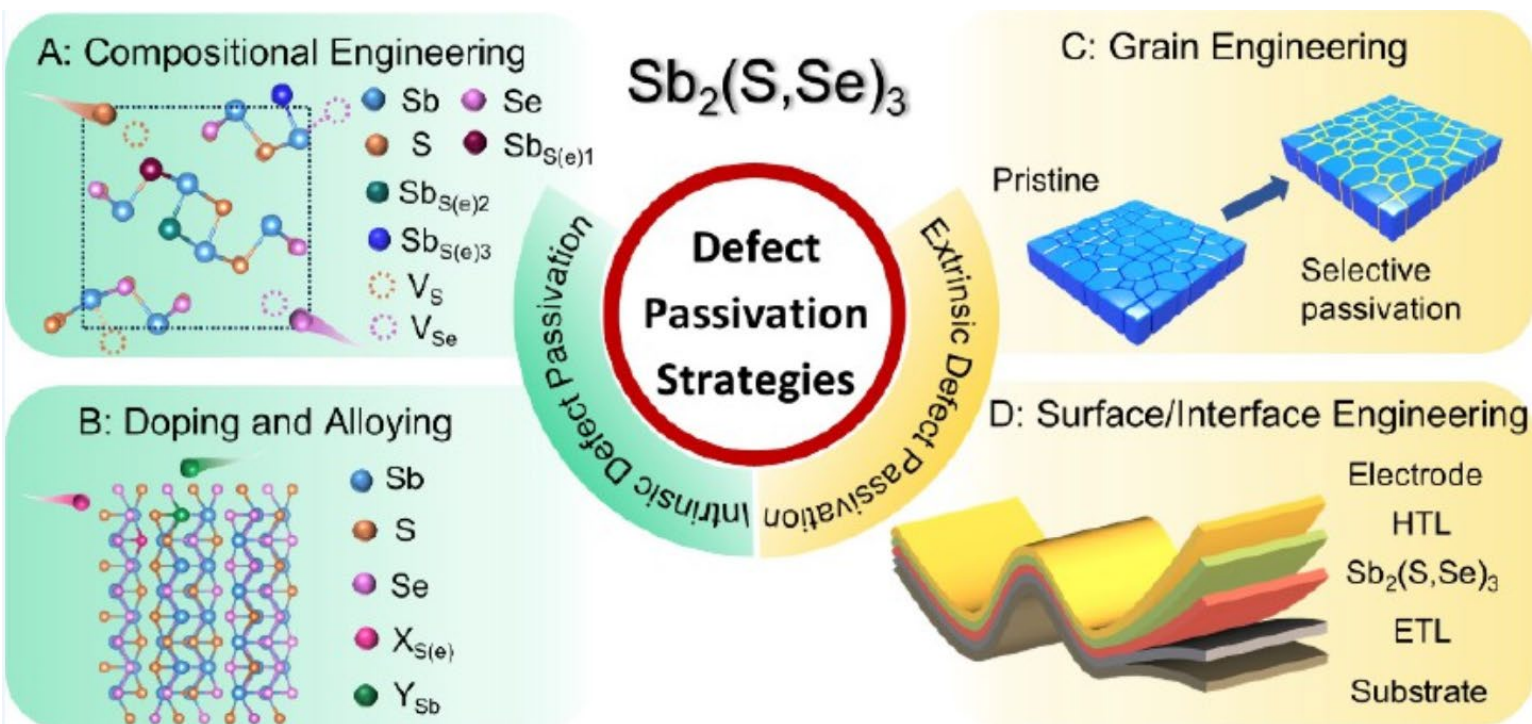
of chemical research

pubs.acs.org/accounts

Article

Unique Defect Characteristics of Antimony Chalcogenide Photovoltaic Materials

Xiaoqi Peng, Zichen Ruan, Changfei Zhu, Shangfeng Yang, and Tao Chen*



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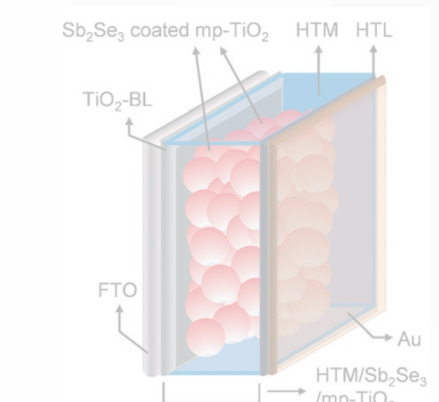
Conclusions and Outlook

p-SbSSe-n Device Structure

Developed ***p-SbSSe-n planar heterojunction*** device structure, which is currently the widely applied high efficiency device structure

Conventional Device Structure

mesoporous structure



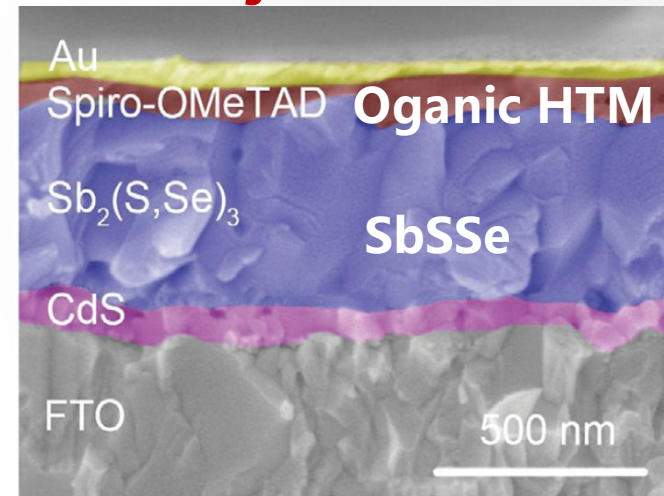
Ref: *Angew. Chem.* 2014.

metal-semiconductor



Ref: *Nat. Energy* 2017.

p-SbSSe-n planar heterojunction



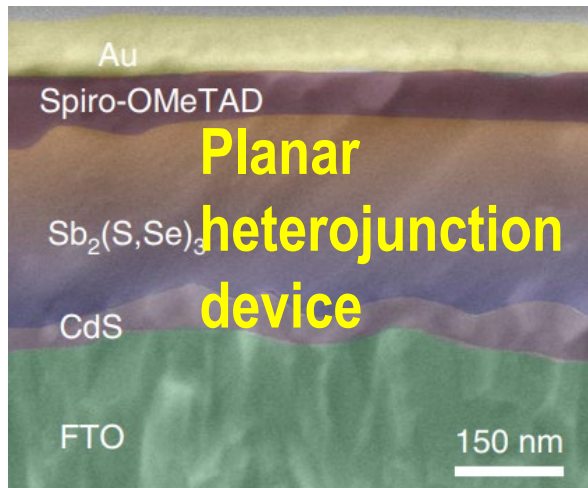
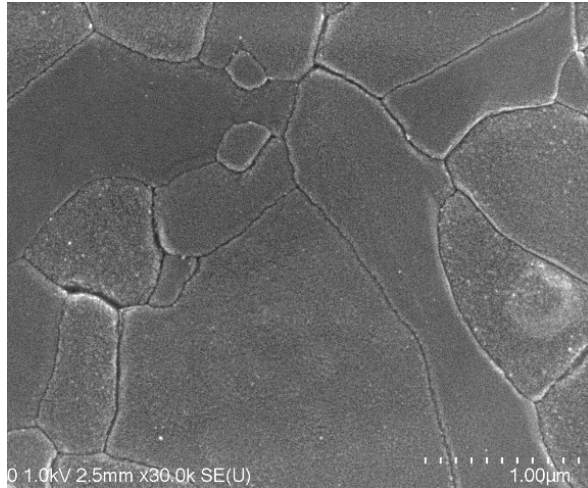
Metal
P-HTM
SbSSe
N-ETM
FTO

Jiang, ..., Tang,* Chen,* *Energy Environ. Sci.*, 2021, 14, 359.

Wang, ..., Chen,* *Nanoscale* 2017, 9, 3386-3390.

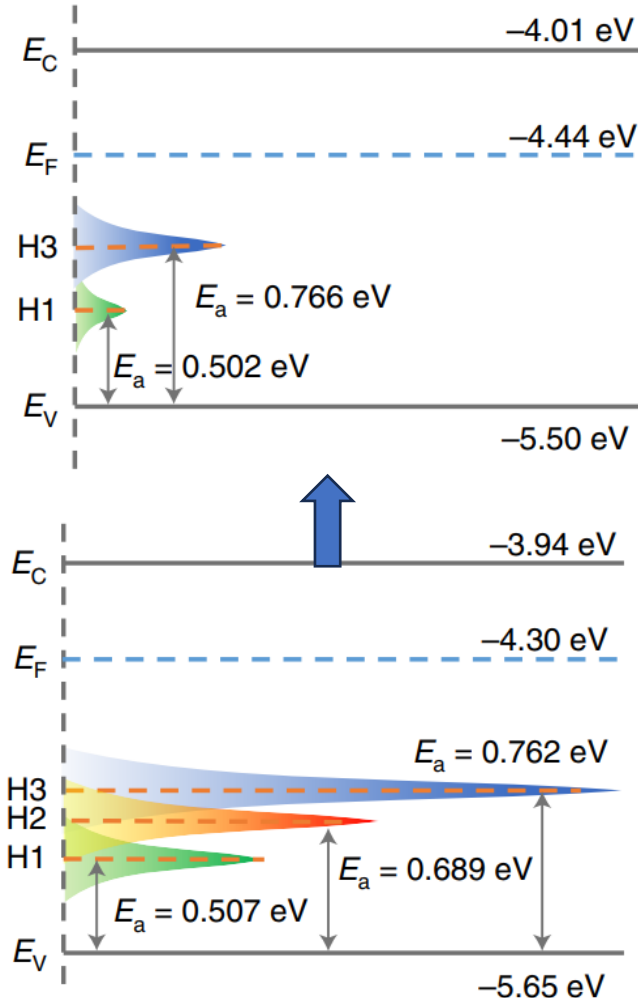
Efficiency Breakthrough: new device structure + hydrothermal deposition

$\text{Sb}_2(\text{S,Se})_3$ Film



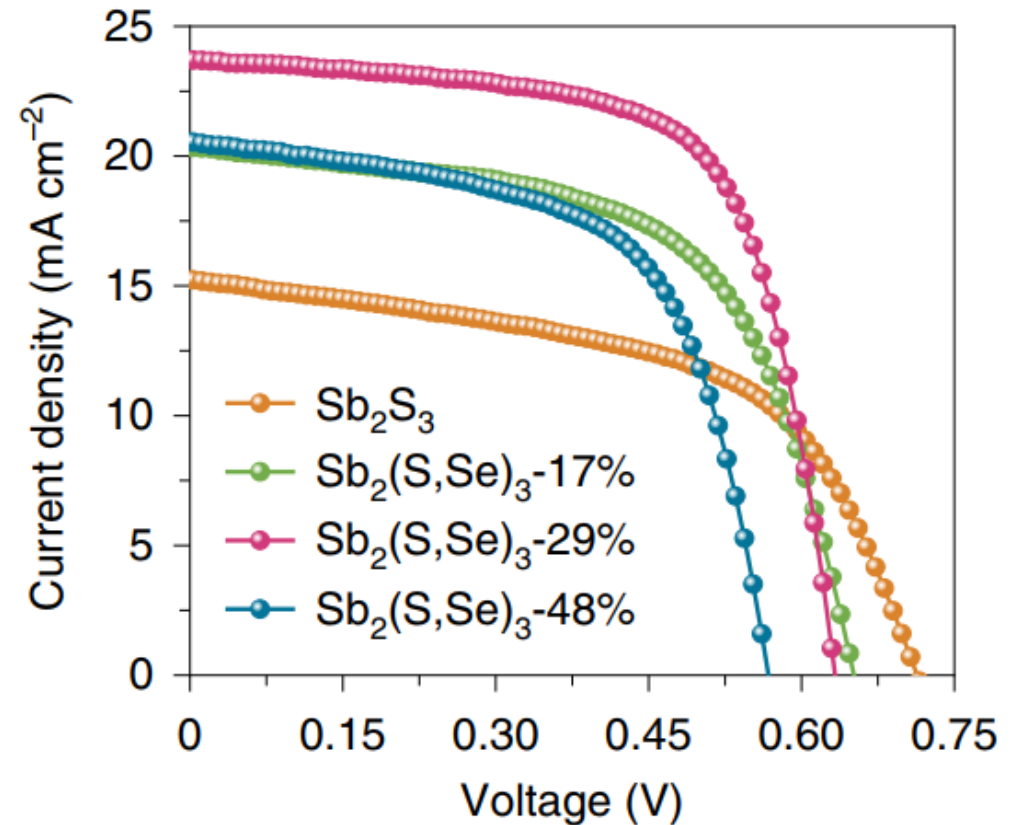
Planar heterojunction device

Low Defect

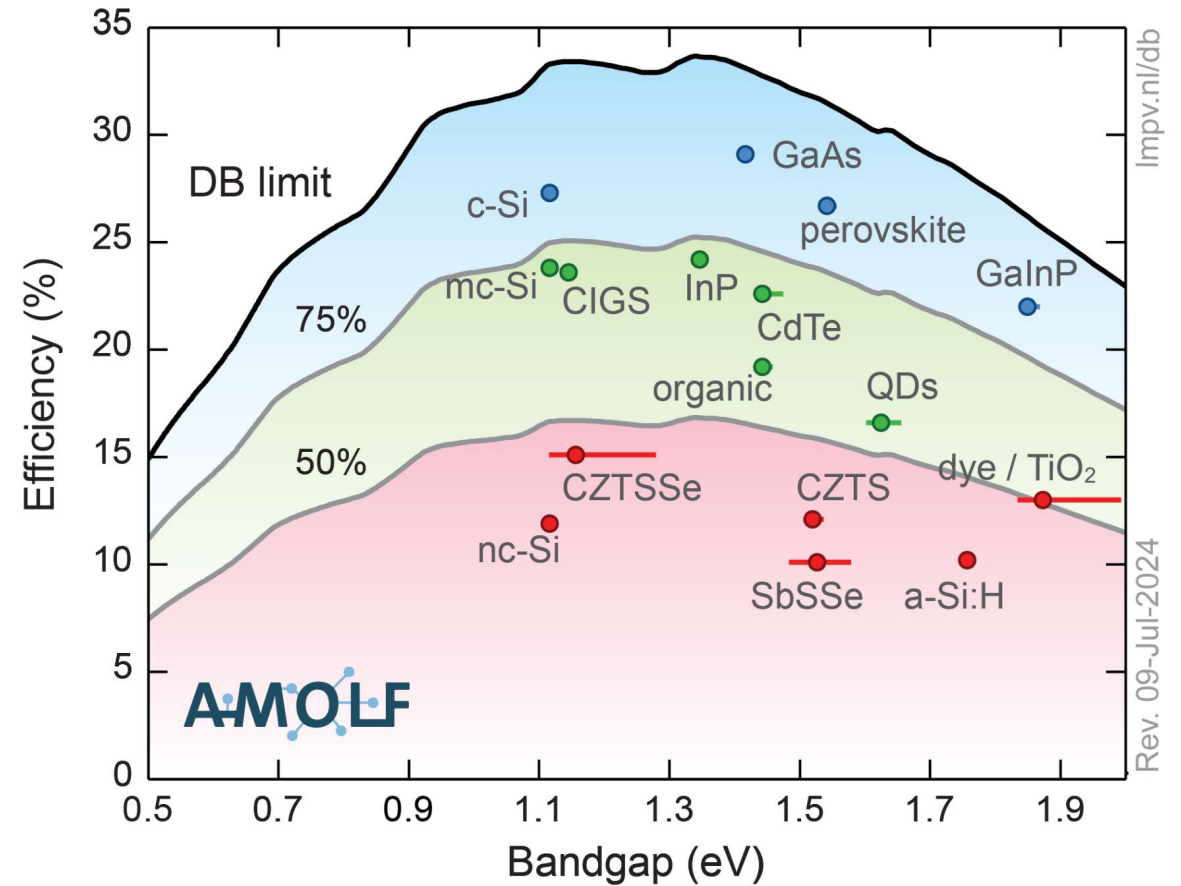
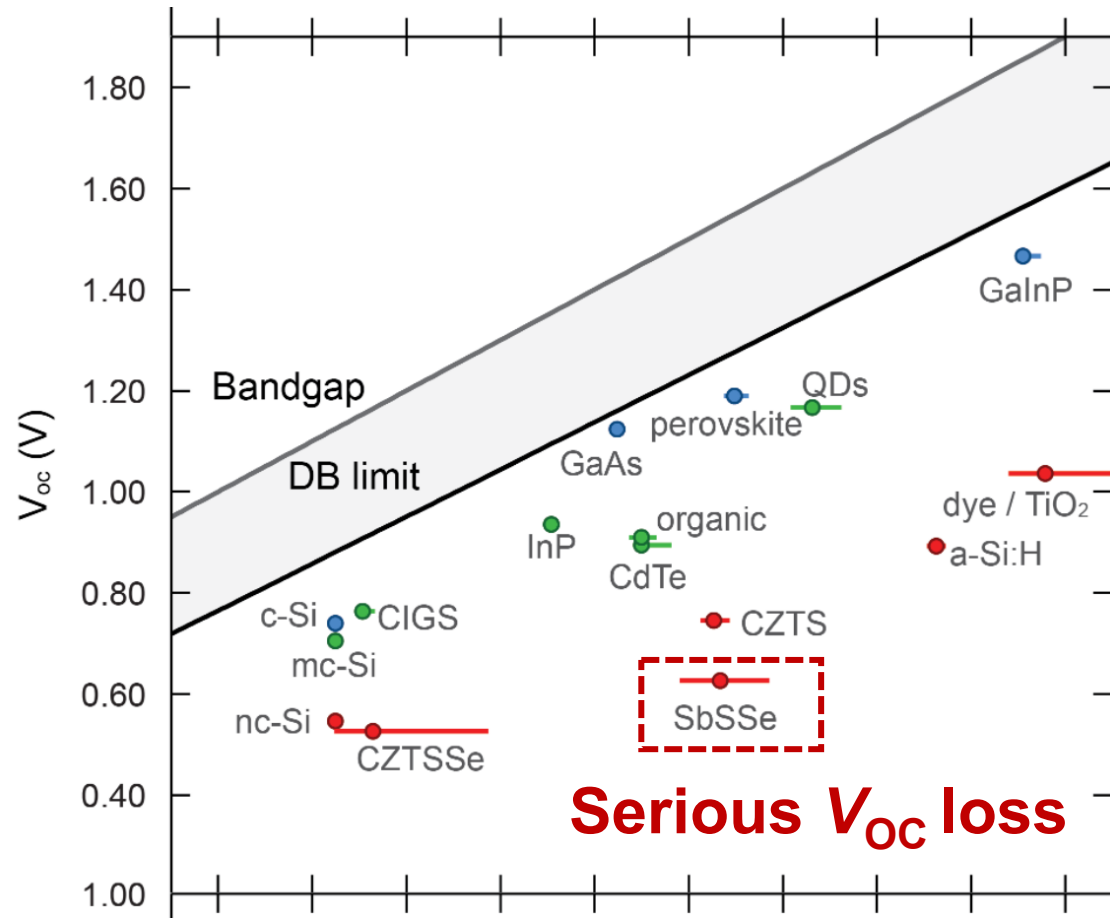


10% landmark efficiency

• *Nat. Energy* 2020, 5, 587.



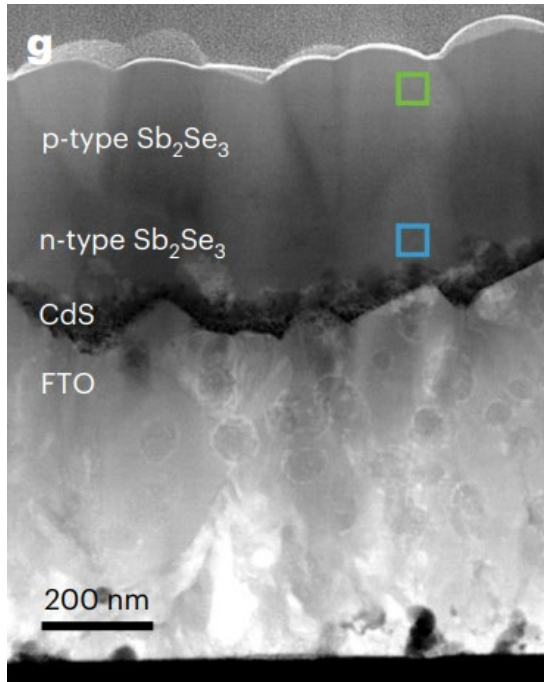
V_{OC} Loss in Sb_2Se_3 Solar Cells



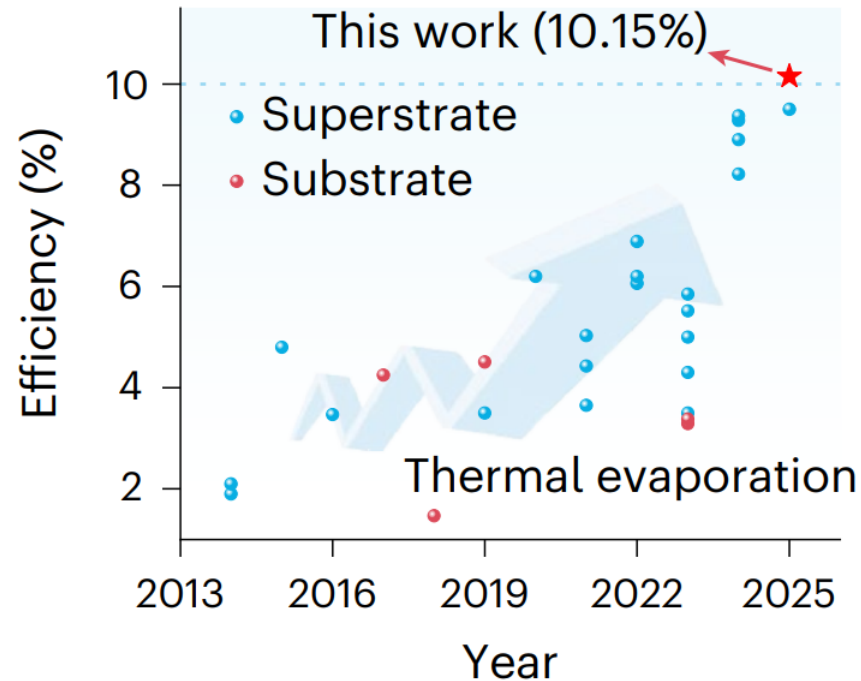
The way to improve V_{OC} : reducing recombination & enhancing internal field

Internal Homojunction Structure

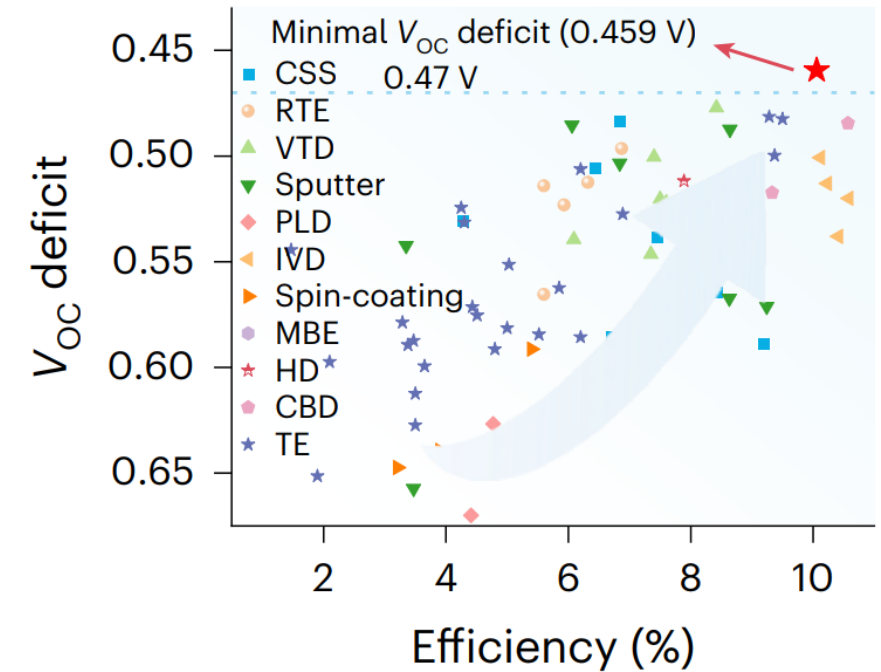
Internal Homojunction $p\text{-Sb}_2\text{Se}_3/n\text{-Sb}_2\text{Se}_3$



High Power Conversion Efficiency



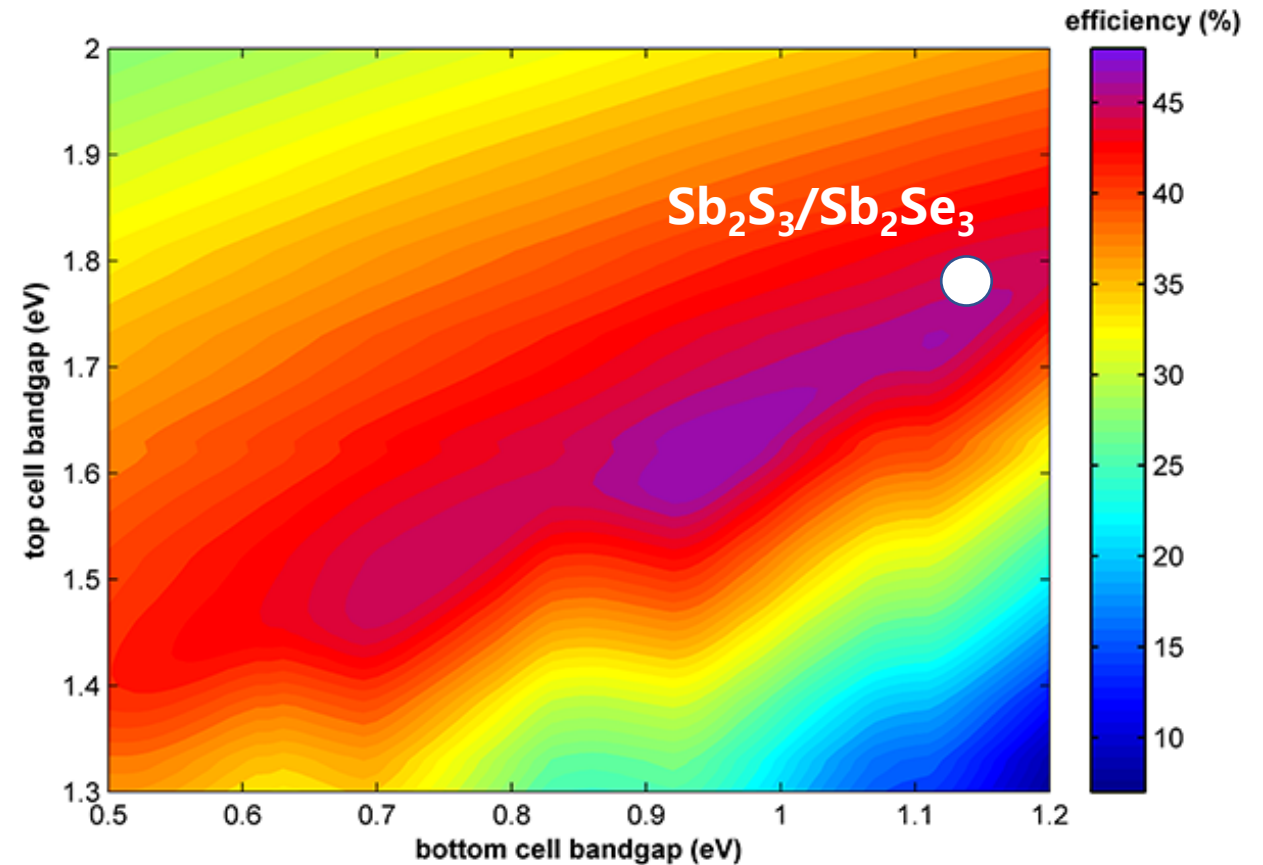
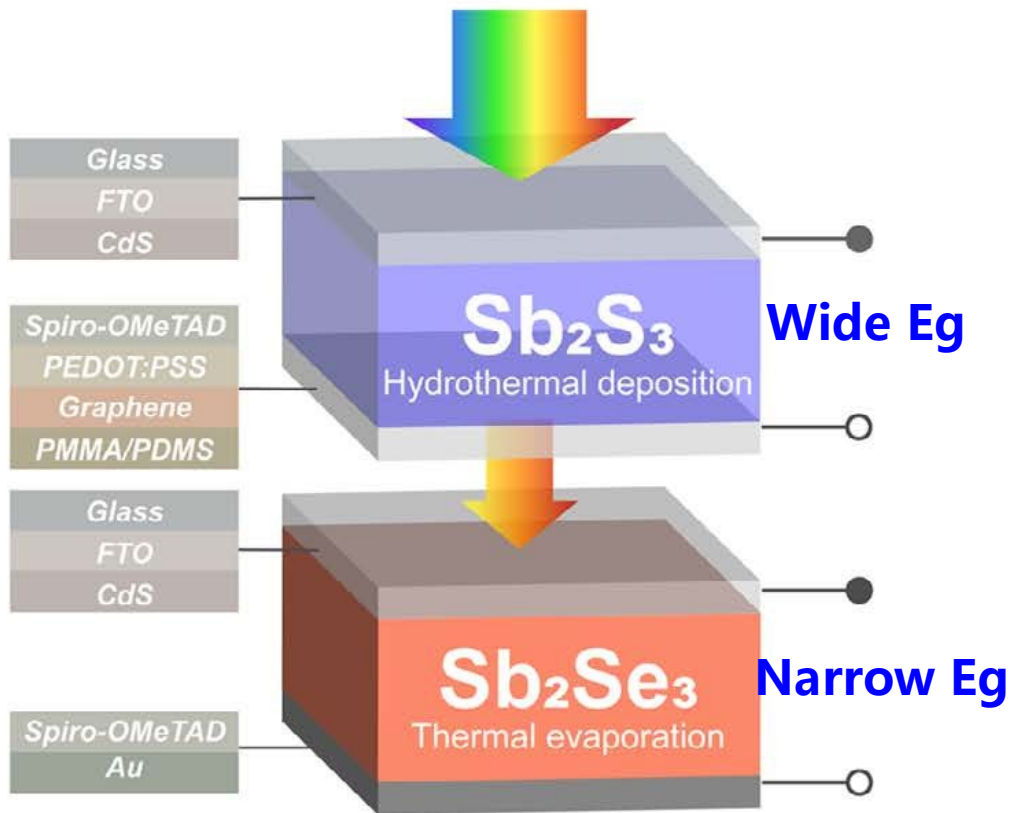
Low V_{OC} Loss



Yang, ..., Tang,* Chen,* *Nature Photonics* 2026, **20**, 644.

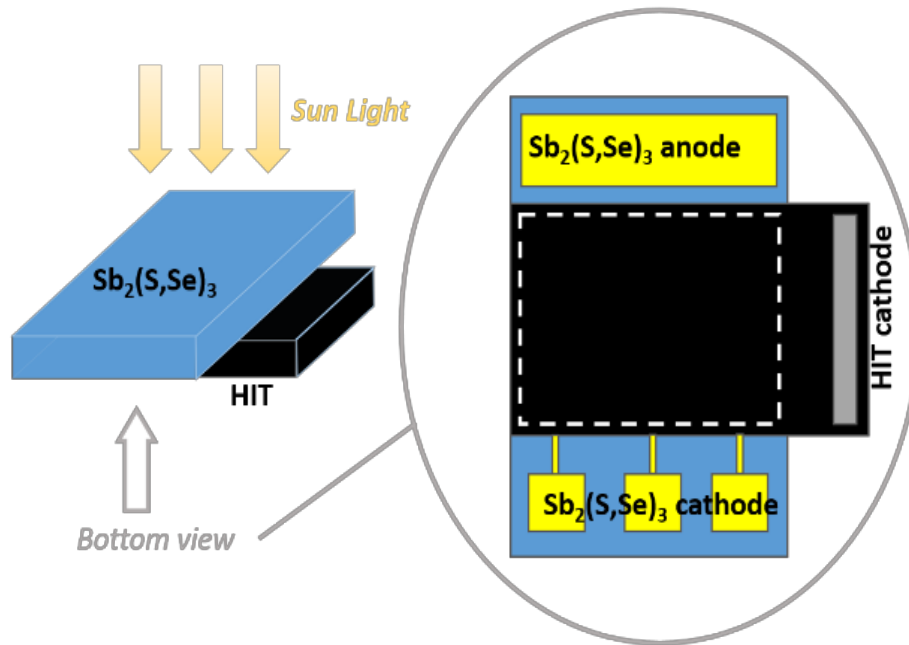
Tandem Device

Perfect bandgap: Sb_2S_3 : 1.8 eV, Sb_2Se_3 : 1.1 eV

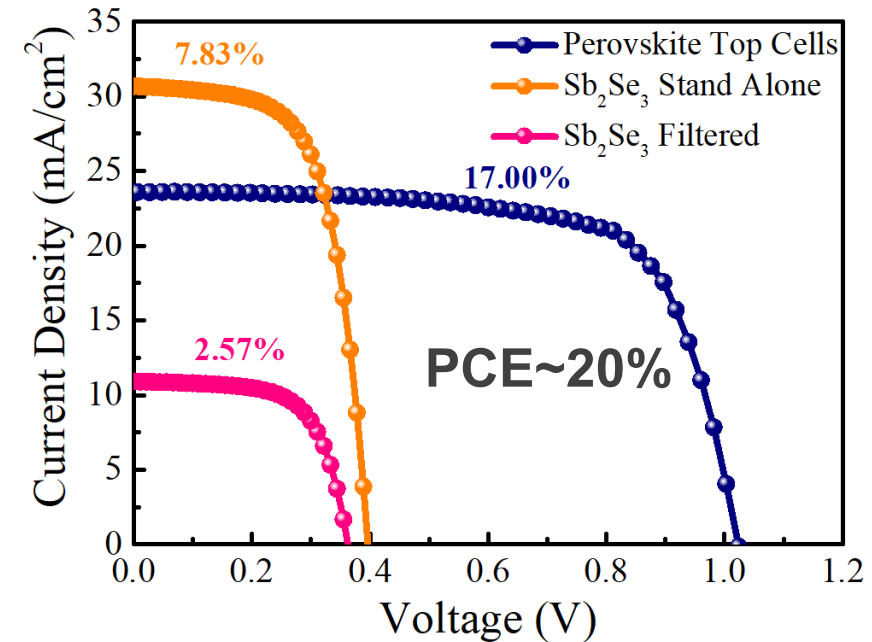


Tandem Device with Si and Perovskite

SbSSe/Si



SbSSe/Perovskite



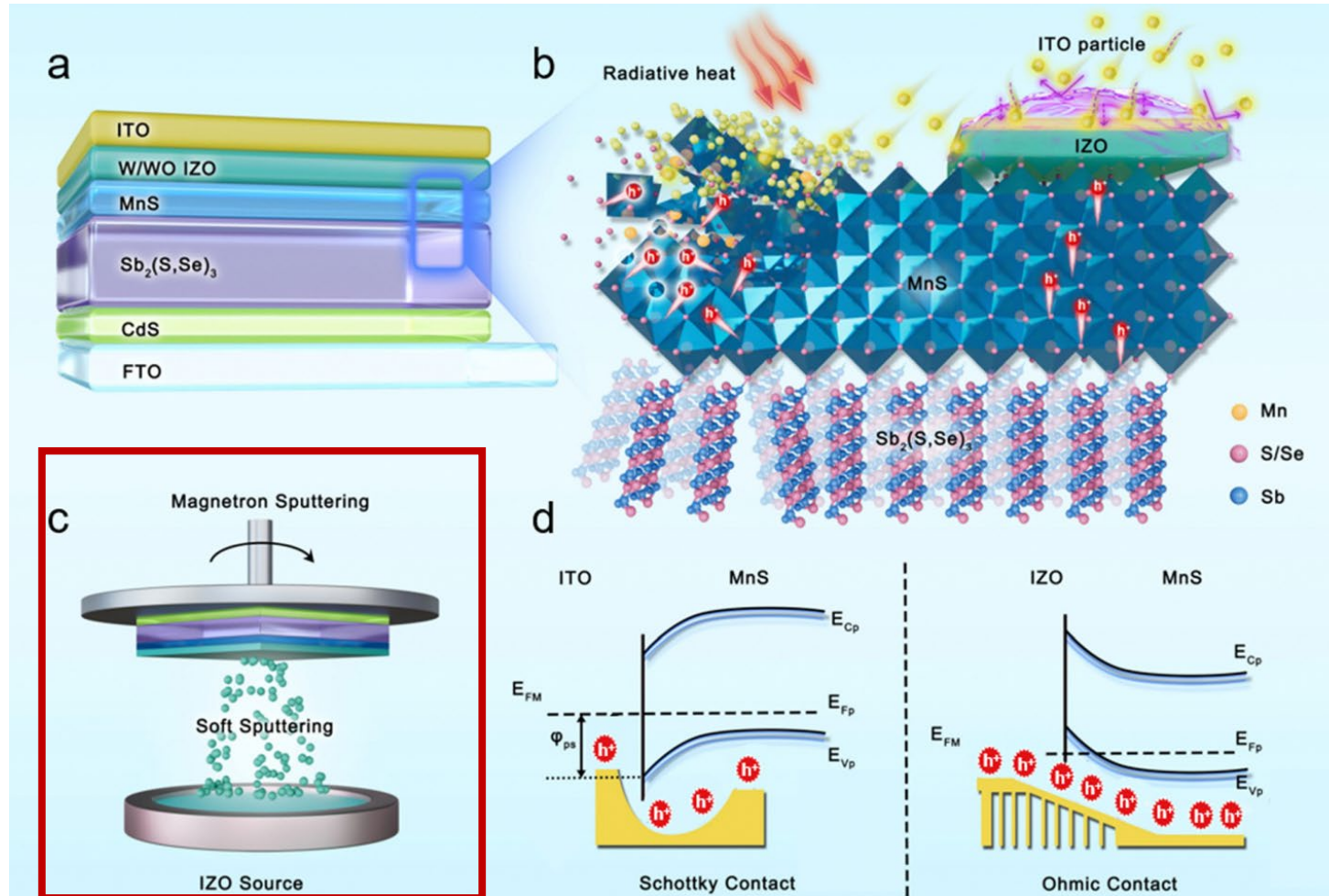
C. Qian,..., B. Hoex,* T. Chen,* X. J. Hao,* **Adv. Mater.** 2023, 2303936. (with Si)

J. W. Zhang, ..., T. Chen,* **Solar RRL**, 2020, 2000048. (All antimony)

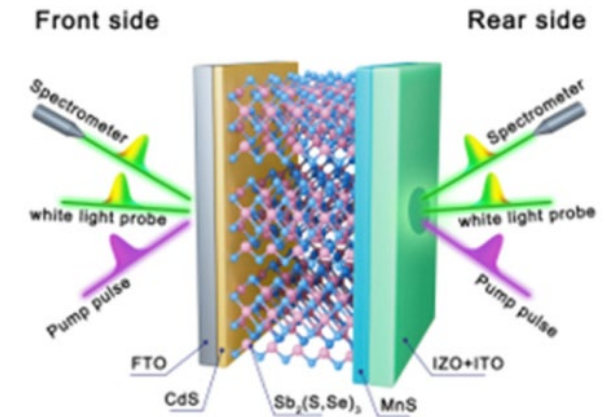
Z. Y. Cai, ..., T. Chen,* **Energy Mater. Device**, 2024, accepted. (with perovskite)

All Inorganic Device

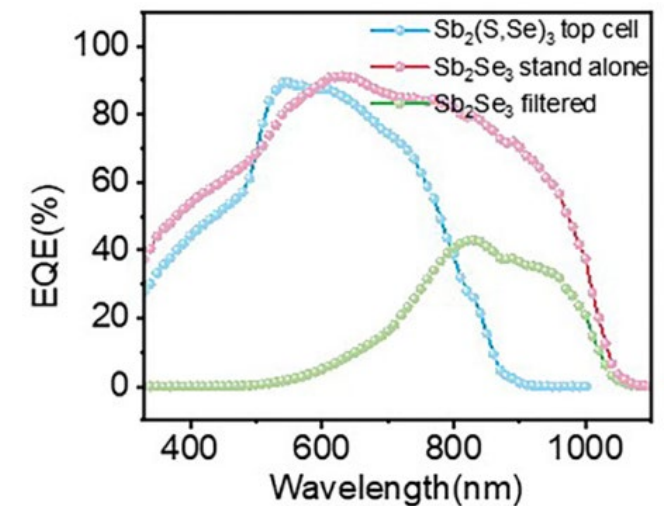
Soft sputtering to alleviate the interfacial damage



Bifacial Solar Cell



Tandem Solar Cell



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Conclusions and Outlook

Conclusions and Outlook

1. The **crystallinity** is not high enough, which generates high transport resistance, either increase the crystallinity or establish interconnection between ribbons to **enhance carrier transport** could further improve the device efficiency.
2. The device structure based planar heterojunction or internal homojunction seem efficient, more efficient hole transporting materials other than **Spiro-OMeTAD** is needed for enhancing the device stability (**all inorganic device** would be better).
3. The bandgap of Sb_2S_3 and Sb_2Se_3 are 1.7 and 1.1 eV, which provide **new opportunities for tandem device** applications with silicon, perovskite, etc..

Acknowledgment

Collaborators:



Group Member:



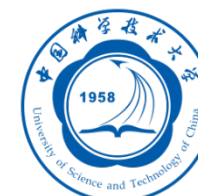
Financial Support



中华人民共和国科学技术部
Ministry of Science and Technology of the People's Republic of China



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Thank you!