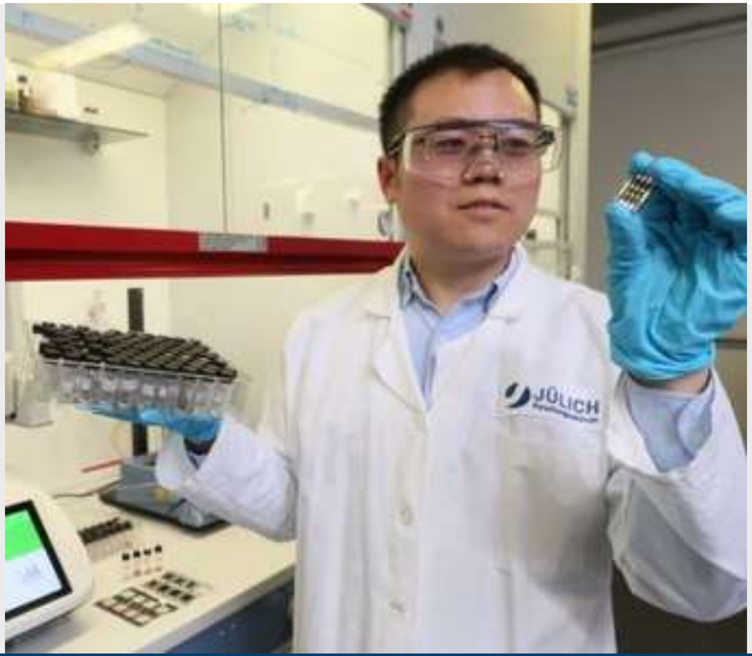
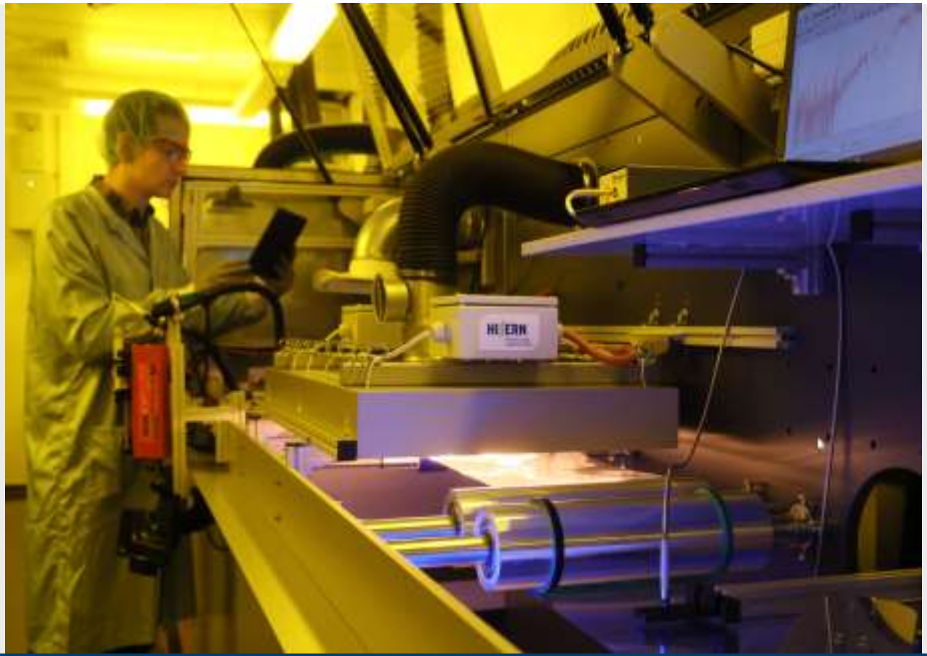




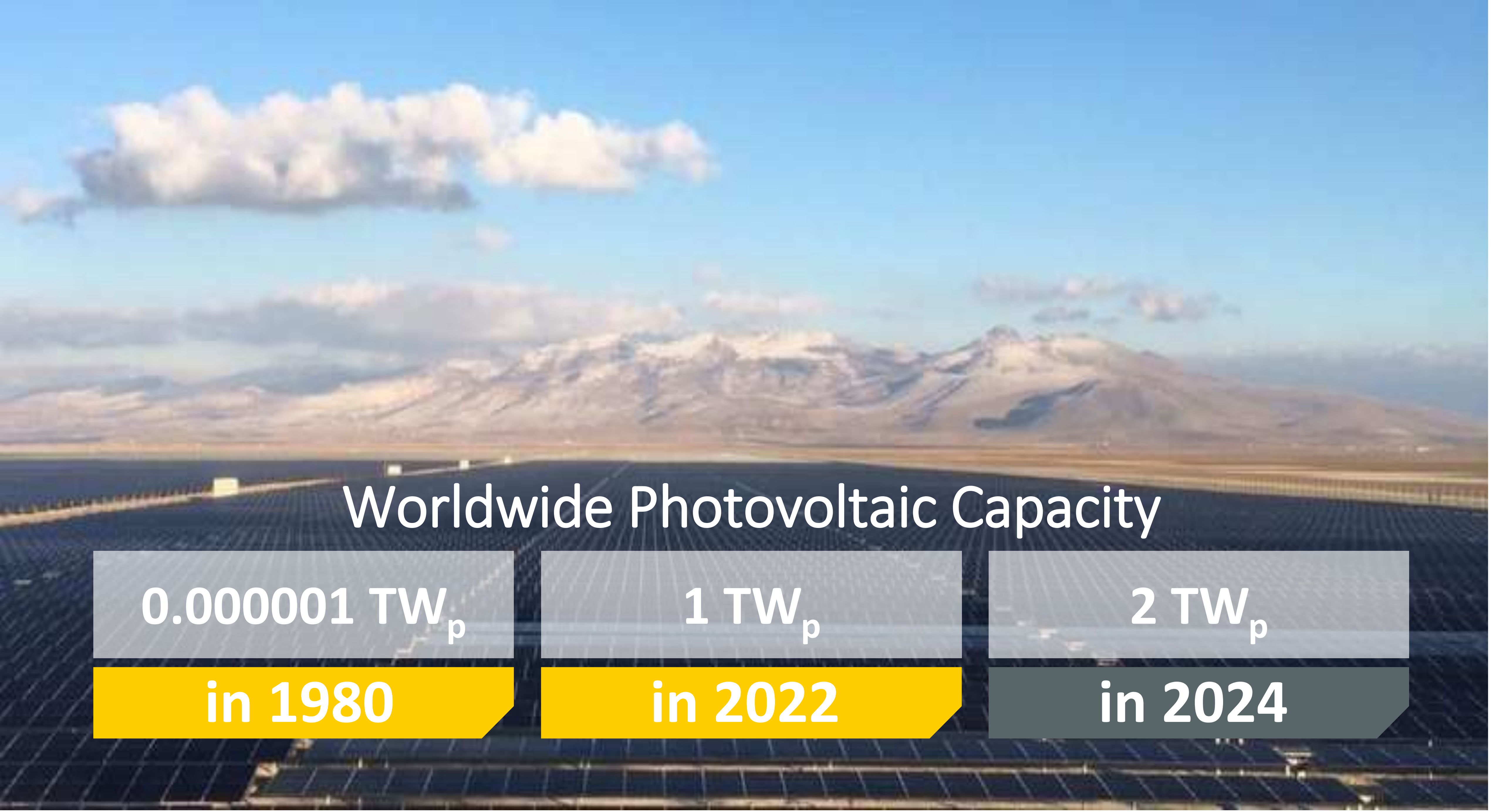

MATERIAL DISCOVERY STRATEGIES FOR EMERGING PHOTOVOLTAICS

WORKSHOP BETWEEN KAST AND LEOPOLDINA „PERSPECTIVES ON ENERGY TRANSITION“

SEOUL, JANUARY 14TH, 2025

CHRISTOPH J. BRABEC

JÜLICH
Forschungszentrum



Worldwide Photovoltaic Capacity

0.000001 TW_p	1 TW_p	2 TW_p
in 1980	in 2022	in 2024

Karapınar Solar Energy Plant, Konya, Turkey. 1,3 GWp on 20 km2 / J. Perlin, From Space to Earth, HARVARD UNIV PR; (2002) / P. Verlinden, J. Renewable Sustainable Energy 12, 053505 (2020)

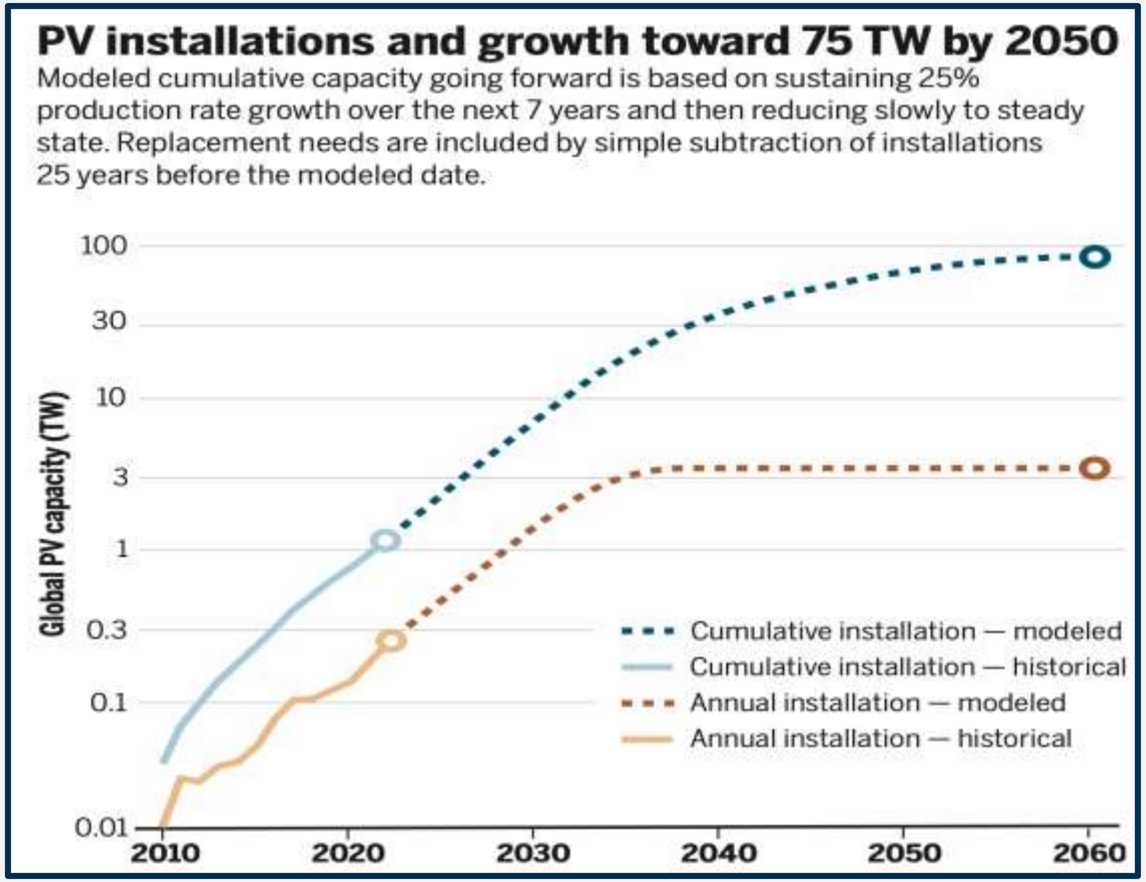
PV TOMORROW: SCALE

Photovoltaics has the power to transform the world´s energy system

2022 saw the first EU Solar Energy Strategy ever, similar in intent as other major economic blocks (US, China, India..):

- Climate change mitigation
- Security of supply / resilience
- Business opportunities

German federal government (BMWK) following up on the EU´s NZIA (net zero industry act)



Deutscher Bundestag Drucksache 20/1630 20. Wahlperiode 02.05.2022

Haegel et al, Science, 2024

PV TOMORROW: EFFICIENCY

Better use of available area for PV to meet 2050 Goals!

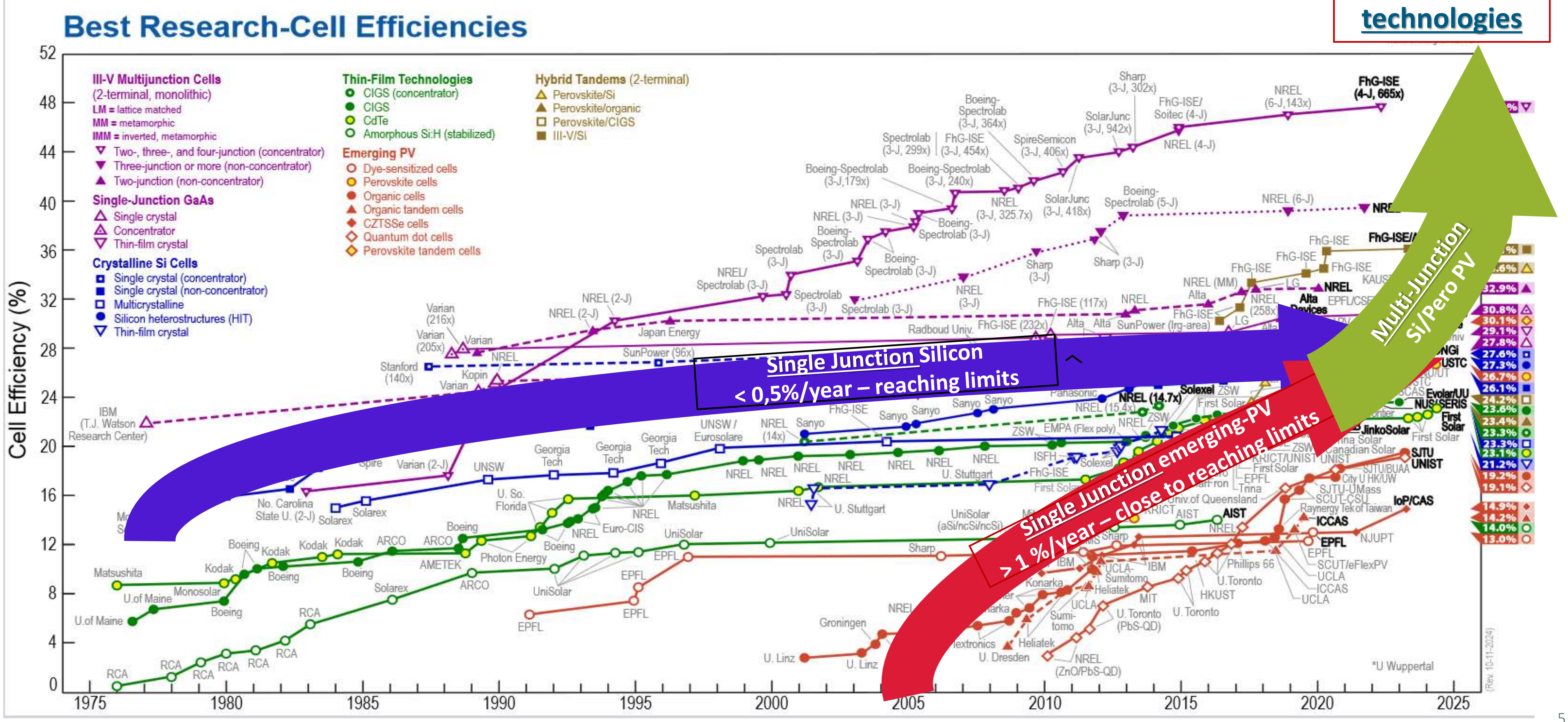
Key figures:

- Efficiency is the key driver for photovoltaics
- Everything is scaling with efficiency:
  - Costs
  - Materials Usage, Sustainability, Recycling
  - Area Usage: Until 2050, we need about 200.000 km^2 "active energy" area and more than 1.000.000 km^2 for energy landscapes
  - Integrability – use energy where you consume, alleviating pressure on grid and storage
- PV will and must improve towards higher efficiency and integrability.

EFFICIENCY: SCALABLE MULTI-JUNCTION PV

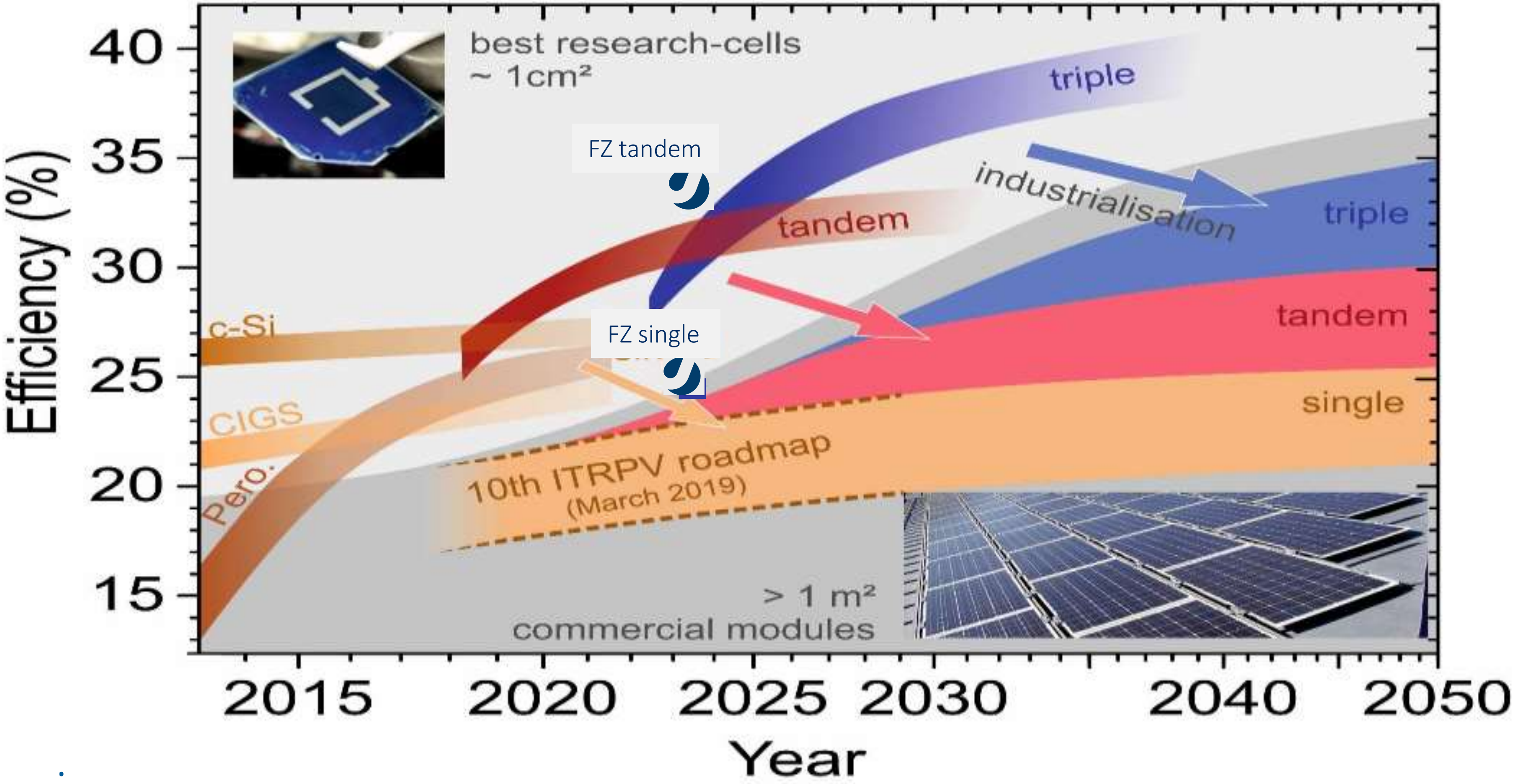
Emerging semiconductors have the potential to accelerate the photovoltaic roadmap

Scalable Multi-junction technologies



FZ STRATEGY IS WELL ALIGNED WITH POV IV

Synergistic cooperation between HZB, KIT and FZJ within MTET



S. Albrecht et al, Nature Energy 2017. This figure was as already presented at the POF IV defense

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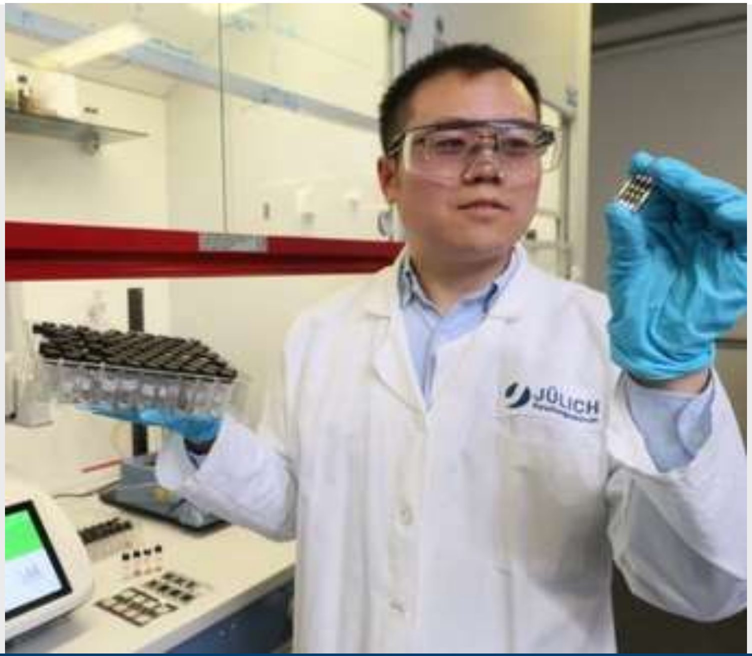

EXAMPLES ON RECENT RESEARCH: MATERIAL DISCOVERY

From **Materials** to Processes to Devices to Demonstration

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Acceleration of Emerging-PV Technologies

Shorten the time to the market by „discovering“ optimized materials and processes

Requires predictive models and inverse design of materials, processes and architectures

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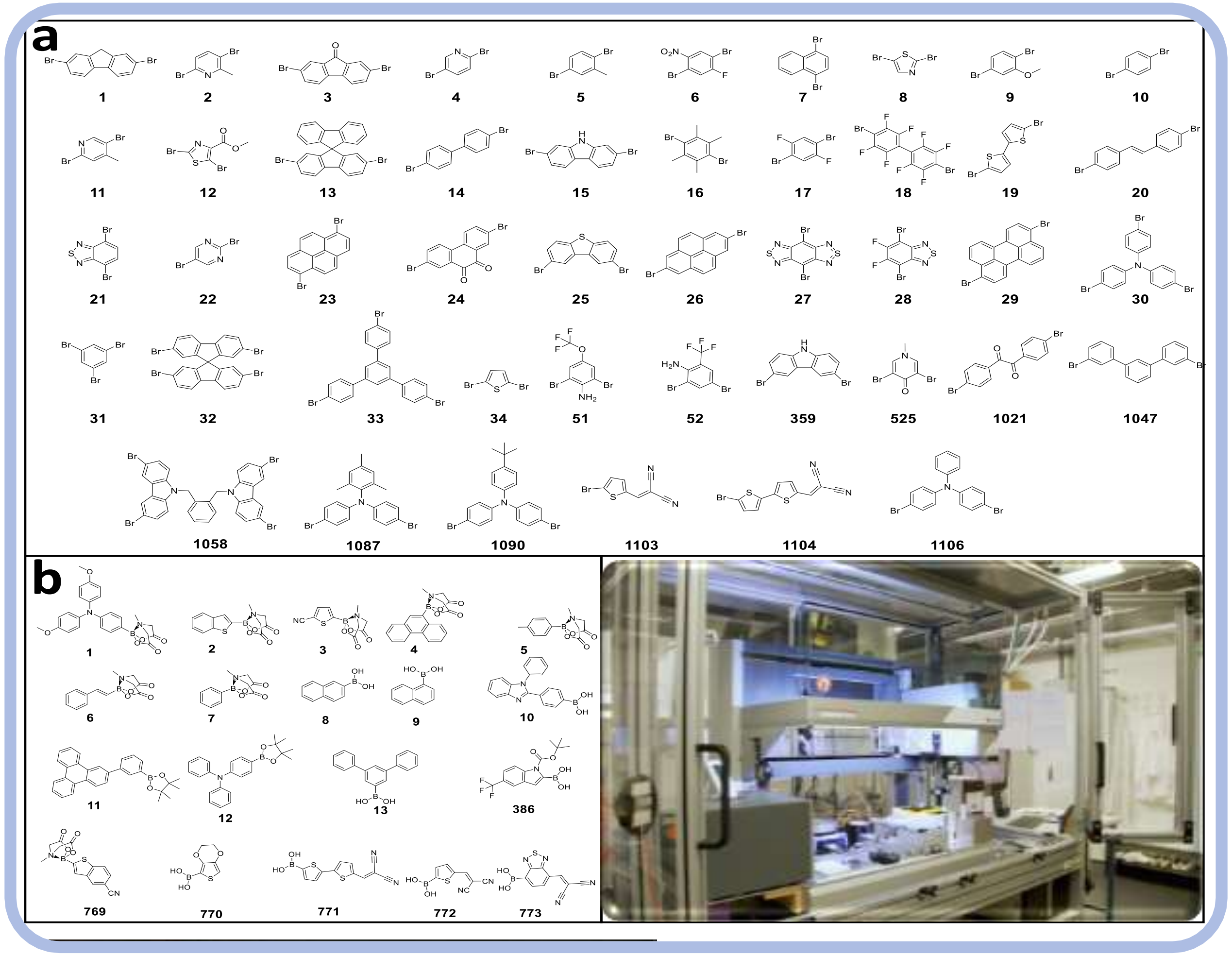
Example 1: A Materials Discovery Workflow

Microwave synthesis of MIDA compounds to build molecular libraries



- Automated synthesis of molecules:
- 1000 A & B candidates (for Suzuki)
- 10^6 molecules: B-A-B type
- 10^9 moelcules: C-B-A-B-C type

- Qualification by DFT
- Analysis by PL, UV/Vis, EC, SCLC,..
- Extended purity analysis
- Proven electronic quality

*J. **Wu** et al., An integrated system built for small-molecule semiconductors via high-throughput approaches, JACS 2023*

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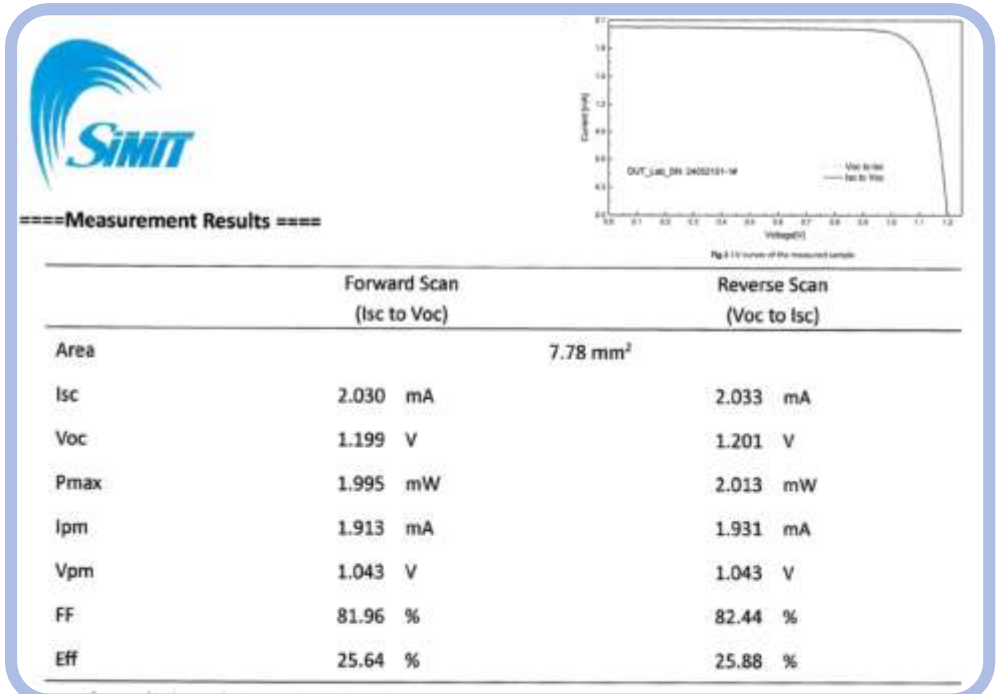
Example 1: A Materials Discovery Workflow

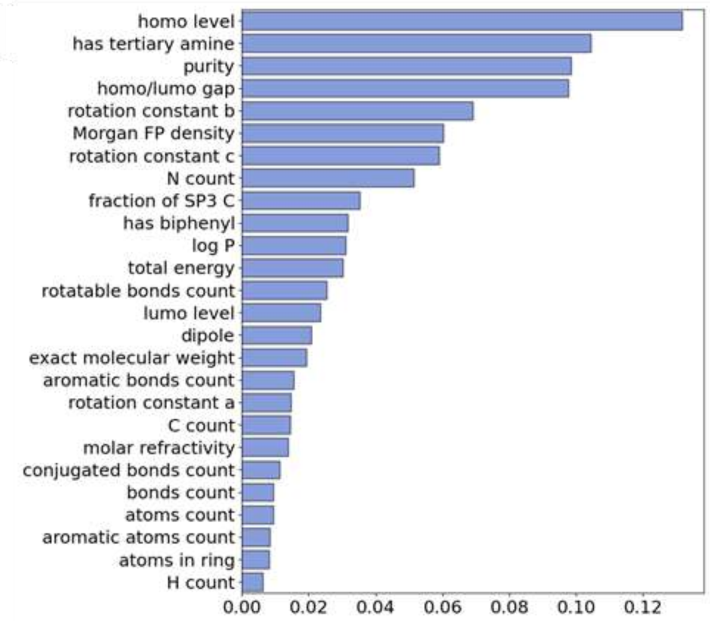
A Paradigm Change in Structure – Property – Functionality Relations

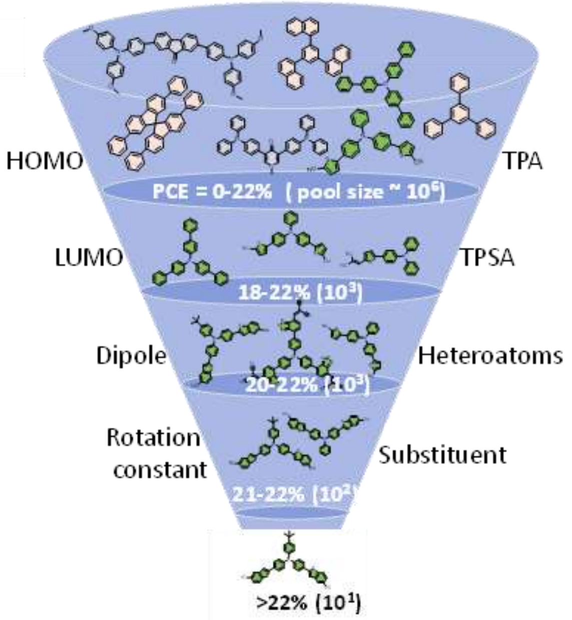


SiMIT

====Measurement Results ====

	Forward Scan (Isc to Voc)		Reverse Scan (Voc to Isc)	
Area		7.78 mm²		
Isc	2.030	mA	2.033	mA
Voc	1.199	V	1.201	V
Pmax	1.995	mW	2.013	mW
Ipm	1.913	mA	1.931	mA
Vpm	1.043	V	1.043	V
FF	81.96	%	82.44	%
Eff	25.64	%	25.88	%





J. Wu et al., An integrated system built for small-molecule semiconductors via high-throughput approaches, JACS 2023
J. Wu et al., An Inverse design workflow discovers HTL tailored for perovskite solar cells, **Science 2024**;
A. Bornschlegl et al, An Automated Workflow to Discover the Structure–Stability Relations for Radiation Hard Molecular Semiconductors, **JACS 2025**

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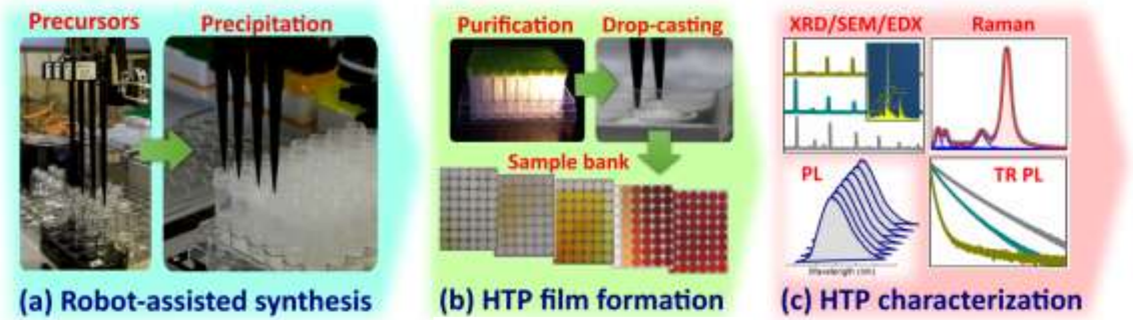
EXAMPLE 2: „GREEN“ SEMICONDUCTOR DISCOVERY

At the hand of Double Perovskites e.g. $Cs_2Ag(Na)M^{III}Cl_6$ and perovskite related materials

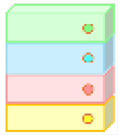


J. Mater. Chem. C, **2022**, 10, 9938
J. Mater. Chem. C, **2023**, 11, 4328

Mater. Adv., **2022**, 3, 7894
ACS Mater. Lett., **2023**, 5, 596

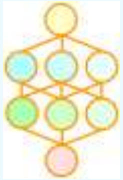
J. Mater. Chem. C, **2024**, 12, 533
J. Mater. Chem. C, **2024**, 12, 8705

Chemistry for Pb-free SC screening workflow

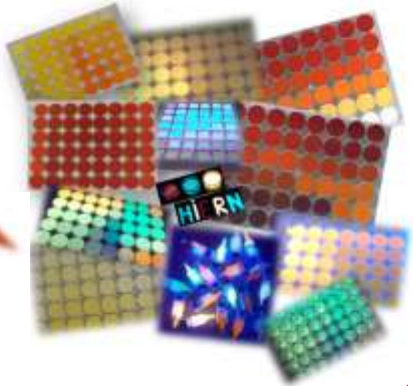


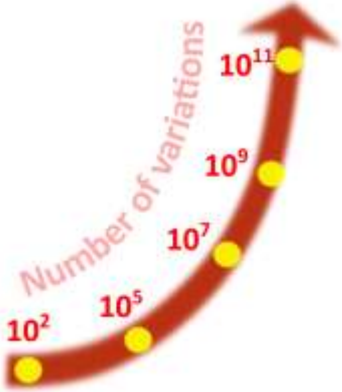
Experimental dataset, ca. 8000 compounds

?



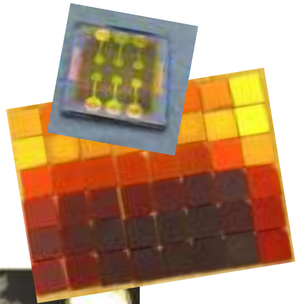
ML-assisted material screening



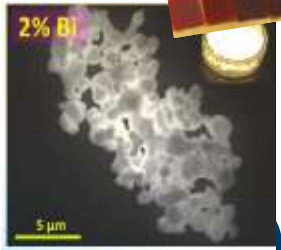


Most promising directions

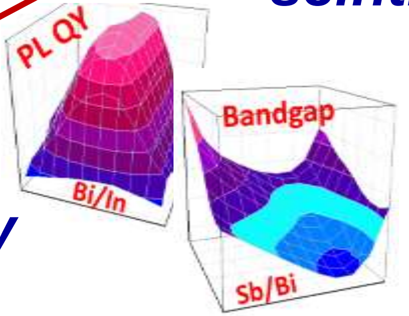
PV absorbers



Phosphors/ scintilators



High-entropy alloys



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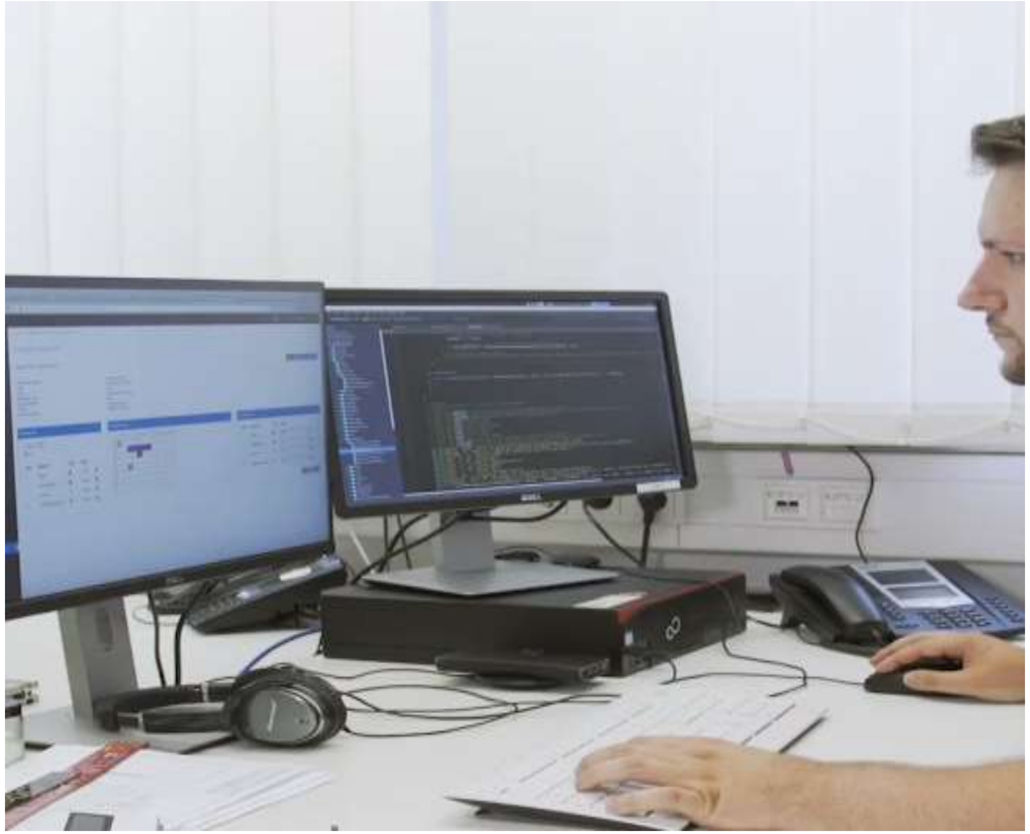
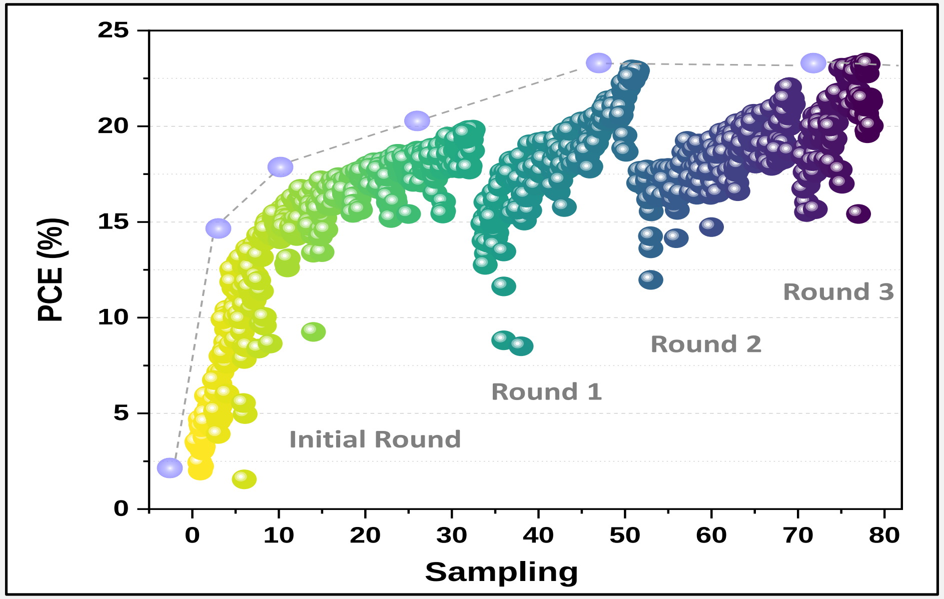
Example 3: Autonomous Device Processing Optimization

Autonomous Bayesian Optimization of Organics (Line 1) and Perovksites (Line 2)

Capable of varying 100´s of processing dimensions with thousands to variations each



- Reducing process dimensions from > 70 to 6: few 100 devices identify optima in a 6d space with > 10^{15} parameter variations.



J. Zhang et al., "*Machine Learning-Driven Autonomous Optimization of Air-Processed Perovskite Solar Cell in 6D Parameter Space*" , AEM, accepted 2024

J. Zhang et al., "*Precise control of process parameters for > 23 % PSC in ambiet air using an automated device acceleration platform",* EES, 2024)

J. Zhang et al., "*Optimizing Perovksite Thin-film Parameter Spaces with a ML guided Robotic Platform for Perovskite Solar Cells "* , AEM 2023

J. Zhang et al., "*Toward Self-Driven Autonomous Matierla and Device Acceleration Platforms for emerging PV Technologies"* , Accounts of Chem Res 2024

J. Zhang et al., "*A self-driving AMADAP Laboratory: Accelerating Discovery and Optimization of emerging perovskite photovoltaics"* , MRS Bulletin, 2024

EXAMPLES ON RECENT RESEARCH: RESPONSIBLE PV

Recycling and closed cycle processes for photovoltaic technologies

From Materials to Processes to Devices to **Demonstration**

MARIUS I PETERS

JÜLICH Forschungszentrum

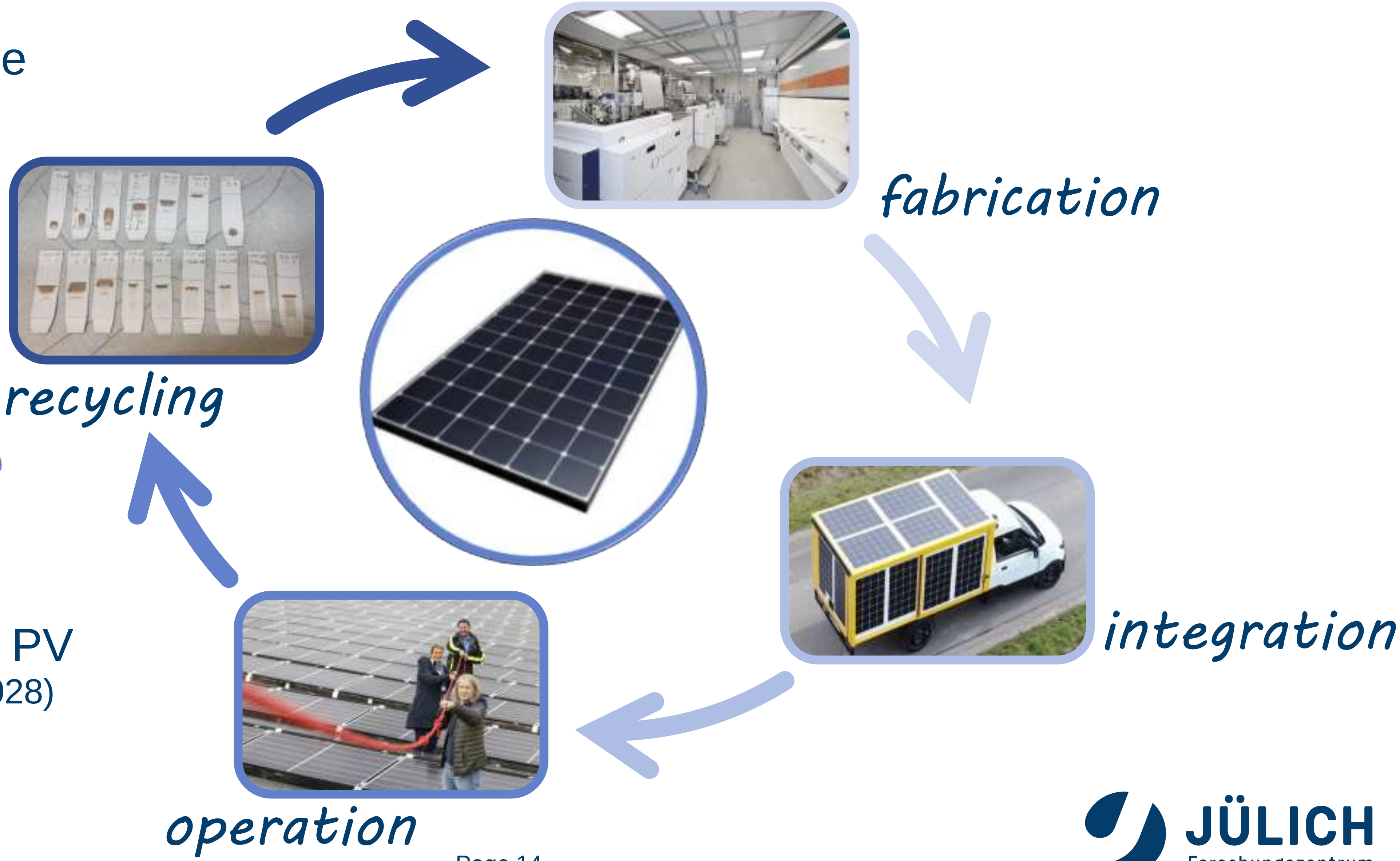
The Lifecycle of a photovoltaic module

Zeitenwende
HZB, FZJ, KIT
(2021 – 2025)

C2C-PV
(2023 – 2028)

Retrieve
(2023 – 2028)

Circular PV
(2025 – 2028)



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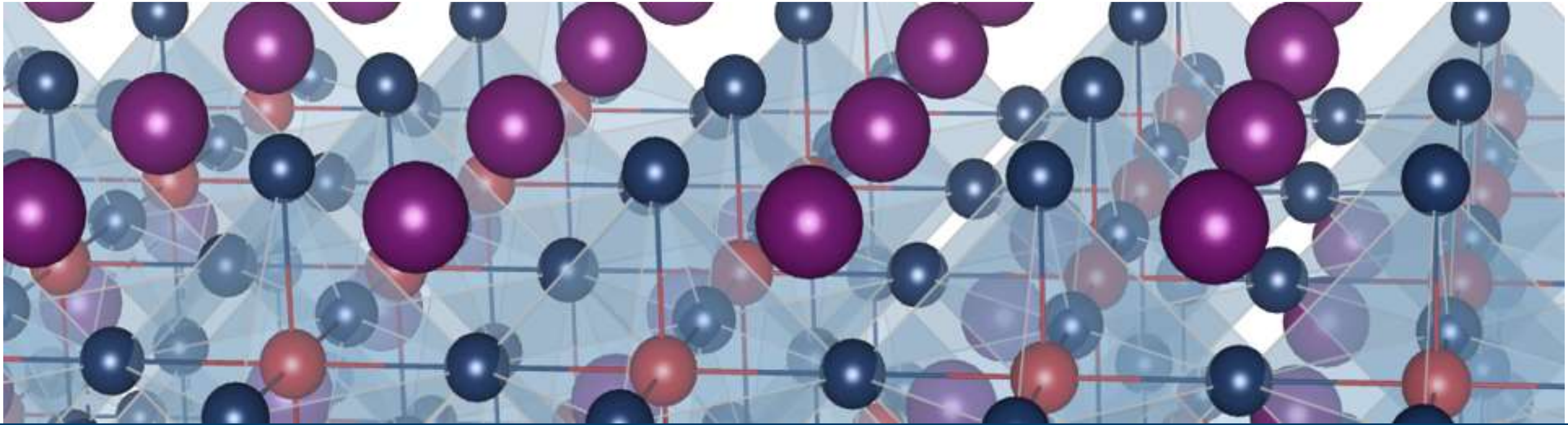

Thank you for your attention!

Prof. Dr. Christoph Brabec

c.brabec@fz-juelich.de

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Organic Photovoltaics - Challenges and Opportunities

Karl Leo

Dresden Integrated Center for
Applied Physics and Photonics (IAPP)
Technische Universität Dresden, 01062 Dresden, Germany
www.iapp.de

KAST 한국과학기술한림원
The Korean Academy of Science and Technology

Leopoldina
Nationale Akademie
der Wissenschaften

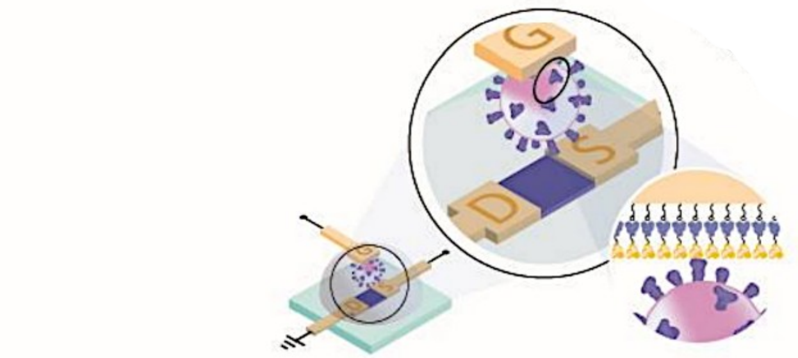
Organic electronics: a path to sustainable electronics

OLED display

Organic photovoltaics

OLED
lighting

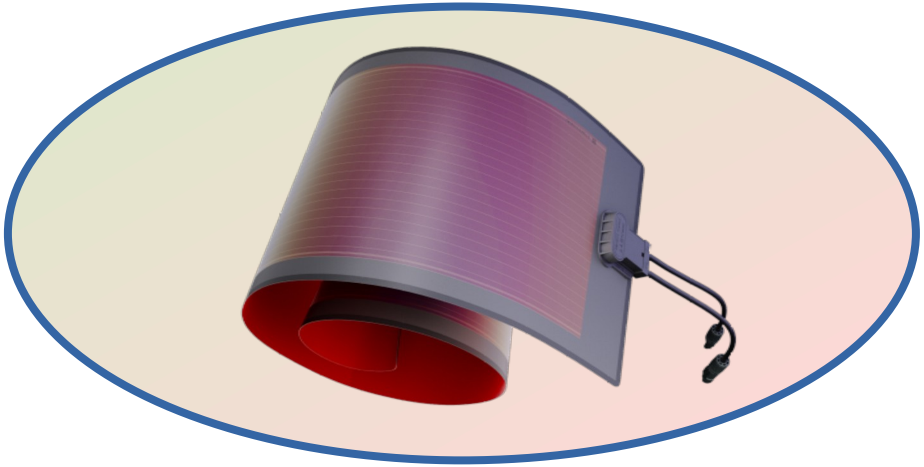
Biosignal monitoring



Organic Photovoltaics

Less than 1mm
Thick film

Flexible & lightweight



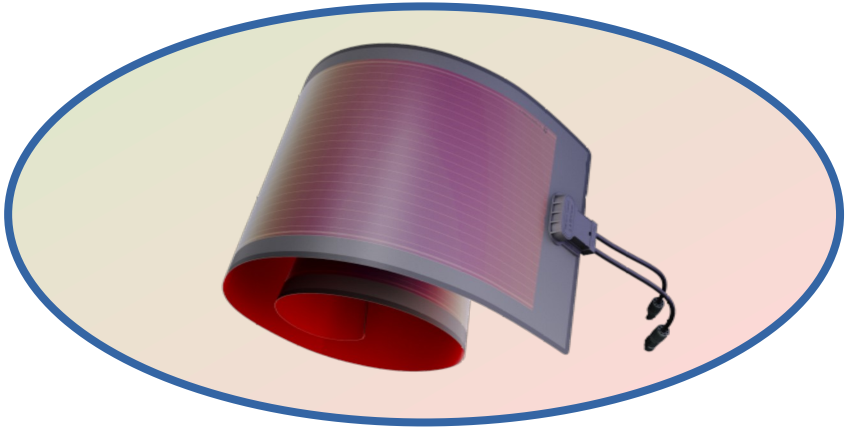
Inexhaustible
non-toxic materials

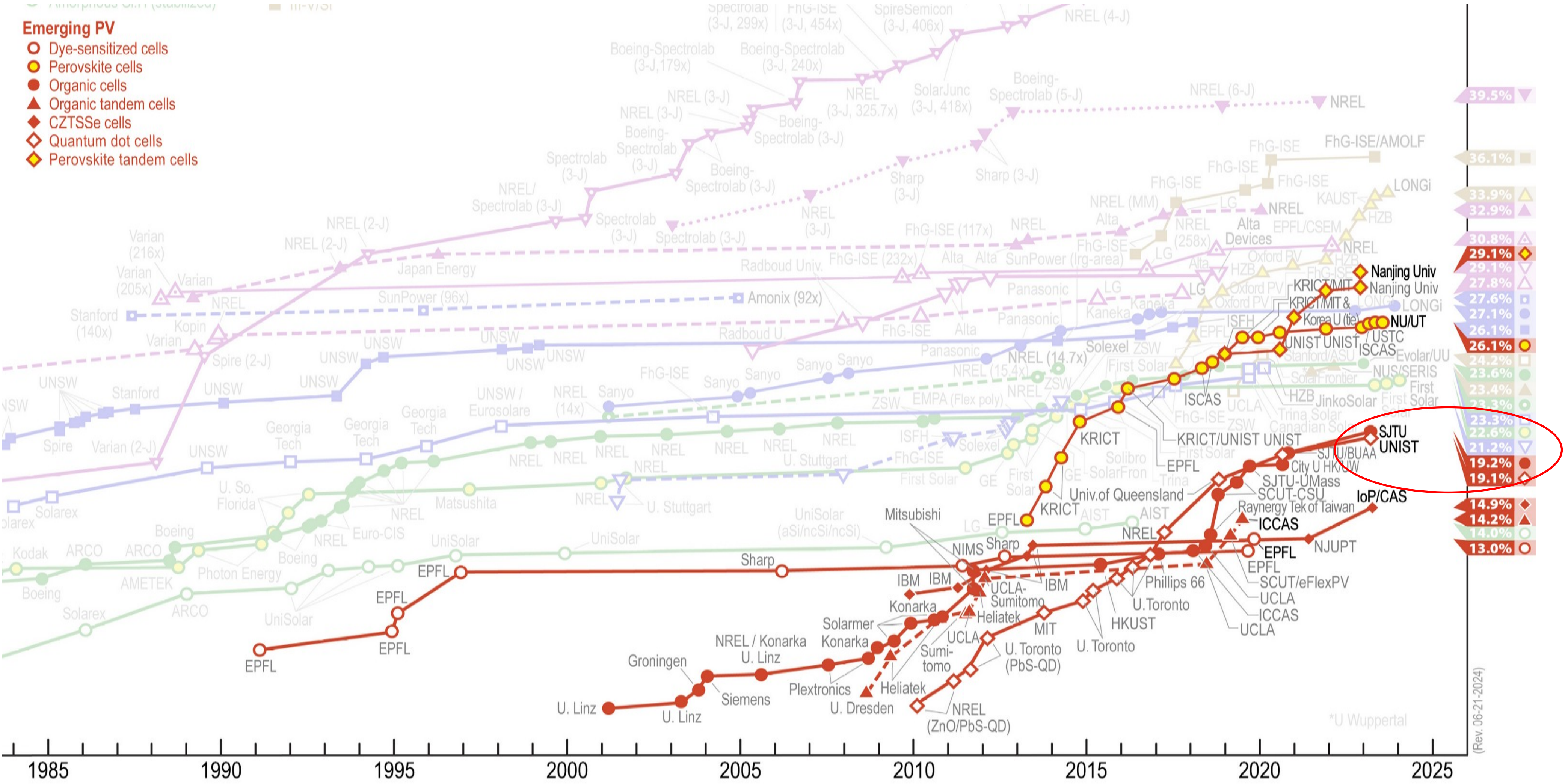
Homogeneous
Surface

Adjustable
Transparency
Levels

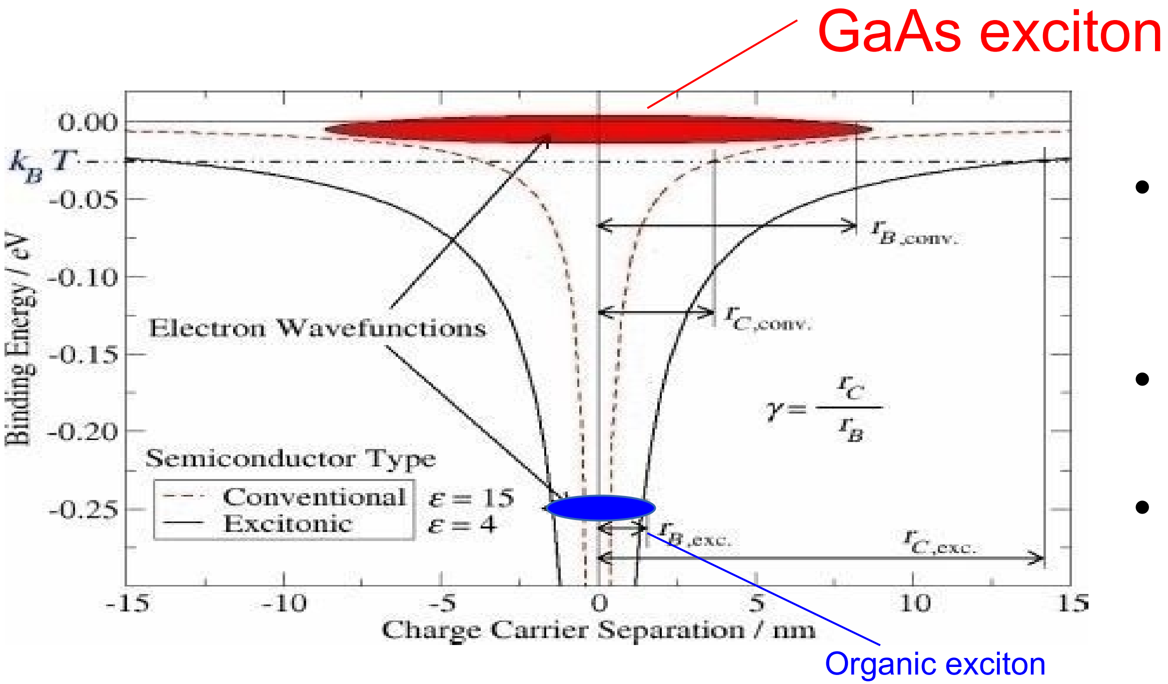
Outline

- Research Challenges in Organic Solar Cells
- Manufacturing of Organic Solar Cells
- Applications




Emerging PV
Dye-sensitized cells
Perovskite cells
Organic cells
Organic tandem cells
CZTSSe cells
Quantum dot cells
Perovskite tandem cells
SJTU
UNIST
IoP/CAS
Nanjing Univ
NU/UT
19.2%
19.1%
14.9%
14.2%
13.0%
29.1%
26.1%
1985
1990
1995
2000
2005
2010
2015
2020
2025

The organic exciton separation problem



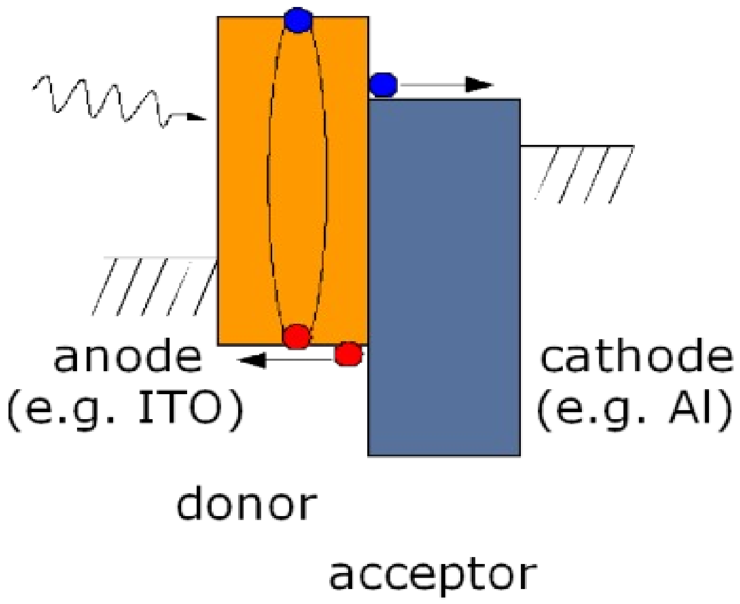
- Absorption leads to tightly bound (0.2 … 0.5 eV) excitons
- Separation in electric field inefficient
- Usual solar cell structure does not work

S. E. Gledhill et al. J. Mat Res. 20, 3167 (2005)

P. Würfel, CHIMIA 61, 770 (2007)

Exciton separation at a heterojunction

Flat heterojunction (FHJ)



C. W. Tang, Appl. Phys. Lett. 48, 183 (1986)

bulk heterojunction (BHJ)

The first organic solar cell

AIP **Applied Physics Letters**

HOME ISSUES INFO FOR AUTHORS COLLECTIONS

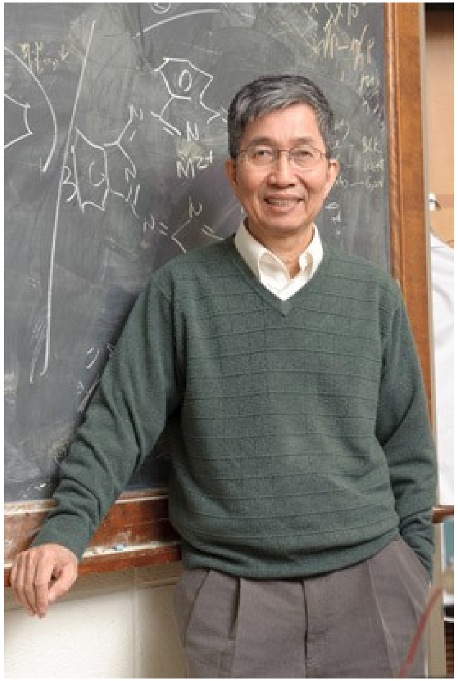
Home > Applied Physics Letters > Volume 48, Issue 2 > 10.1063/1.96937

No Access . Published Online: 04 August 1998 Accepted: October 1985

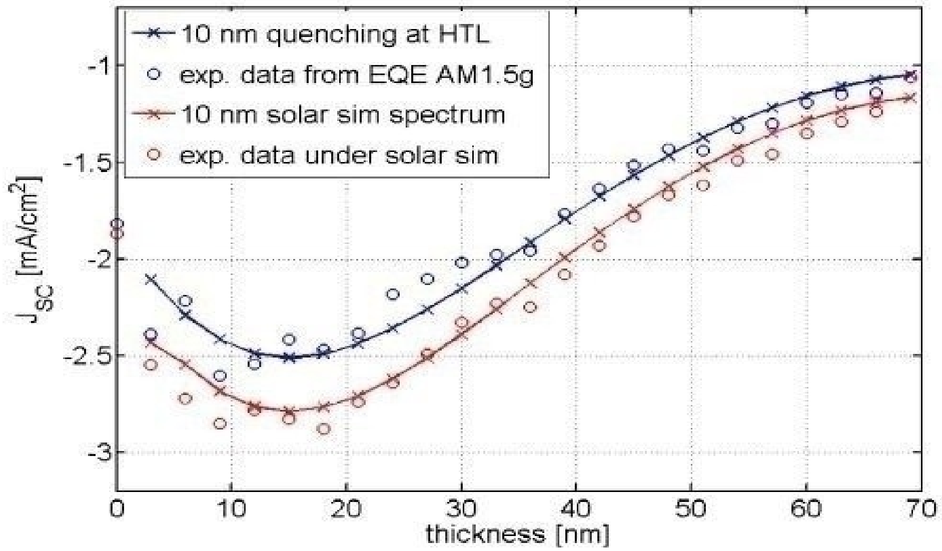
Two-layer organic photovoltaic cell

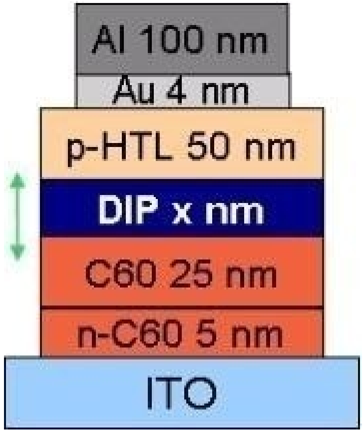
Appl. Phys. Lett. **48**, 183 (1986); https://doi.org/10.1063/1.96937

C. W. Tang



Exciton diffusion length



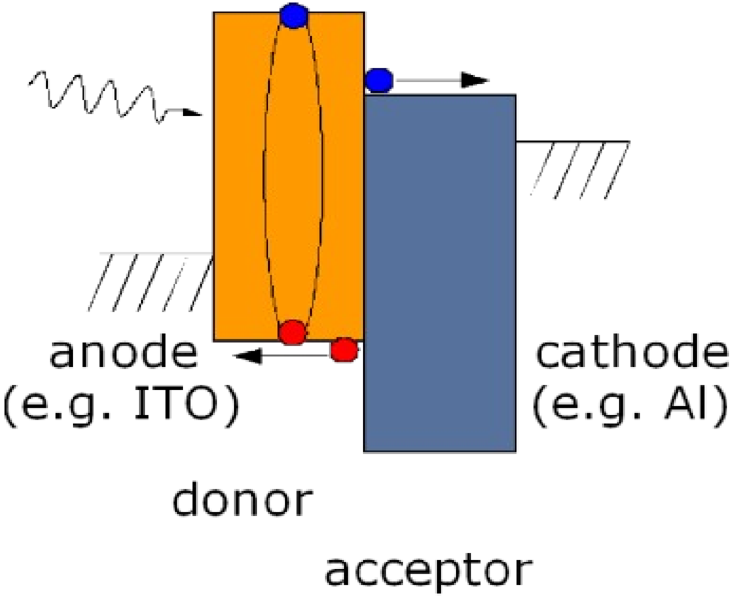


Exciton diffusion length L_D = (10 ±1) nm:

Much smaller than absorption length!

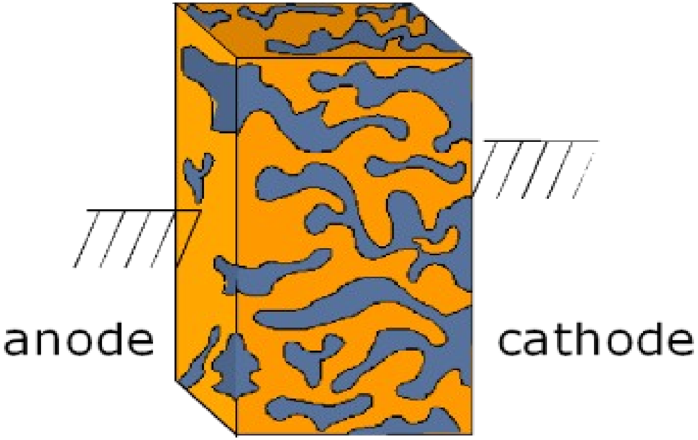
Exciton separation at a heterojunction

Flat heterojunction (FHJ)



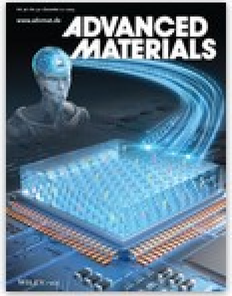
C. W. Tang, Appl. Phys. Lett. 48, 183 (1986)

bulk heterojunction (BHJ)



M. Hiramoto et al., Appl. Phys. Lett. 58, 1062 (1991)
N.S. Sariciftci et al., Science 258, 1474 (1992)
J. J. Hall et al., Nature 376, 498 (1995)
G. Yu et al. Science 270, 1789 (1995)

ADVANCED MATERIALS



Volume 36, Issue 50
December 12, 2024
2402834

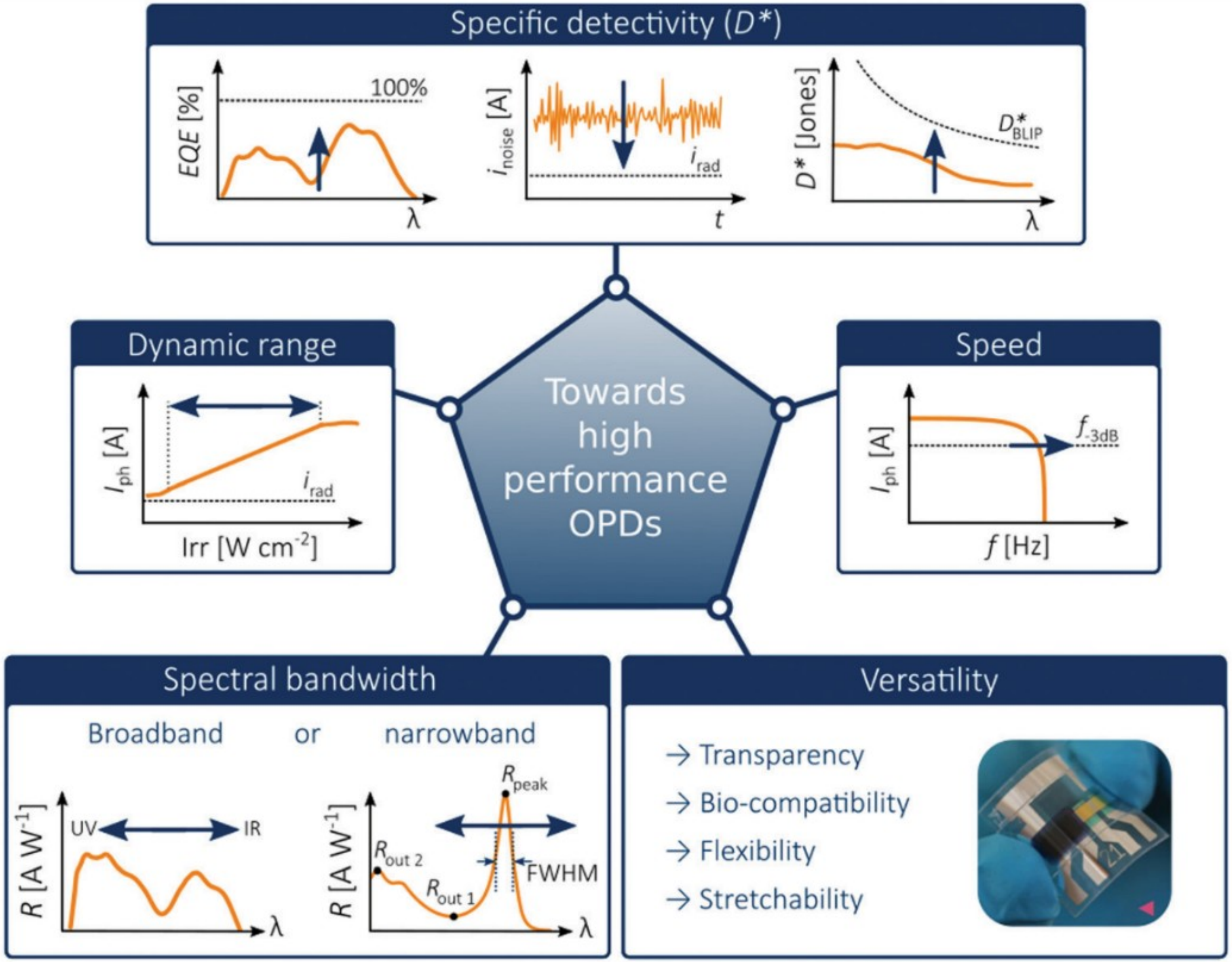
Research Article | Open Access

Sensitive Self-Driven Single-Component Organic Photodetector Based on Vapor-Deposited Small Molecules

J. Wolansky et al., https://doi.org/10.1002/adma.202402834

With Banerji (Bern, CH) and Ortmann (Munich) groups

Organic Photodectors



Y. Wang et al., Mater. Horiz., 2022, 9, 220

RESEARCH ARTICLE

ADVANCED FUNCTIONAL MATERIALS
www.afm-journal.de

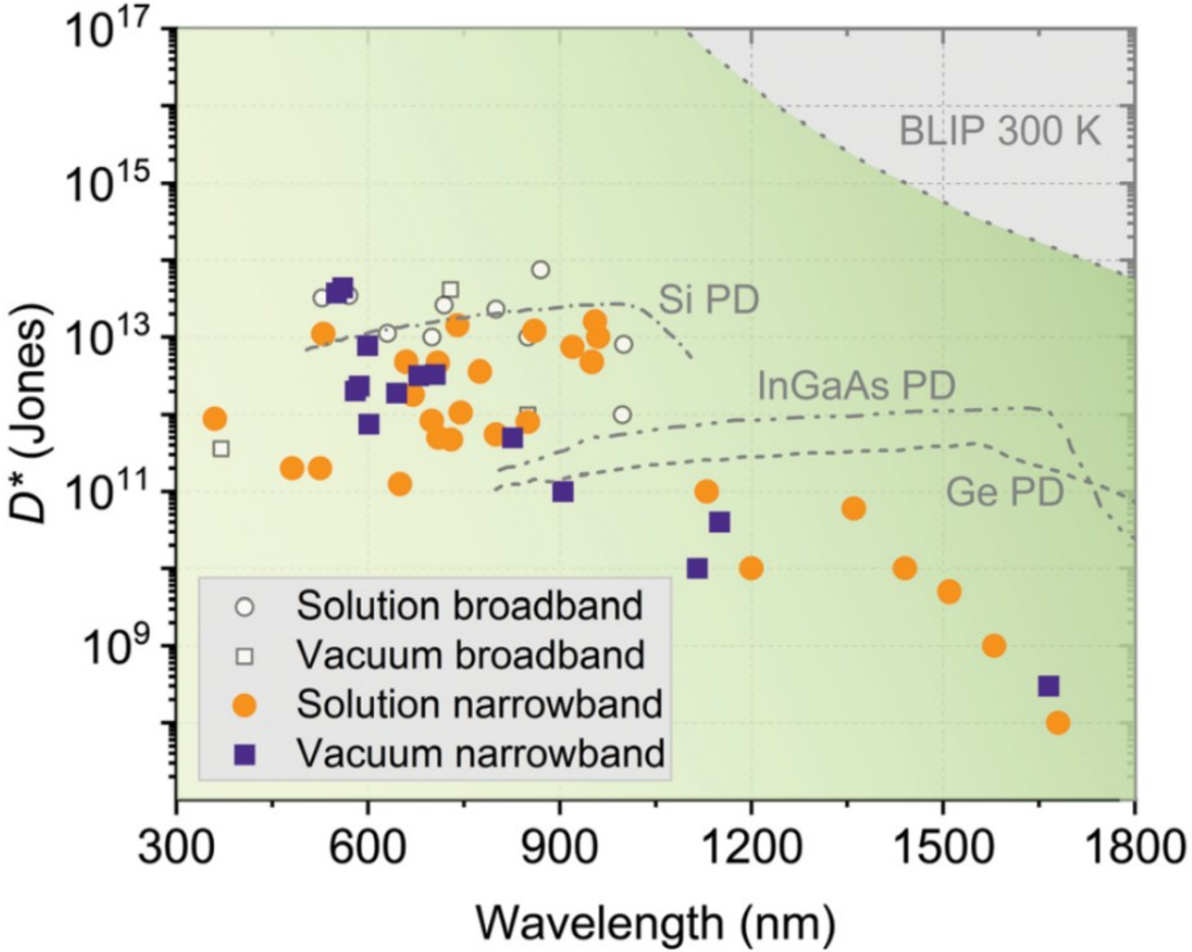
High-Performance Filterless Blue Narrowband Organic Photodetectors

T. Zhang et al., Adv. Funct. Mater. 2024, 34, 2308719, DOI: 10.1002/adfm.202308719

Performance of Organic Photodetectors

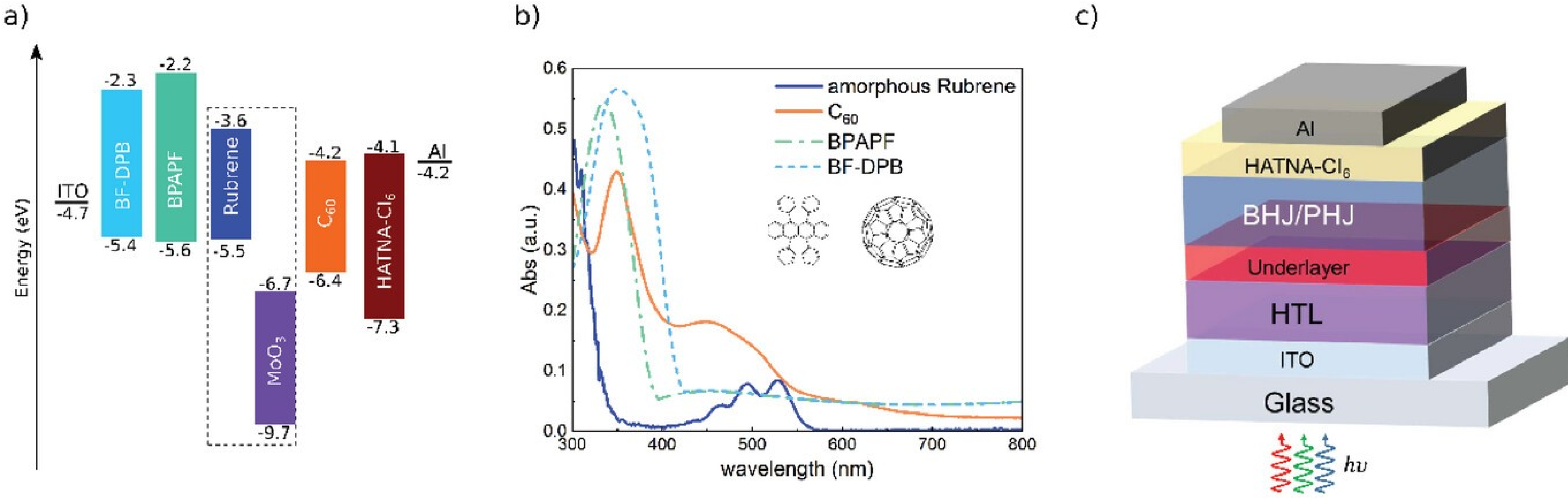
$$D^* = \frac{q\lambda \mathrm{EQE}}{hcS_\mathrm{n}} \quad (\mathrm{cm\ Hz^{1/2}\ W^{-1}\ or\ Jones})$$

With S_n spectral noise density
(which is mainly determined by dark current)



Y. Wang et al., Mater. Horiz., 2022, 9, 220

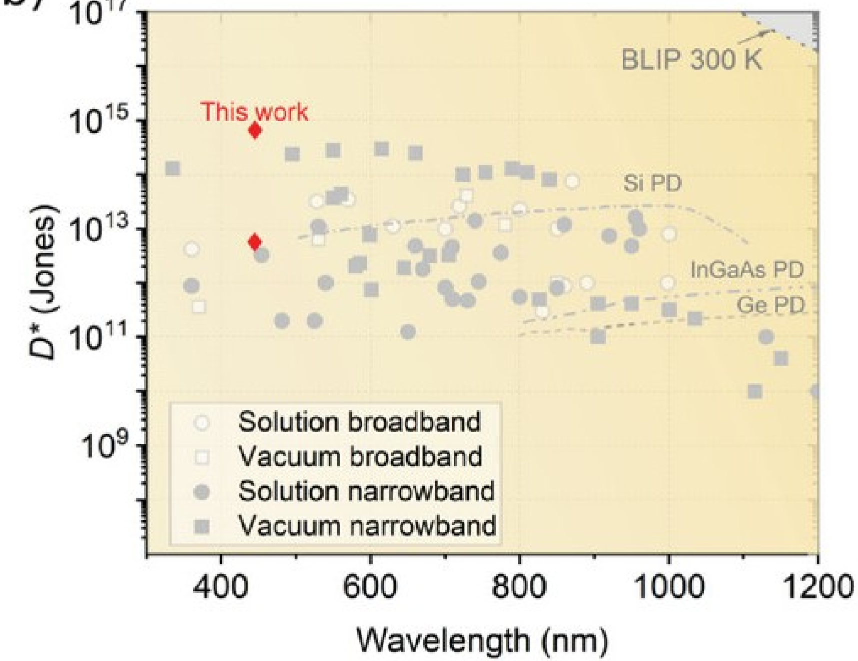
Rubrene organic photodiodes

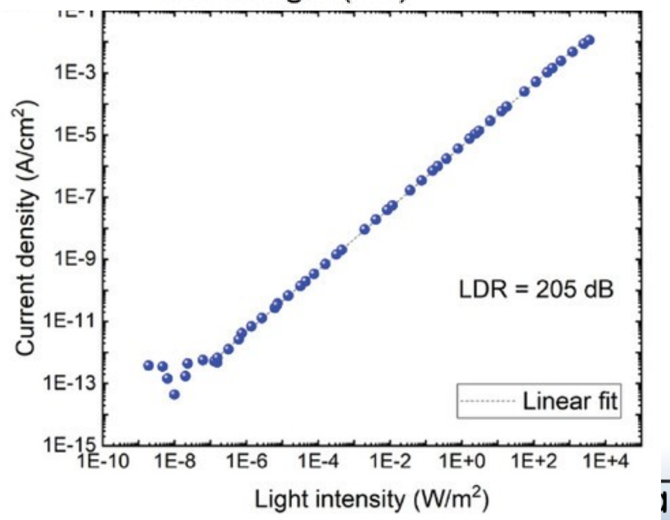


T. Zhang et al., High-Performance Filterless Blue Narrowband Organic Photodetectors, Adv. Funct. Mat. **34**, 2308719 (2024)

Extremely high detectivity

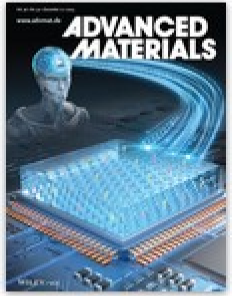
- Specific detectivity (D*) reaching record-high value of 6.35 × 10^{14} Jones
- Better than silicon photodiodes
- Excellent linear dynamic range (LDR)





T. Zhang et al., High-Performance Filterless Blue Narrowband Organic Photodetectors, Adv. Funct. Mat. **34**, 2308719 (2024)

ADVANCED MATERIALS



Volume 36, Issue 50
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2402834

Research Article | Open Access

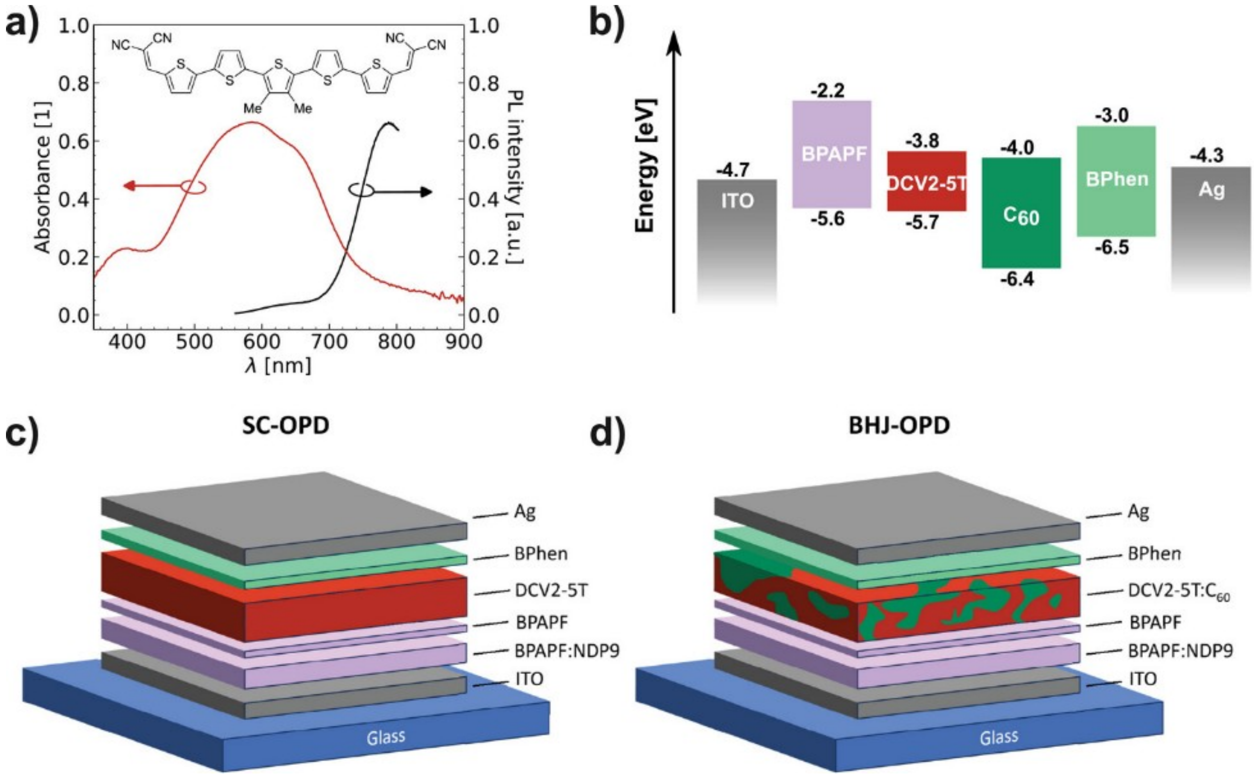
Sensitive Self-Driven Single-Component Organic Photodetector Based on Vapor-Deposited Small Molecules

J. Wolansky et al., https://doi.org/10.1002/adma.202402834

With Banerji (Bern, CH) and Ortmann (Munich) groups

Single-Component vs bulk heterojunction

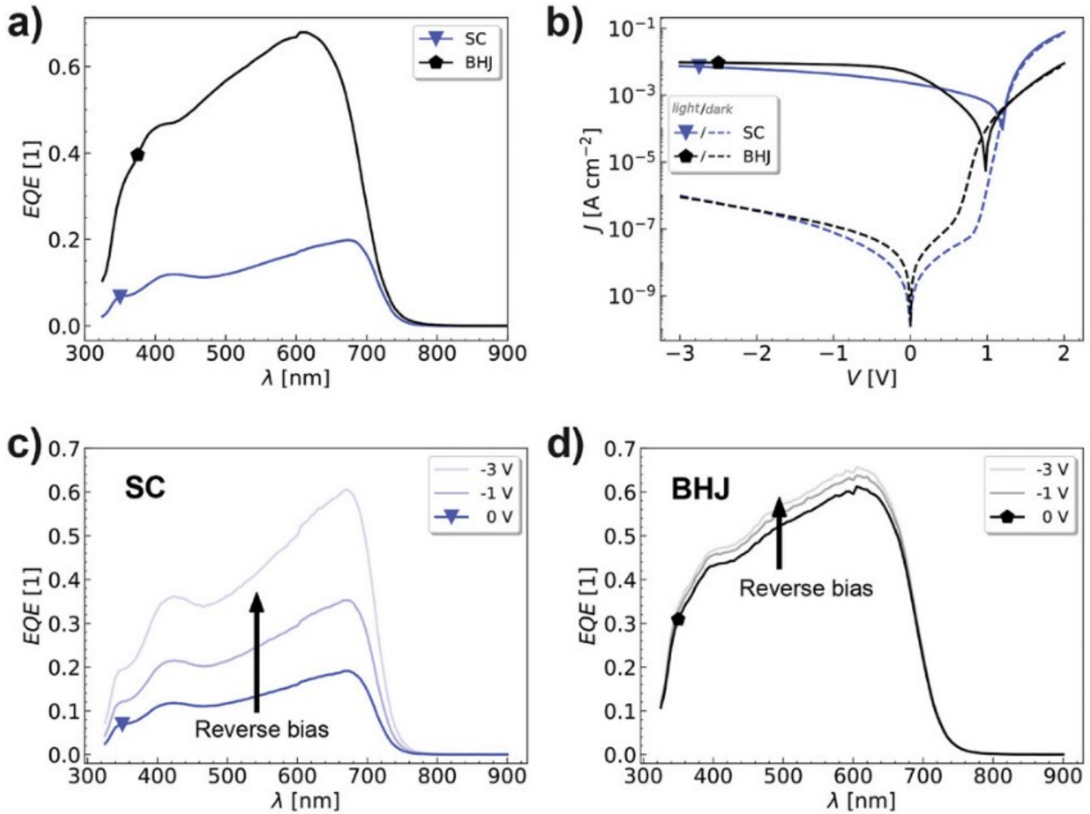
- Thiophene donor (from Bäuerle group, Ulm)
- Around 10% efficiency, high voltage loss in BHJ



J. Wolansky et al., https://doi.org/10.1002/adma.202402834

SC vs BHJ: External Quantum Efficiency

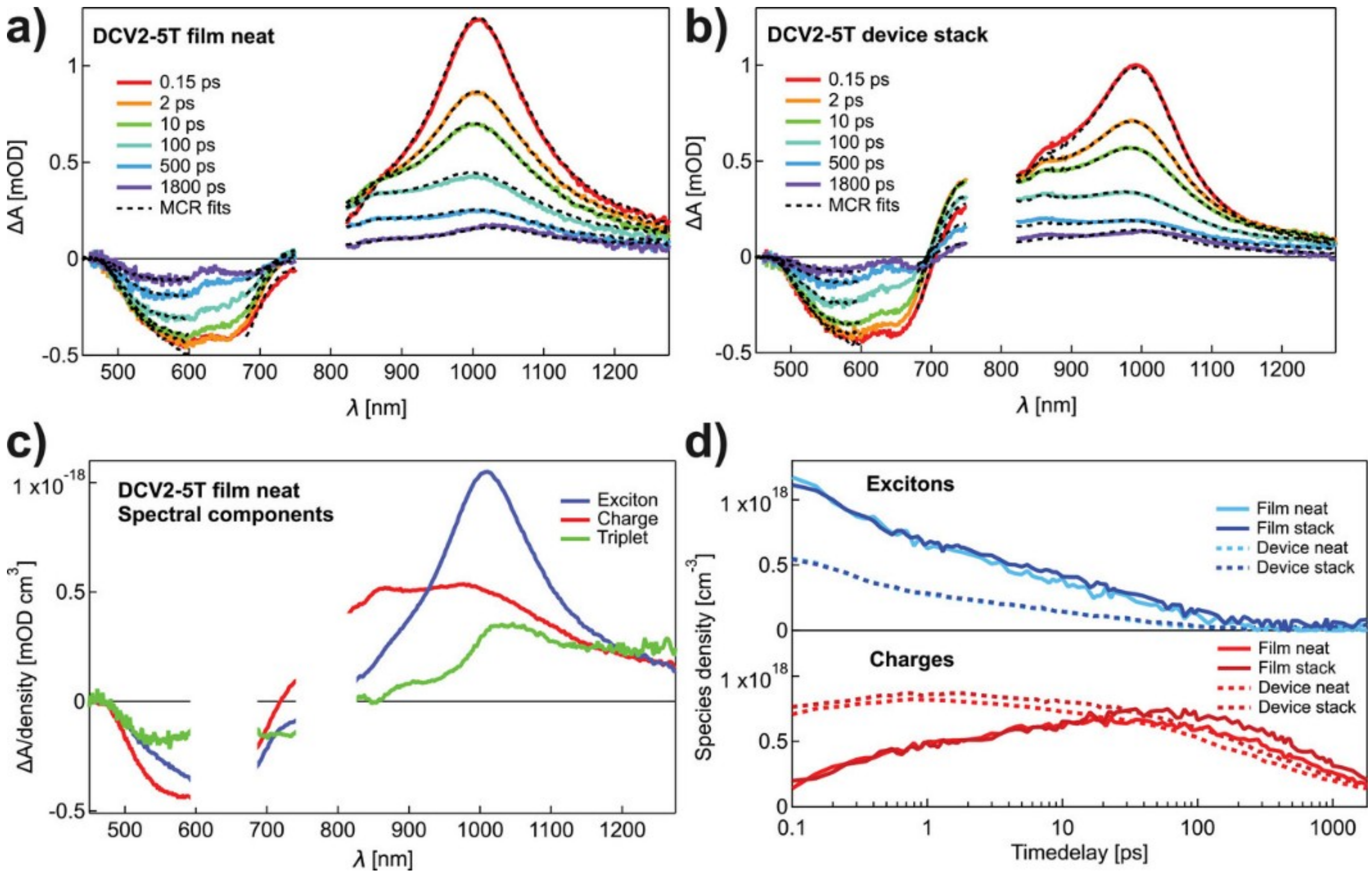
- Fairly high quantum efficiency even without heterojunction
- Small electric field separates excitons almost completely!
- Excellent detectors: specific detectivities of $1 \cdot 10^{13}$ Jones



J. Wolansky et al., https://doi.org/10.1002/adma.202402834

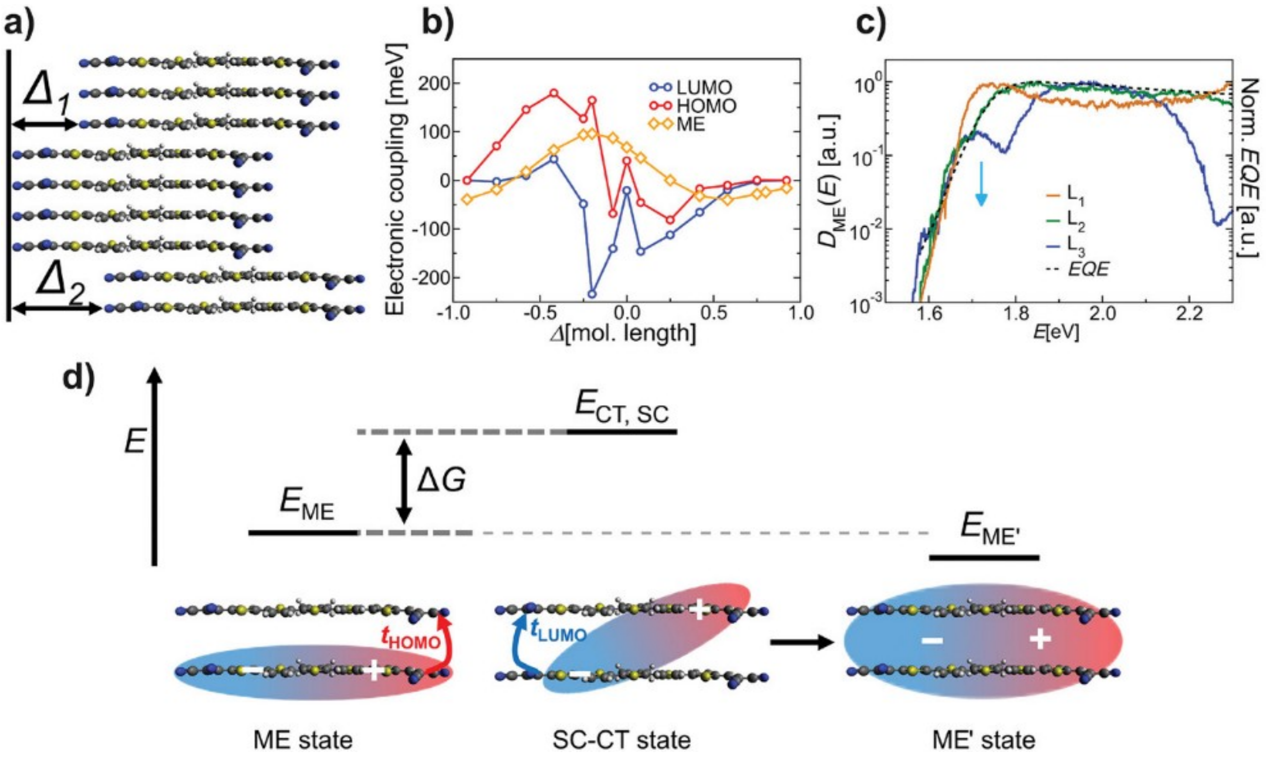
Transient Absorption Study (Banerji group)

- Almost instantaneous (<1ps) carrier generation
- Observed in neat film and device stack
- Stronger in device stack with electrodes: confirms field dependence



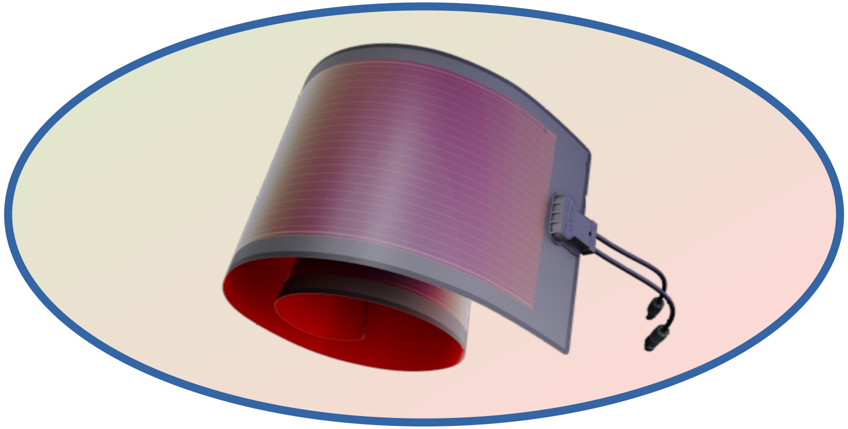
Theoretical interpretation (Ortmann group)

- Strong electronic coupling of molecular exciton and charge transfer states
- Coupling depends on lateral shift Δ of the molecular π-stack
- Disorder in Δ supports exciton separation

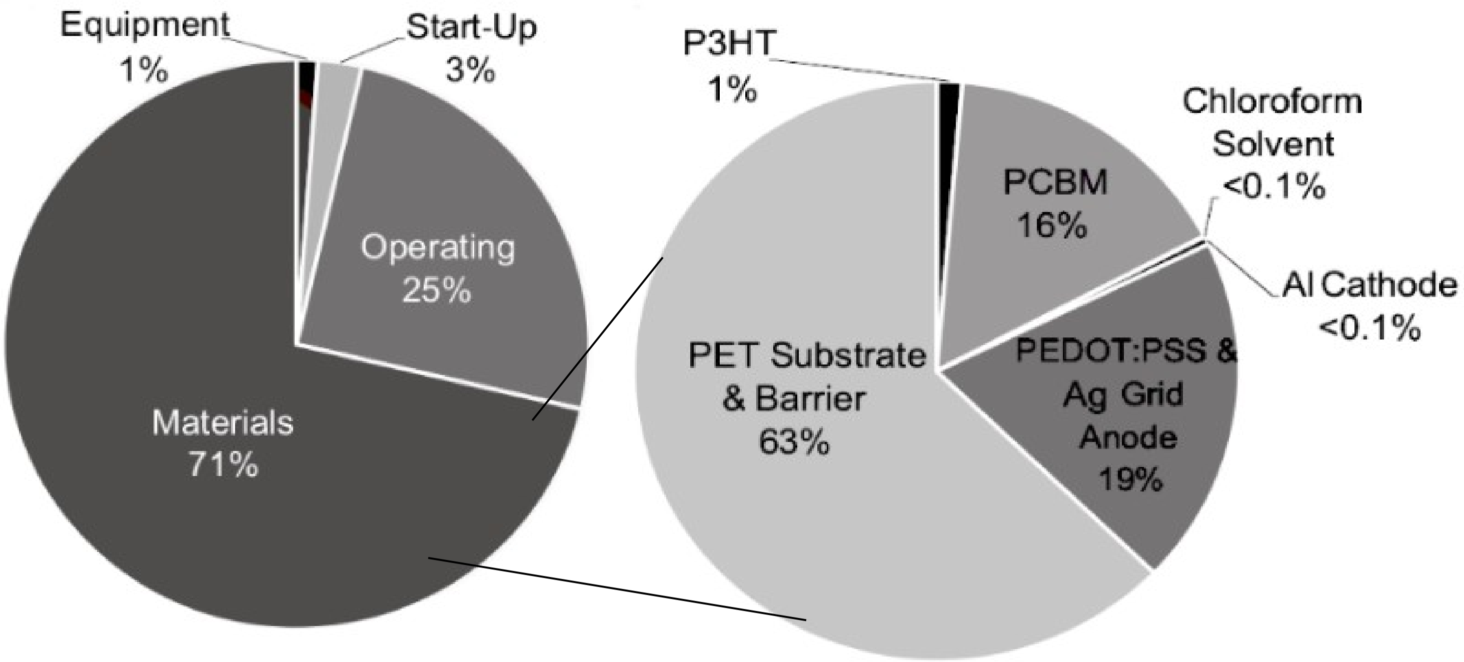


Outline

- Research Challenges in Organic Solar Cells
- Manufacturing of Organic Solar Cells
- Applications



Cost distribution



Total cost: 7.80 (±2) US$/m^2 ≈ 0.05US$/Watt$_{peak}$ ≈ 0.02US$/kWh*

* if system cost can be scaled similarly

C.J. Mulligan et al. / Solar Energy Materials & Solar Cells 120 (2014) 9–17

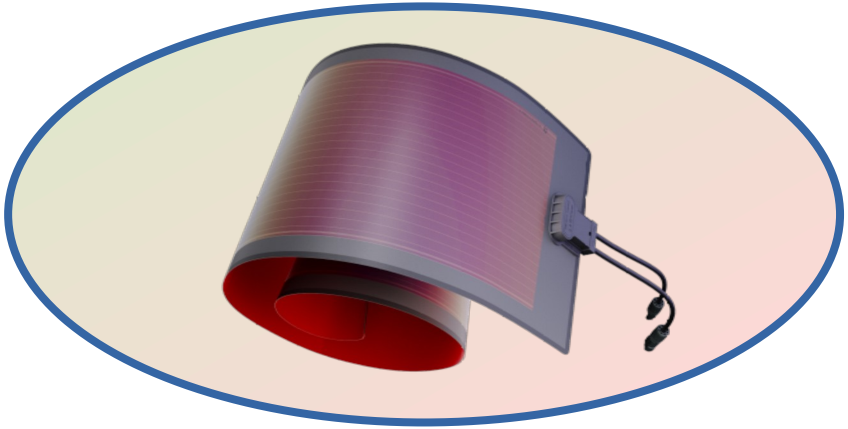

Heliatek
Dresden Mass Manufacturing Line
5,000 m² floor space
~1 million m²/year capacity

Carbon Dioxide Budget (Heliatek analysis)

- Manufacturing: 16 kg CO_2 per m^2
- Results in 7-9g CO_2 per kWh (in central Europe, better in southern locations)
- Energy fed back after 3 months operation, 4-10x better than crystalline silicon
- Southern locations: Lowest CO_2 footprint of any energy generating technology!

Outline

- Research Challenges in Organic Solar Cells
- Manufacturing of Organic Solar Cells
- Applications



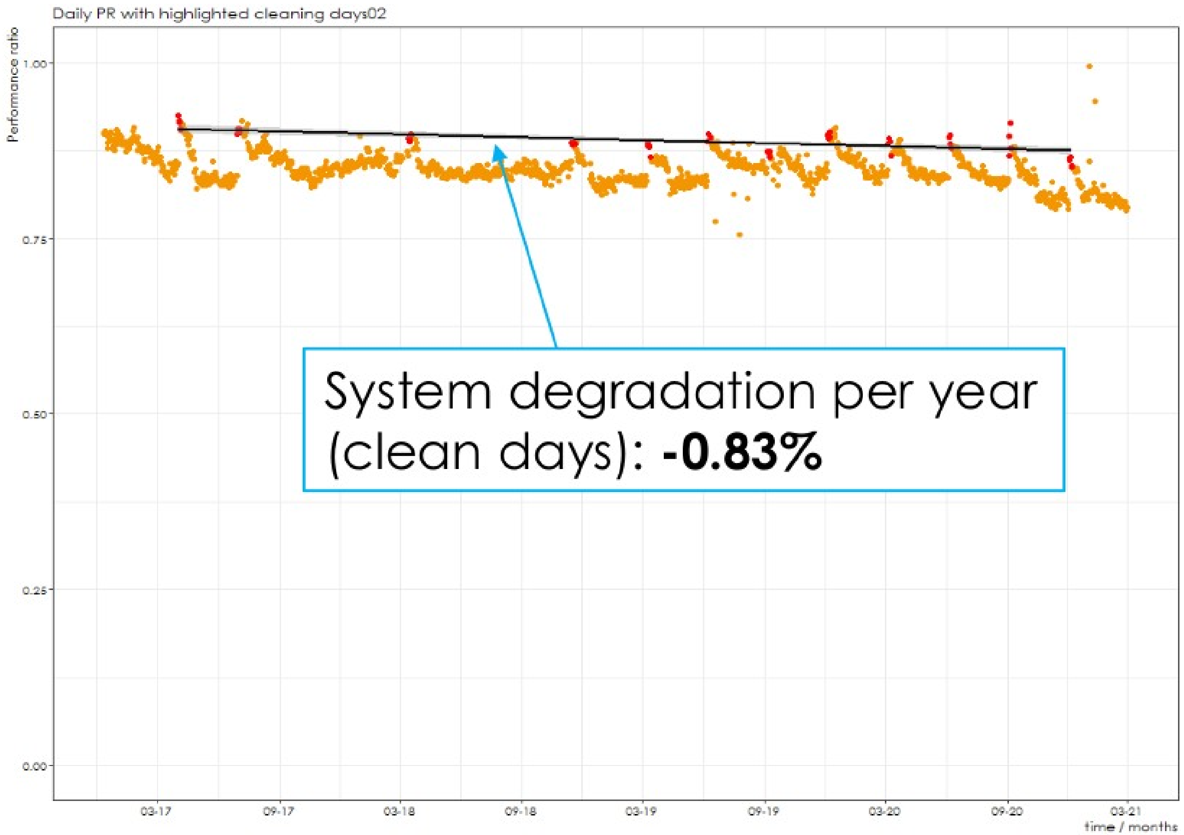
Transparent BIPV installations: Singapore

Heliatek
INDEPENDENT. GREEN. FUTURE.

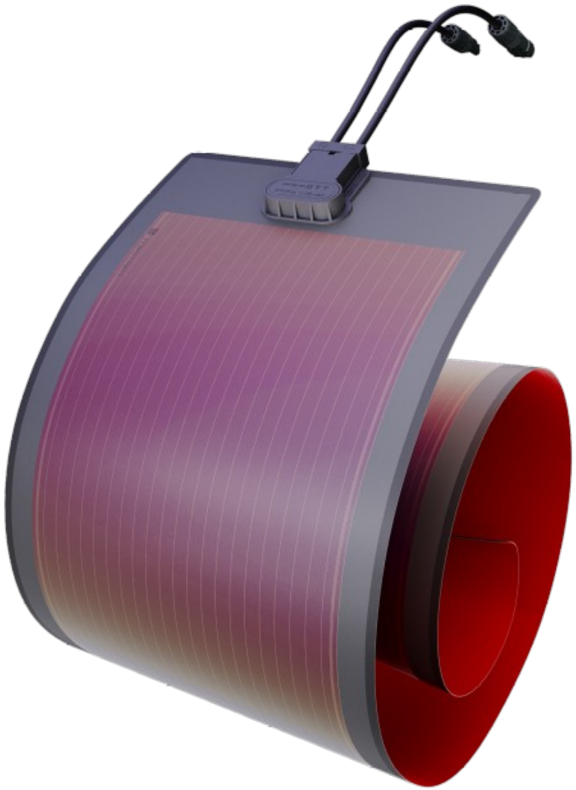
Lifetime >20 years expected in outdoor environment

Seris Outdoor Module Testing in Singapore

- **Test:**
  - Nominal module power: 22 Wp
  - Test period: From Dec 2016 onwards (ongoing)
  - Data saved daily
- **Finding:**
  - Performance ratio decreases only **< 1 % per year**



Heliatek reaches IEC 61215 certication (first OPV)



Installation on metal façades at Erlanger Stadtwerke (ESTW)

Erlangen
Germany

May 2024

The installation consists of 99 modules with a total capacity of 5.5 kWp on a metal facade.

Tanks and façade of a high-rack warehouse

Arnsberg-Müschede
Germany

September 2024

Two-part installation with 180 modules on tanks and 528 modules on the facade of a high-rack warehouse. The installation has a total capacity of 39 kWp.

World's largest Organic PV plant: 37.7kW$_p$
SAMSUNG Advanced Institute of Technology, Suwon, South Korea

Heliatek
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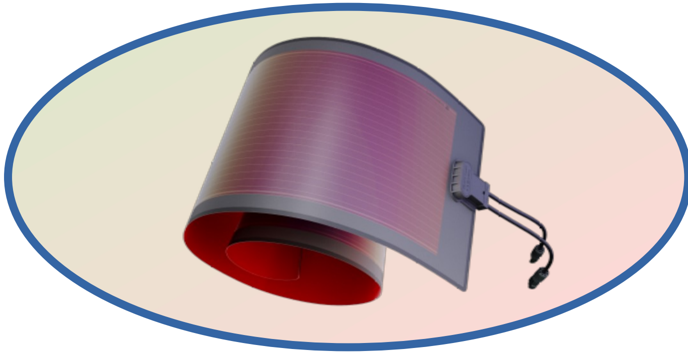
Conclusions

- Organic photovoltaics: promising in terms of materials and environment
- Certified modules commercially produced
- Main challenge: raise module efficiency to 20+ percent



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SENORICS

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Michel Panhans
Sebastian Hutsch

TUM

Natalie Banerji
Cedric Hoffmann

Bundesministerium für Bildung und Forschung

DFG

Freistaat SACHSEN

And many, many more I cannot personally mention!

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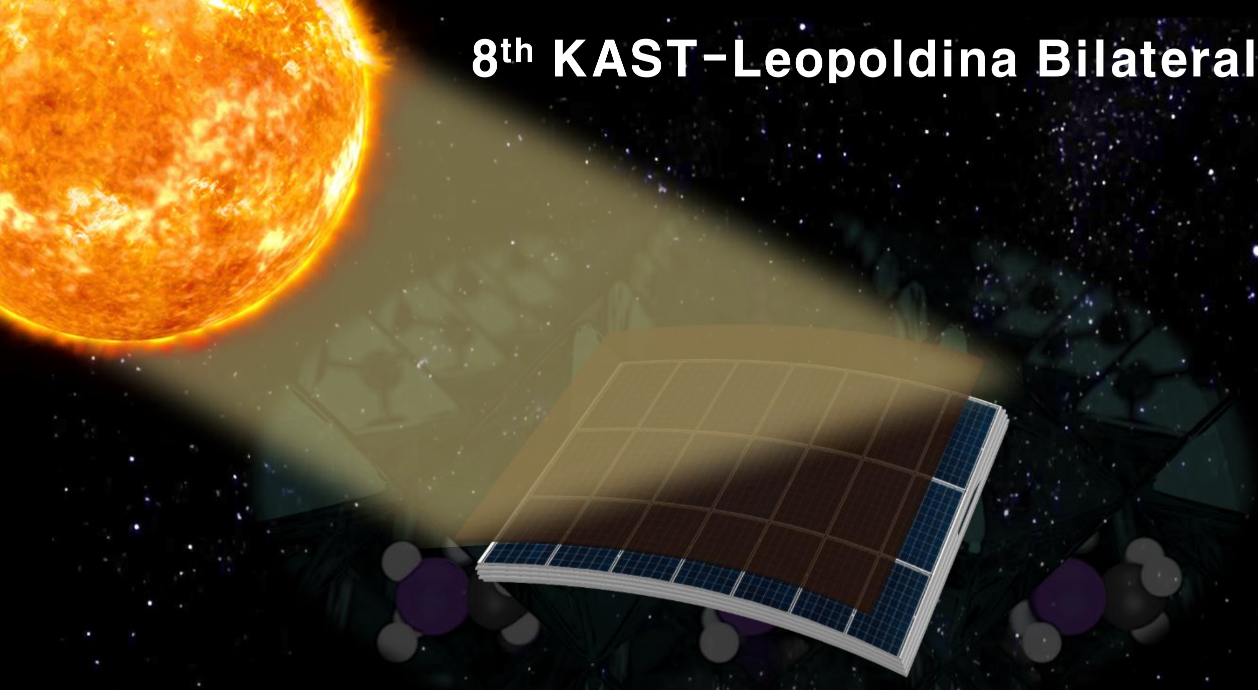
8th KAST-Leopoldina Bilateral Symp., Jan. 14-15, 2025



Perovskite-based Tandems:
Perovskite/Si 2J and beyond

Department of Materials Science and Engineering
Seoul National University

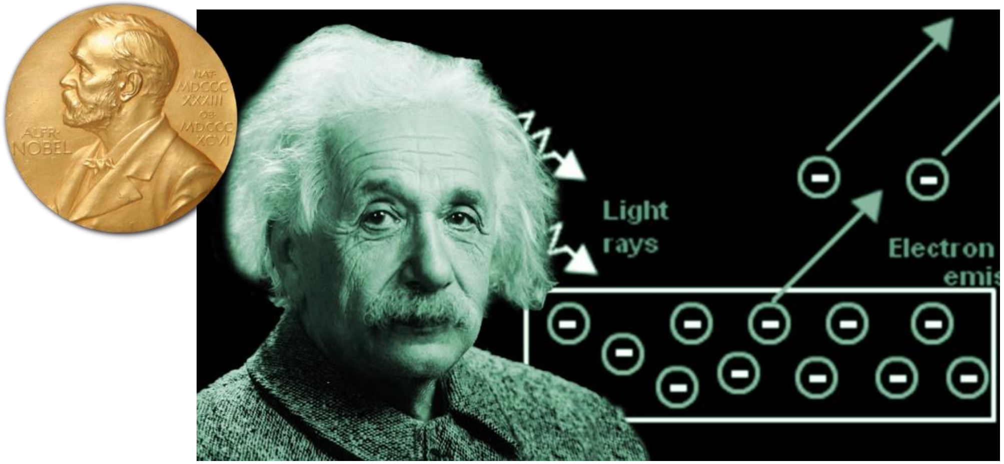
Jin Young Kim

Contents

- Introduction of perovskite-based tandem PVs
- 2-/3-terminal subcell characterization platforms
- Progresses in PVSK/Si 2J tandems
- PVSK-based tandems beyond PVSK/Si 2J
- Summary and outlook

Theoretical background

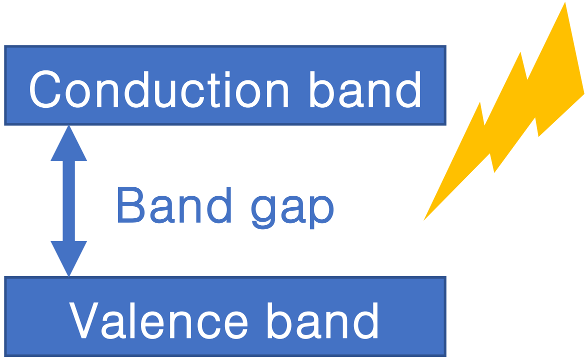
Photoelectric effect



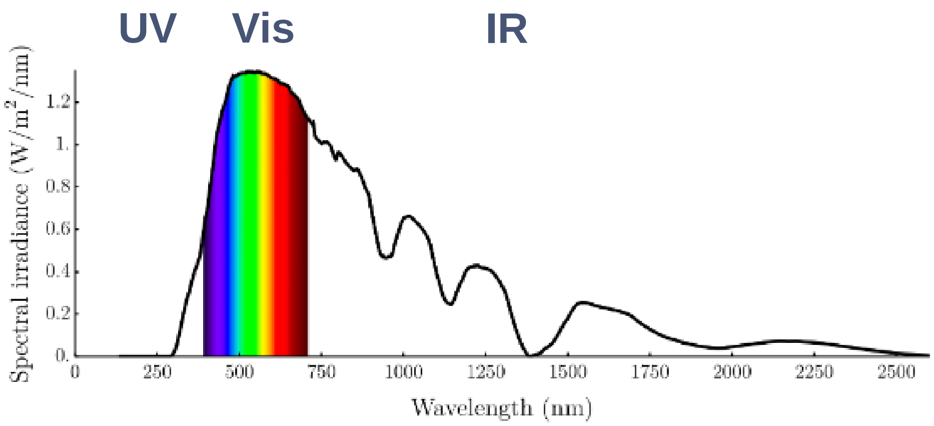
Photon → Electron

Nobel prize in Physics (1921)

Photovoltaic effect



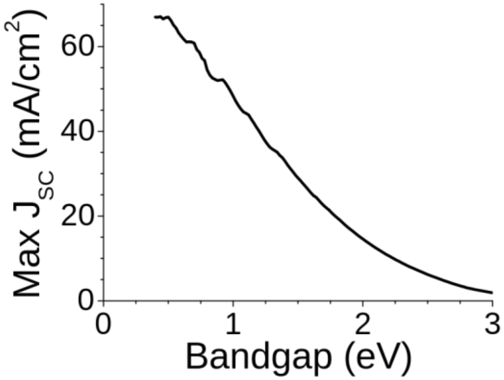
Semiconductor

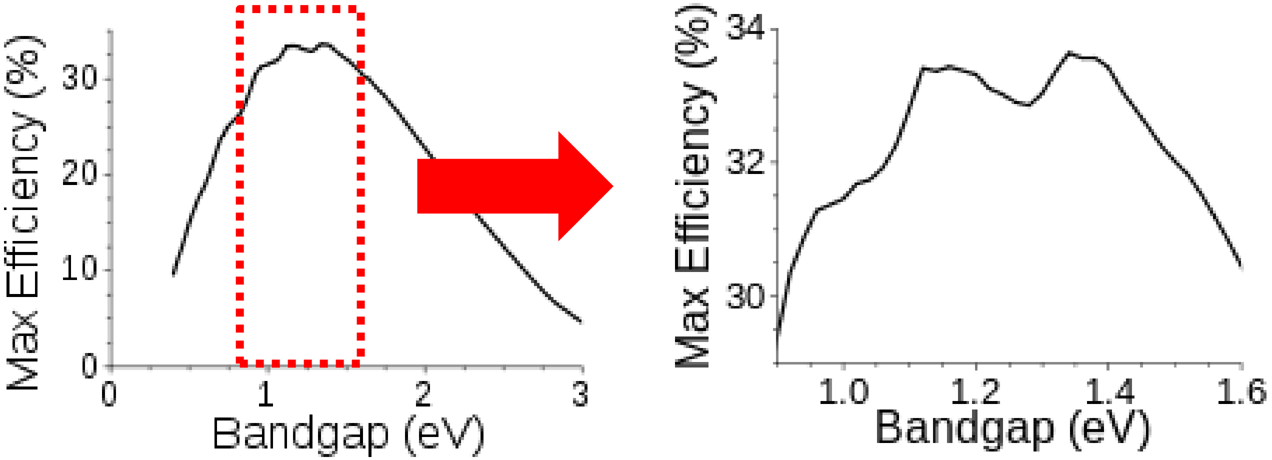


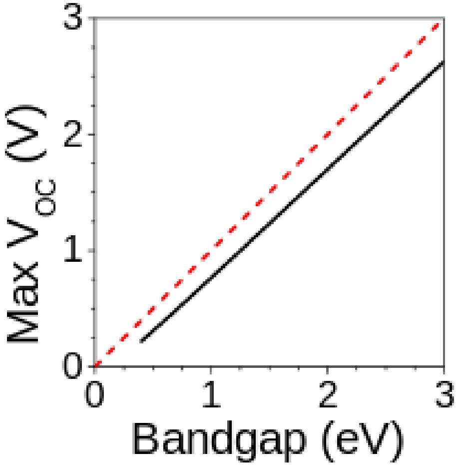
Solar spectrum

Shockley-Queisser limit

- William Shockley and Hans J. Queisser, "Detailed Balance Limit of Efficiency of p-n Junction Solar Cells", Journal of Applied Physics, Volume 32, pp. 510-519 (1961)
- The Shockley-Queisser limit for the efficiency of a solar cell, without concentration of solar radiation.
- The curve is wiggly because of absorption bands in the atmosphere.

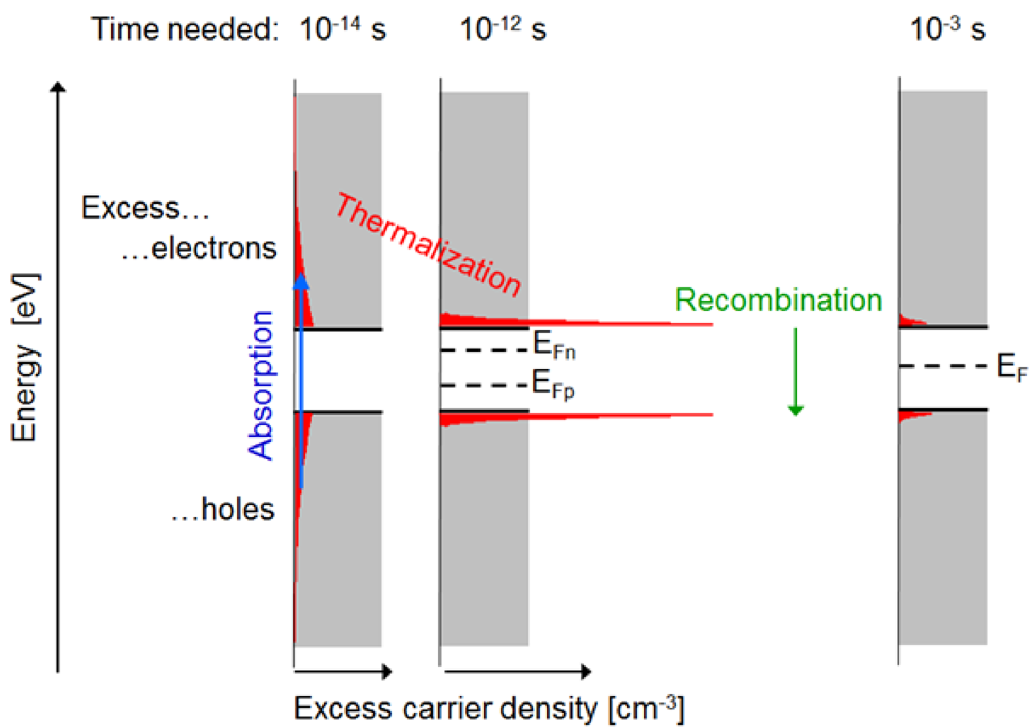




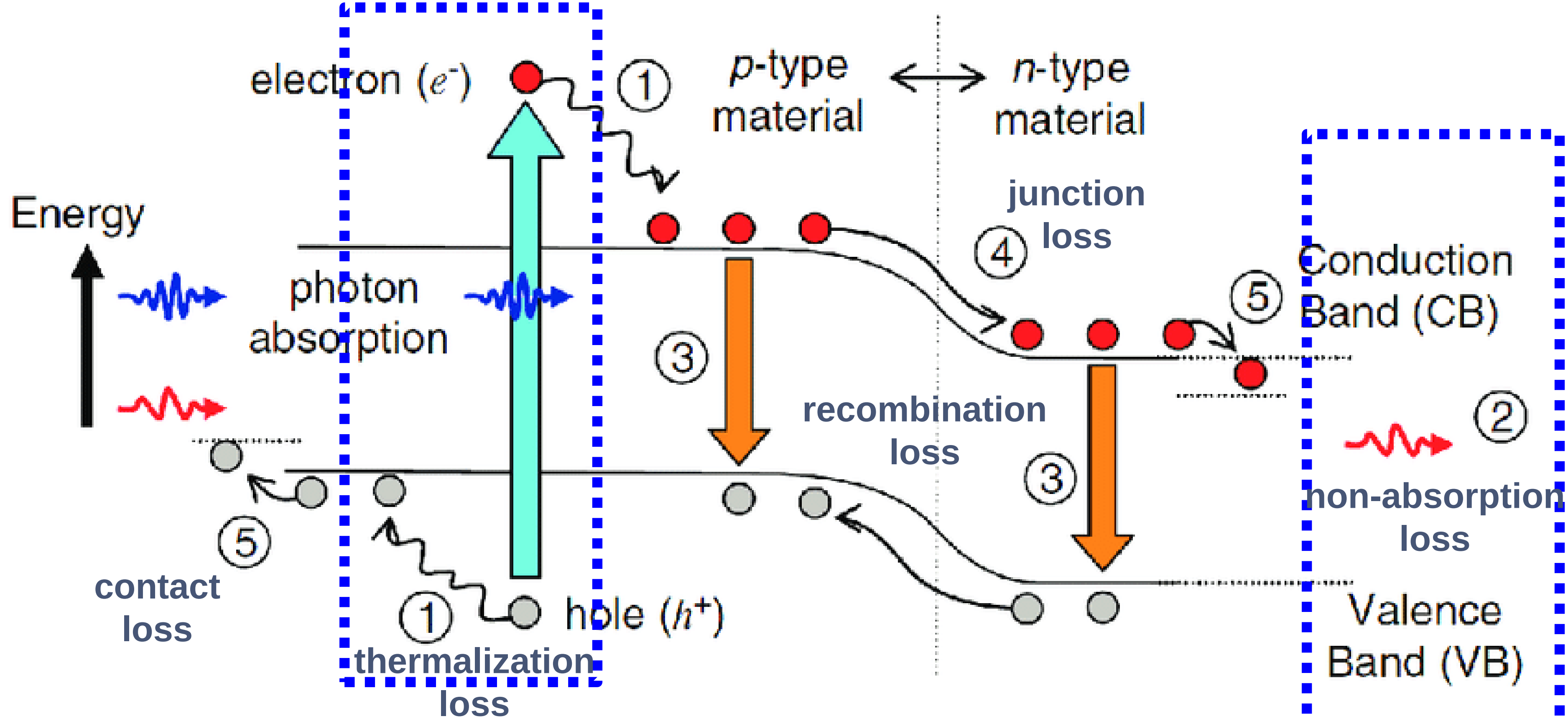


Thermalization

- When photons with energy higher than E_g are absorbed, they generate carriers with higher kinetic energy ("**hot**" carriers), but that energy is **quickly lost (~ ps)** and only E_g of potential energy remains.
- The photogenerated carriers lose any extra kinetic energy by **thermalization** or **cooling**.
- Microscopically, they undergo repeated collisions with the lattice, giving up some of their kinetic energy to **produce phonons** while they decay into a lower energy state, until they are in **thermal equilibrium with the ambient**.



Energy loss mechanisms in PVs

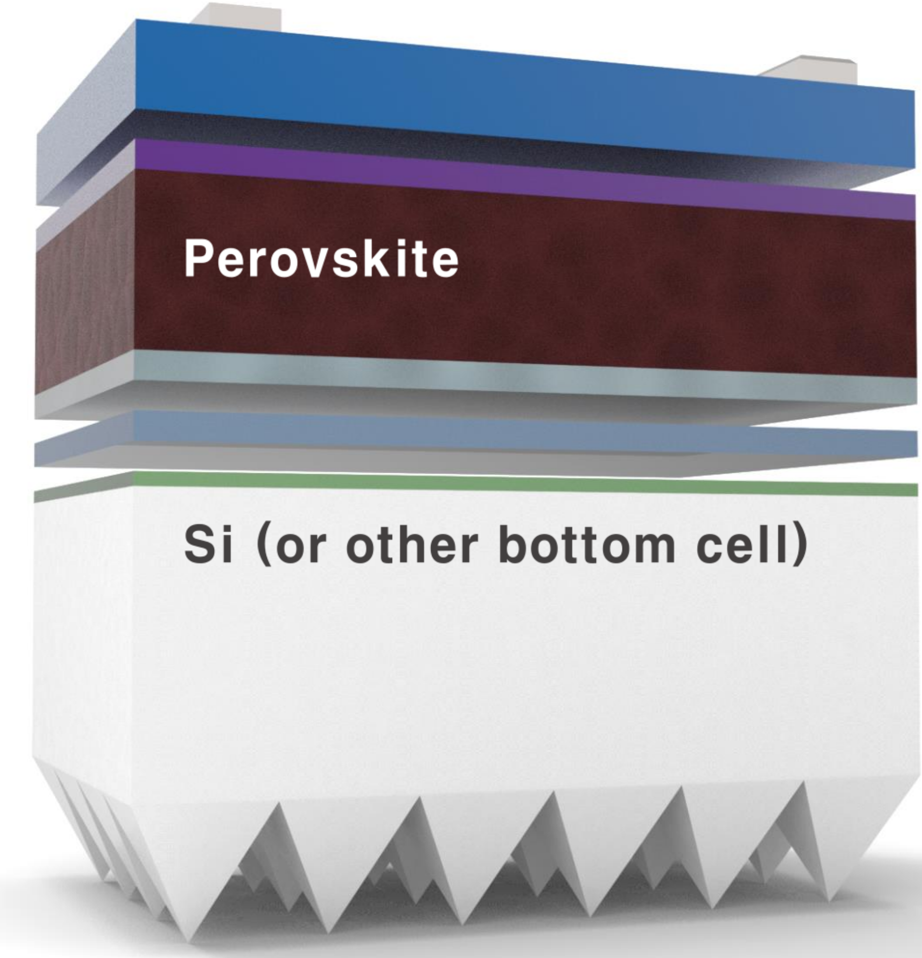


Two inevitable loss mechanisms

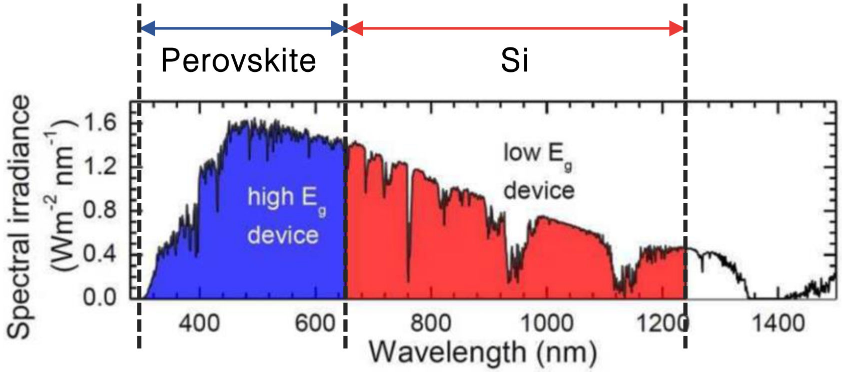
① **Thermalization of hot carriers**

② **Non-absorption of low energy photons**

Perovskite-Si tandem solar cell



[Perovskite/Si tandem solar cell]



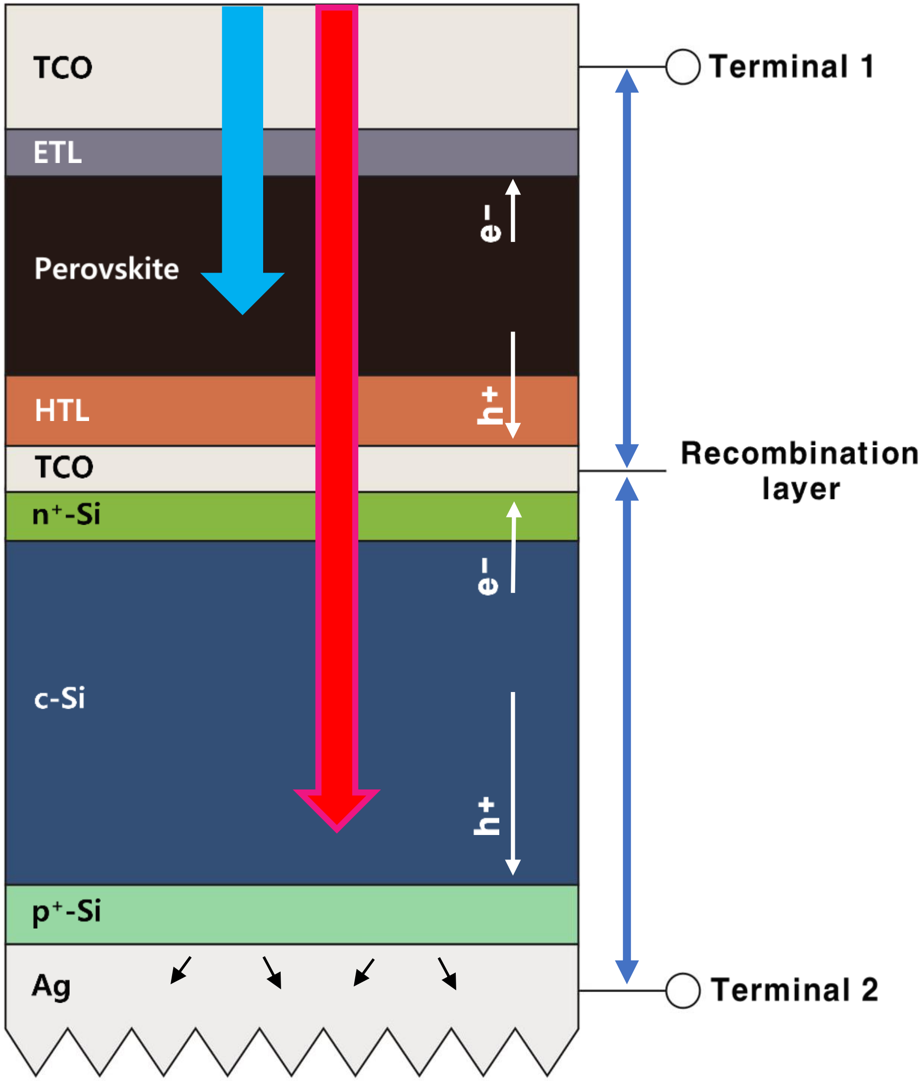
[Solar spectrum]

- High E photons: Perovskite top cell
- Low E photons: Si bottom cell

High efficiency (>35%)

due to less thermalization loss

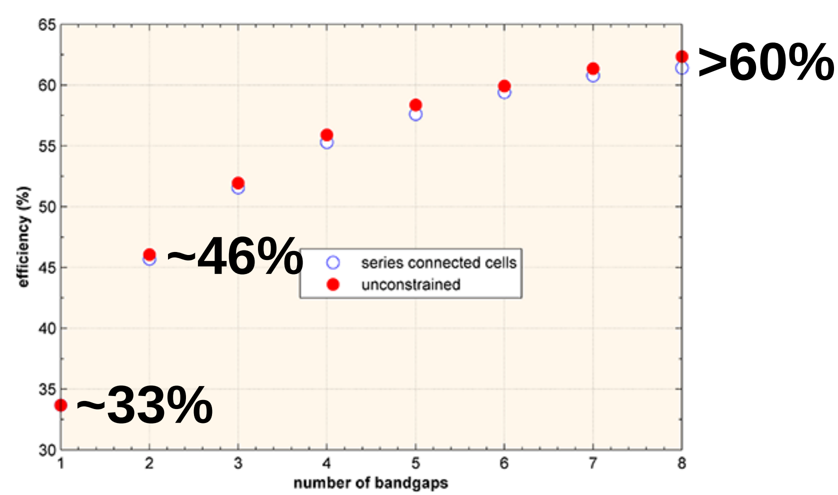
Perovskite-Si tandem solar cell



[Perovskite/Si Tandem]

Series connected subcells

- $V_{tandem} = V_{top} + V_{bottom}$
  → **Increasing subcell voltage!**
- $J_{tandem} = J_{top} * J_{bottom} / (J_{top} + J_{bottom})$
  → **Matching subcell current!**
- **PCE_{tandem} > PCE_{top} & PCE_{bottom}**

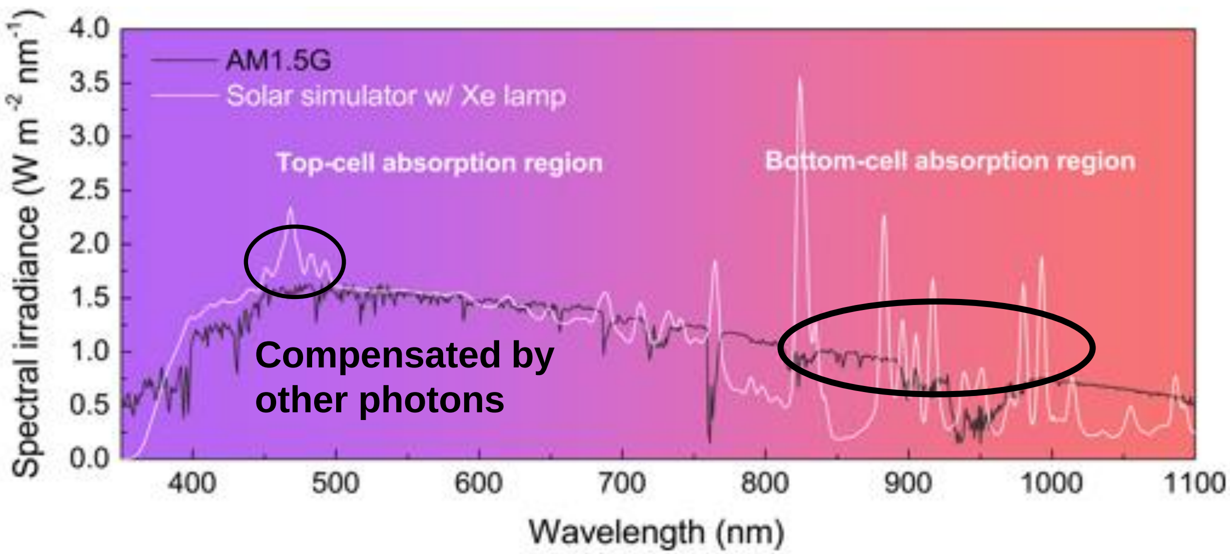


Issues for tandem characterization

Optical issues:

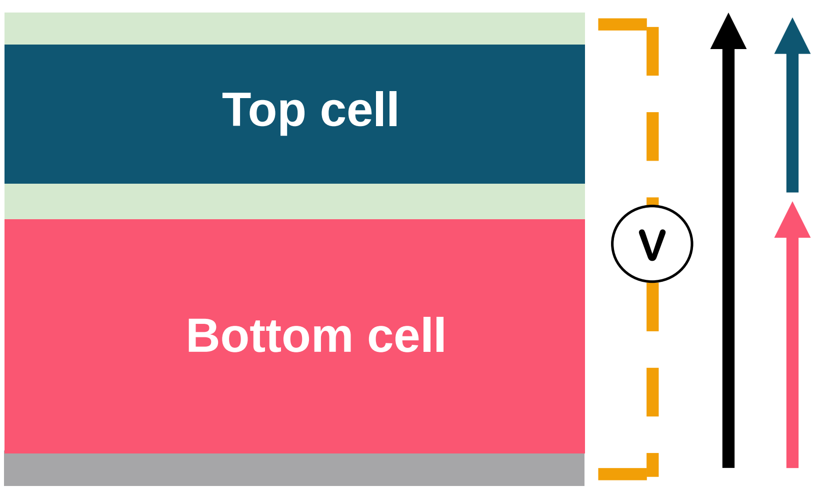
Spectral mismatch

→ Accurate EQE measurement required!



Electrical issues:

Decoupling between subcells is difficult in monolithic devices

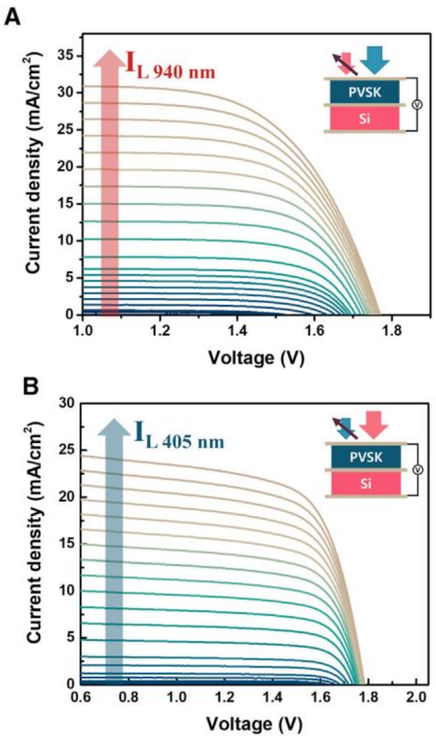


$V_{Tandem} = V_{Top} + V_{bottom}$

$J_{Tandem} = J_{Top} = J_{Bottom}$

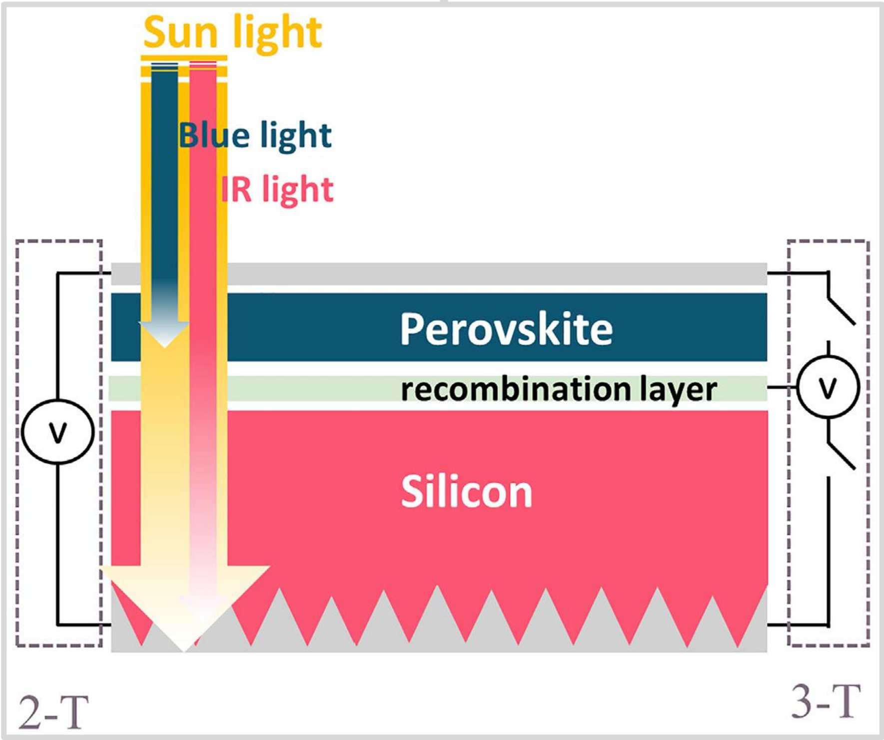
2-T/3-T subcell characterization platform

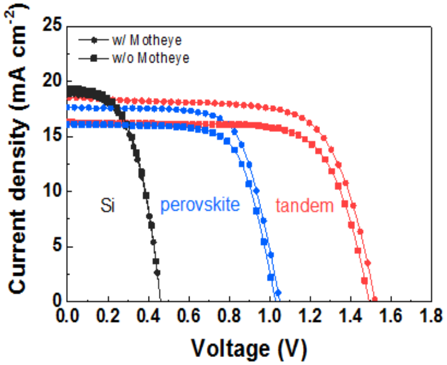
2-T platform
(subcell-selective light bias)

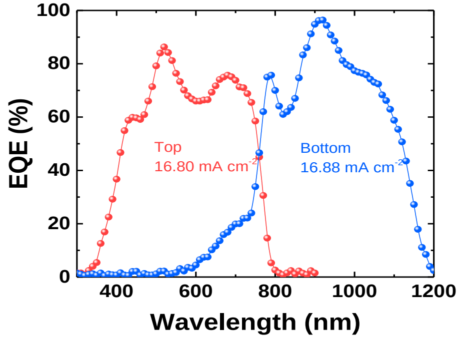


Cell Rep. Phys.Sci., 3, 101076 (2022)

3-T platform
(direct contact to subcells)





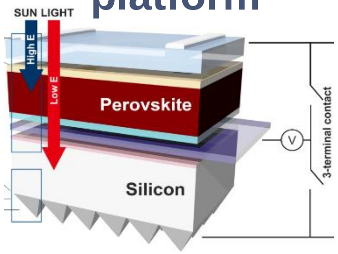


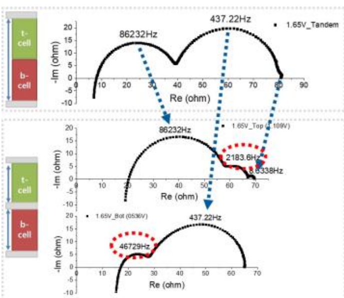
Joule 3, 807-818 (2019)

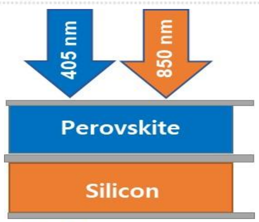
- **2-/3-terminal platforms** for accurate subcell characterization (*e.g.*, EQE without being disturbed by spectral mismatch, and thus accurate J_{SC} values)

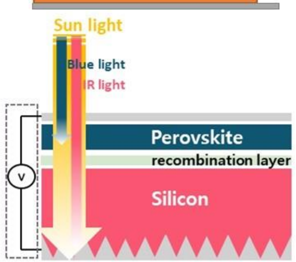
Progress summary

Measurement platform





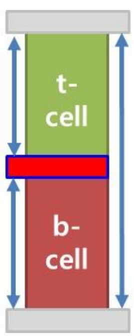


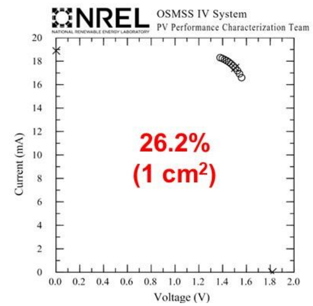


Joule 3, 807-818 (2019)
Cell Rep. Phys.Sci., 3, 101076 (2022)

Photon management (recombination layer, 23.4%)

Joule 3, 807-818 (2019)



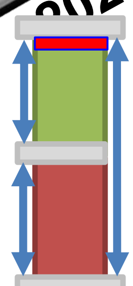


Grain boundary passivation (26.7%)

Science, 368, 155-160 (2020)

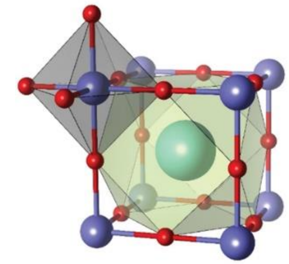
Photon management (window layer, 25.6%)

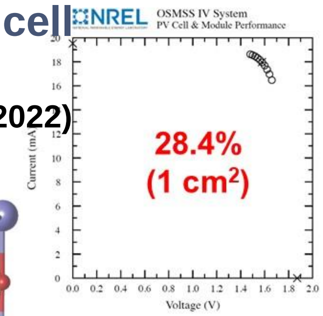
Adv. Optical Mater., 9, 2100788 (2021)



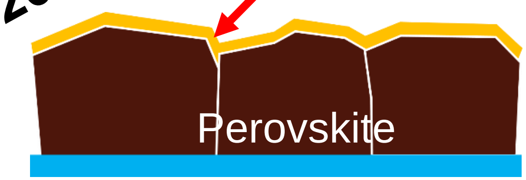
Pure-halide top cell (29.4%)

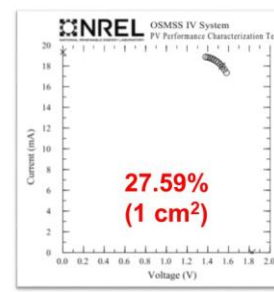
Joule, 6, 2390-2405 (2022)



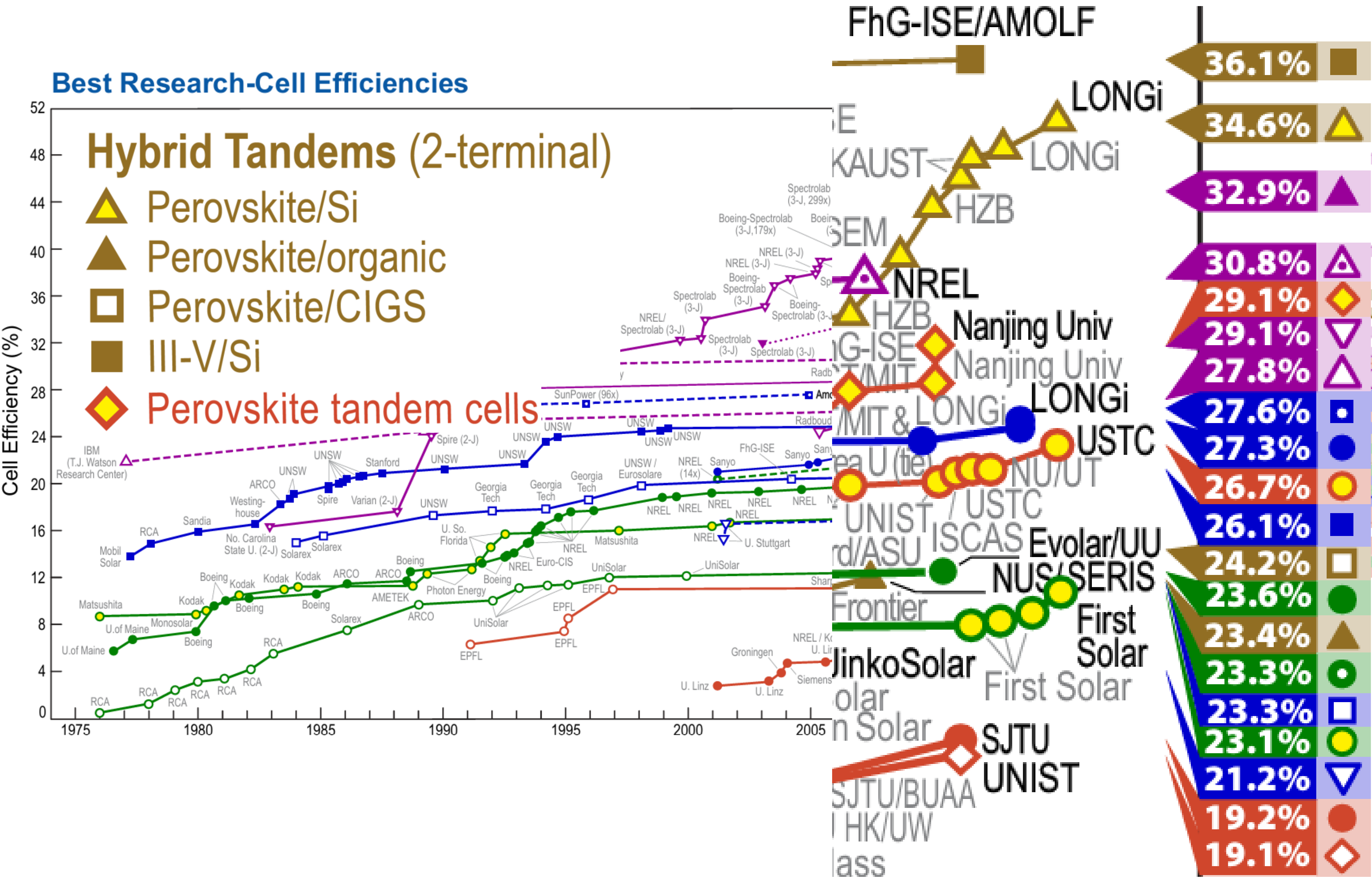


Top surface passivation (28.0%)



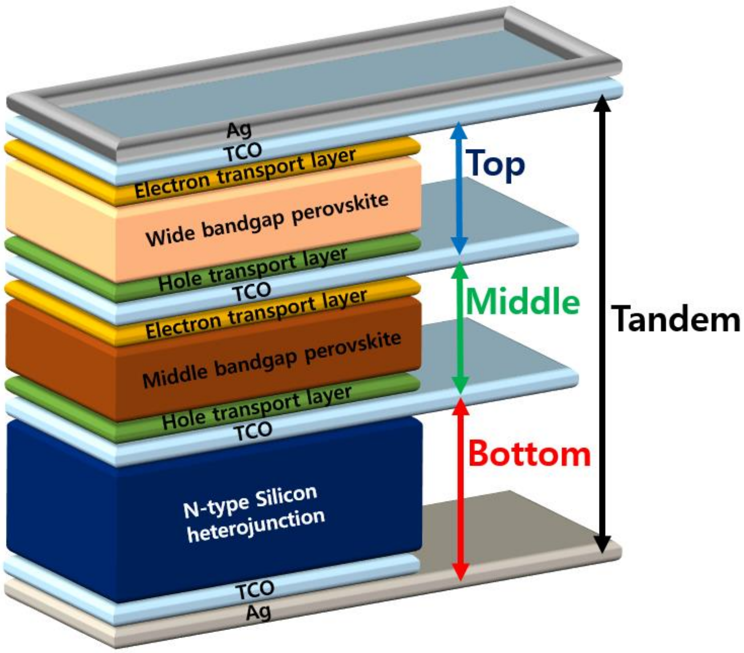


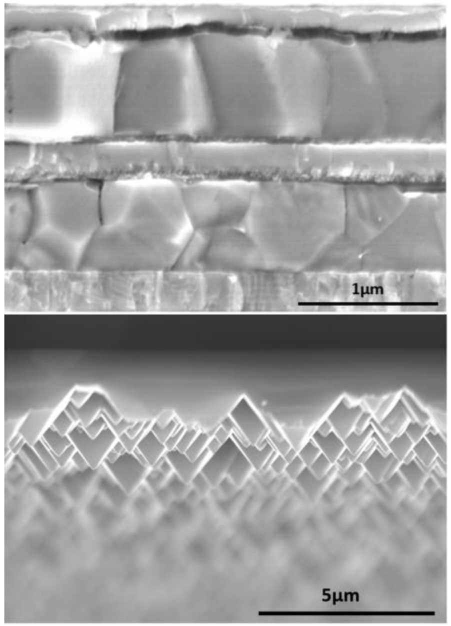
New NREL efficiency chart



Contents

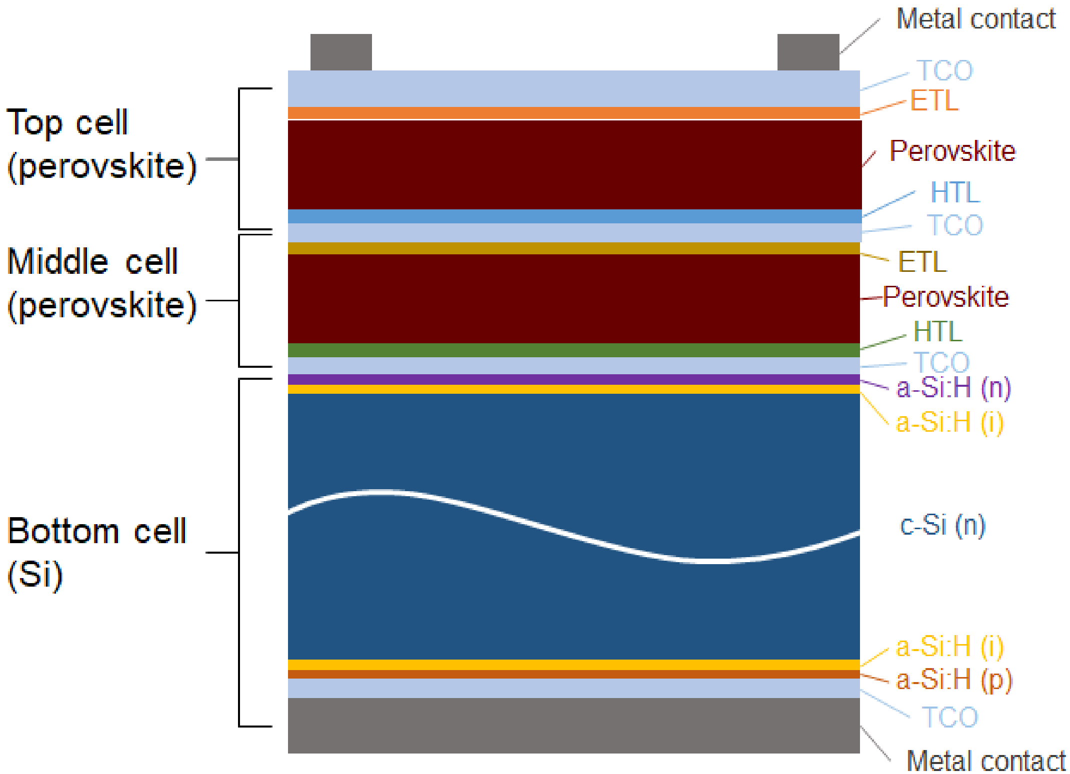
- Tandems beyond perovskite/Si 2J tandems
  - Perovskite/perovskite/Si 3J tandems

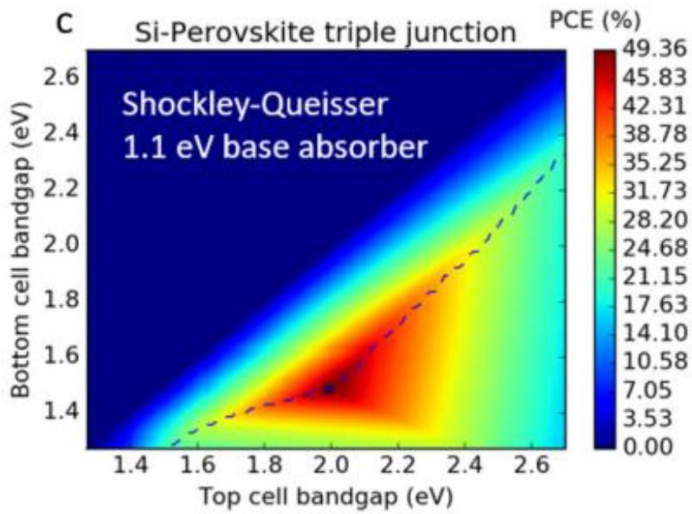




Choi et al., ACS Energy Lett., 8, 3141-3146 (2023)

Perovskite-based 3J tandem



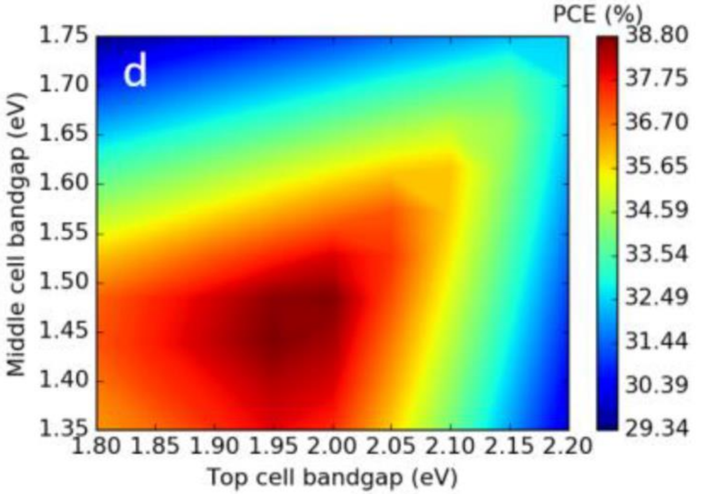


- **SQ limit: 49.36%**
- **Considering interfacial layers: 38.8%**

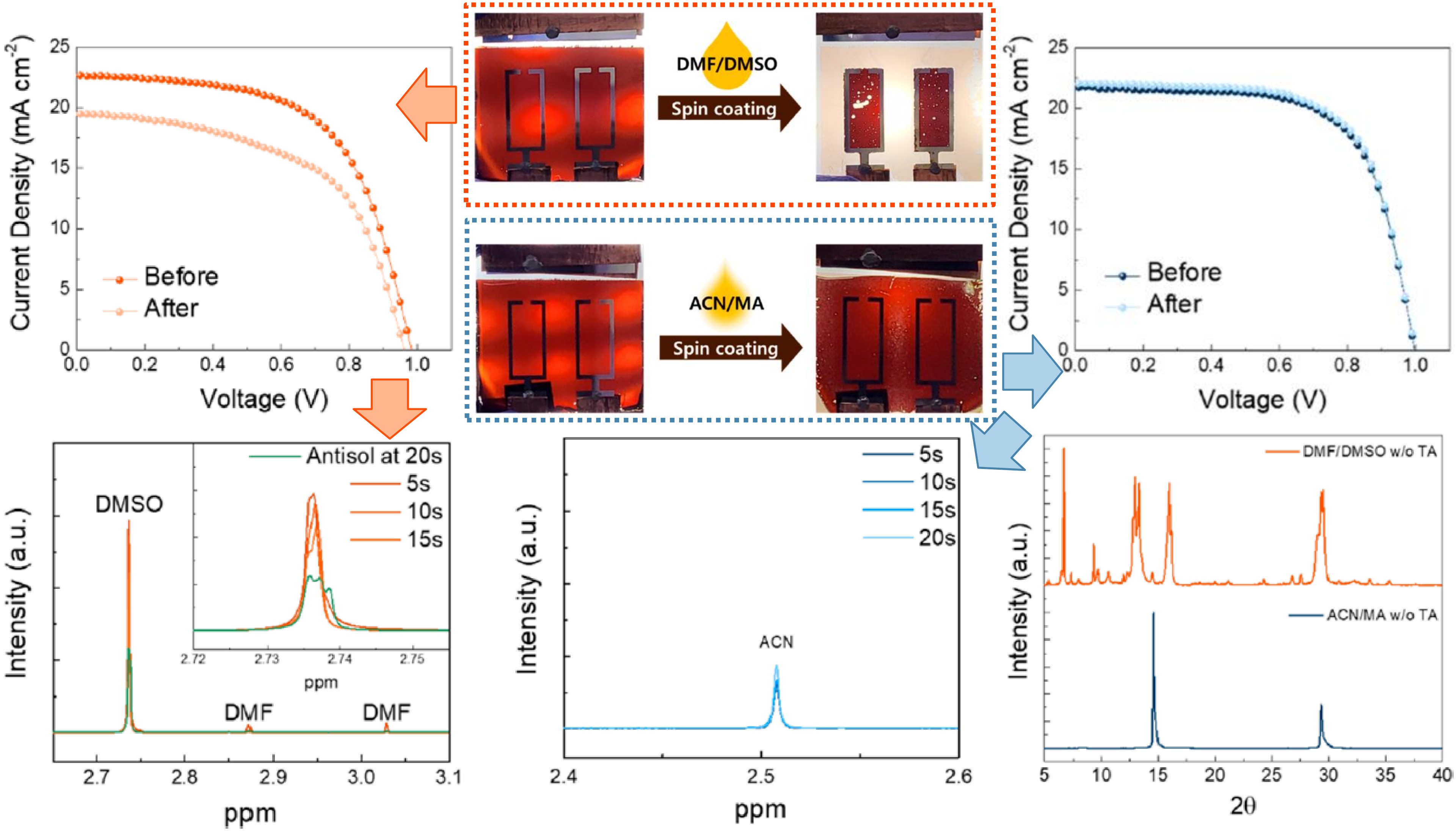
top cell / middle cell / bottom cell

~ 2.0 eV / ~1.5 eV / 1.1 eV (c-Si)

- Poor performance and photo-instability of top cells
- Middle cell degradation during top cell processing



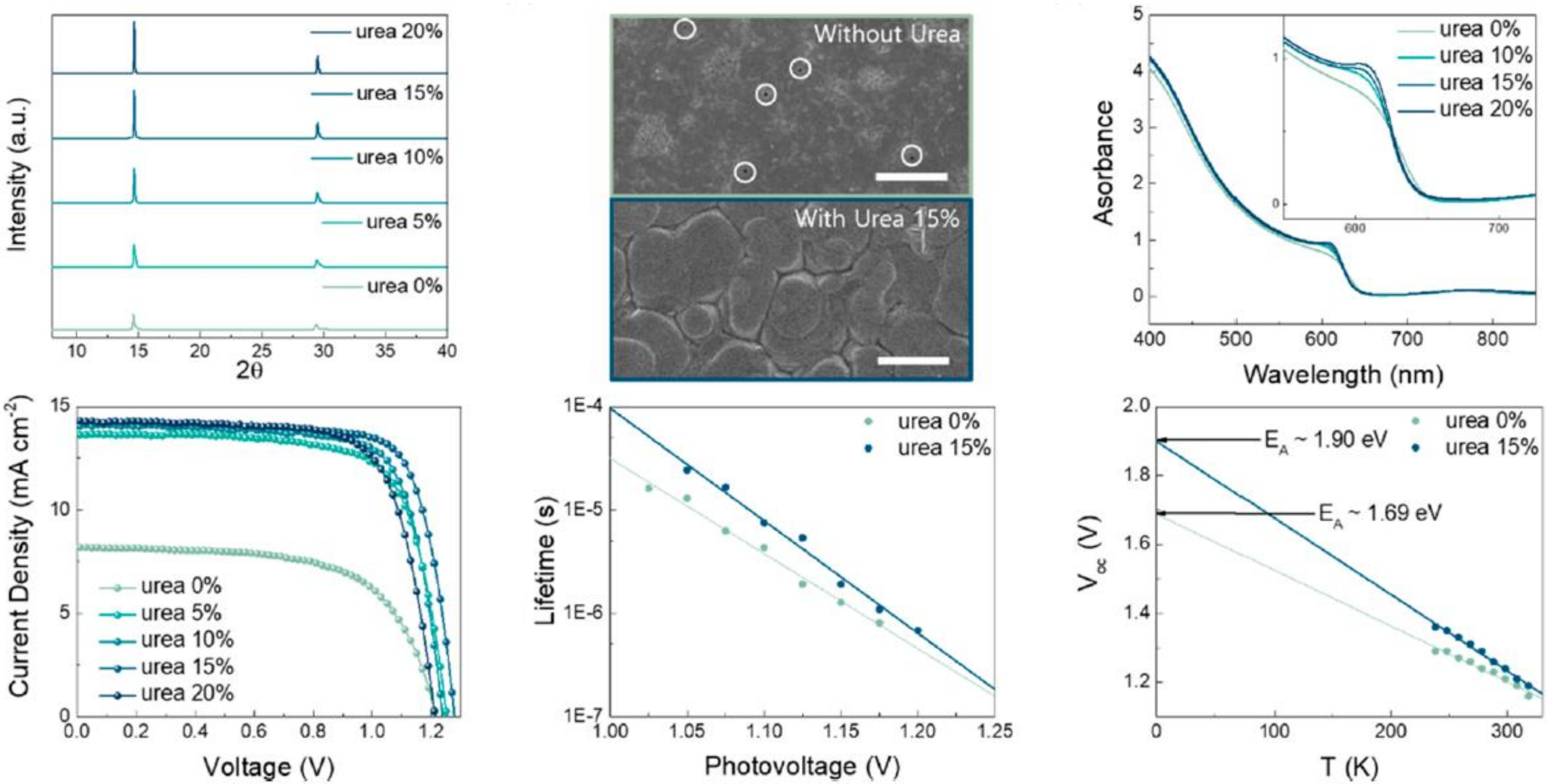
Volatile solvents for PVSK tandems



- New **volatile solvent** mixture prevents degradation of the underneath subcell.

Choi et al., ACS Energy Lett., 8, 3141-3146 (2023)

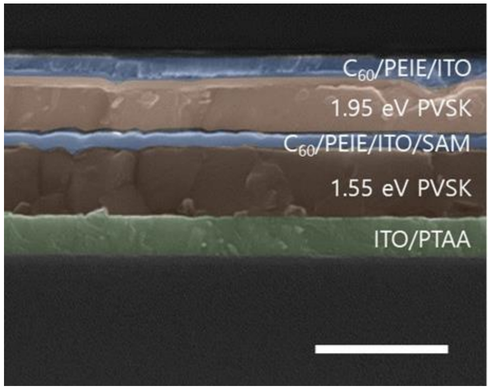
Enhanced crystallinity by Urea additive

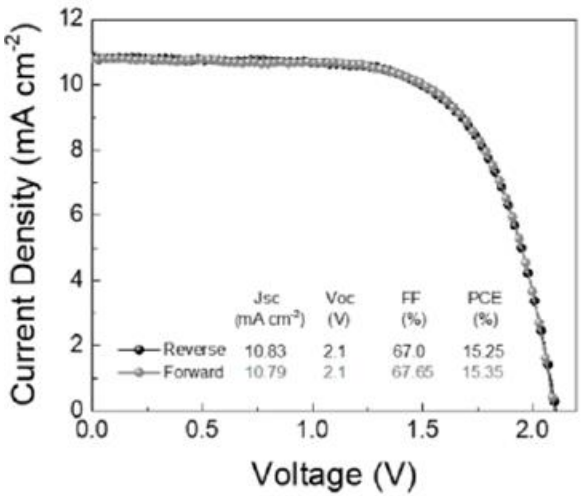


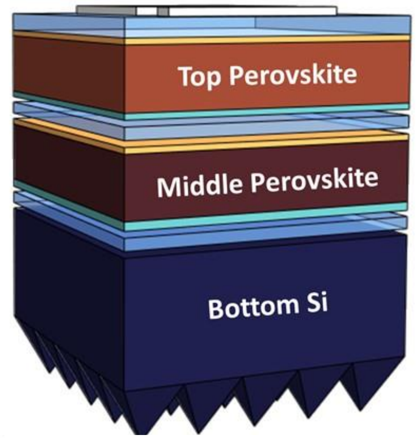
- Addition of **Urea** significantly **enhanced the crystallinity** of 1.96 eV PVSK films.
- Enhanced **light absorption** and **defect passivation** → Improved PV performances

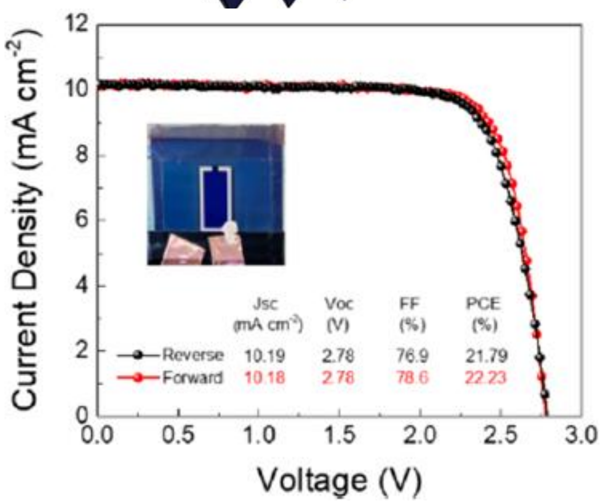
Choi et al., ACS Energy Lett., 8, 3141-3146 (2023)

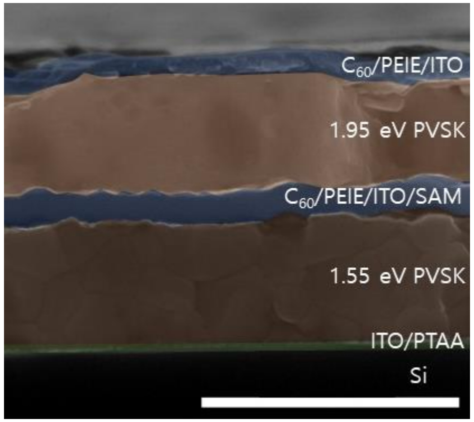
Perovskite/perovskite/Si 3J tandems

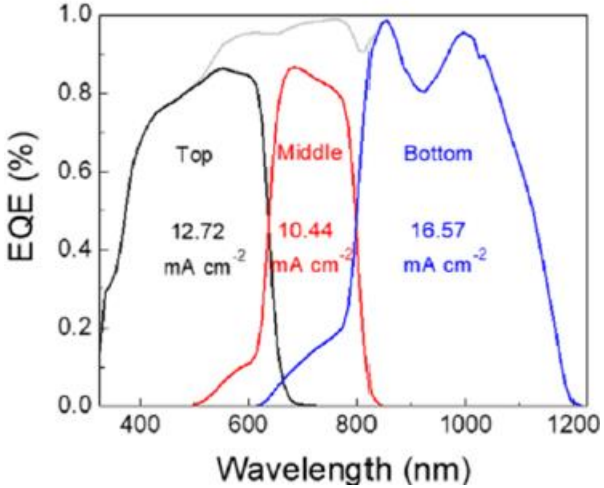










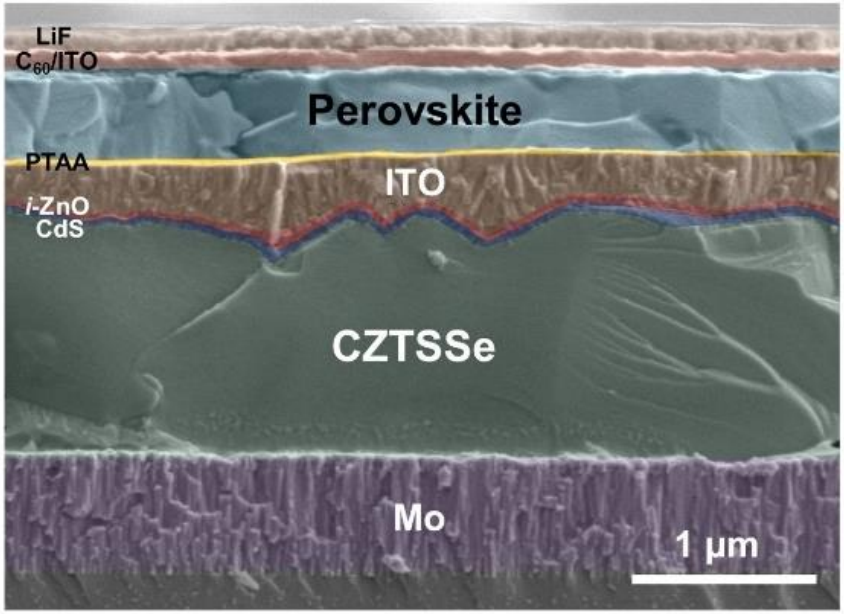


Choi et al., ACS Energy Lett., 8, 3141-3146 (2023)

- Perovskite(1.95eV)/perovskite(1.55eV) 2J tandem with 15.35% efficiency could be prepared as a results of the **solvent/additive engineering**.
- Final 3J tandem exhibited a high conversion efficiency of **22.23%**.

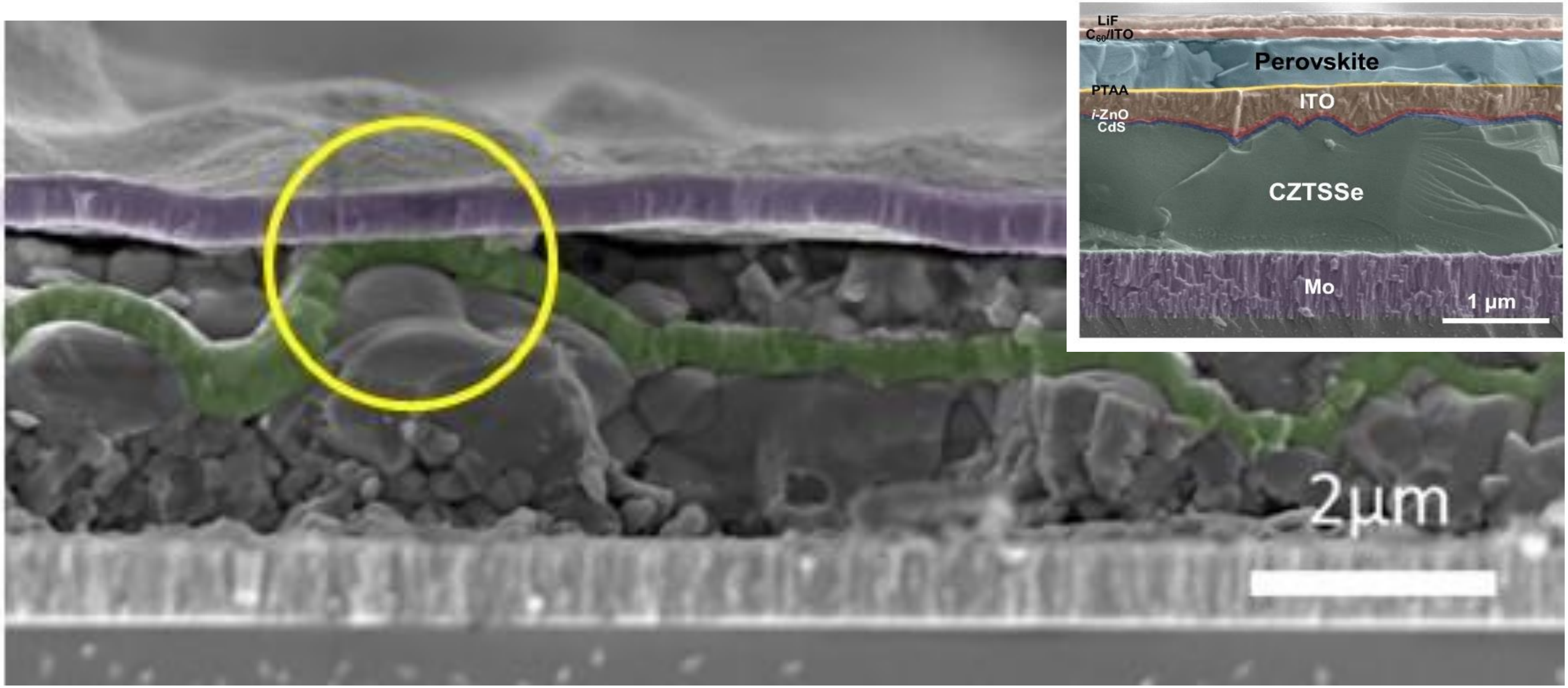
Contents

- Tandems beyond perovskite/Si 2J tandems
  - Perovskite/CZTSSe 2J tandems



Song et al.,ChemSusChem, 15, e202102350 (2022)
Hwang et al., Energy Environ. Mater., e12489 (2024)
Hwang et al., Small, 20, 2307175 (2024)

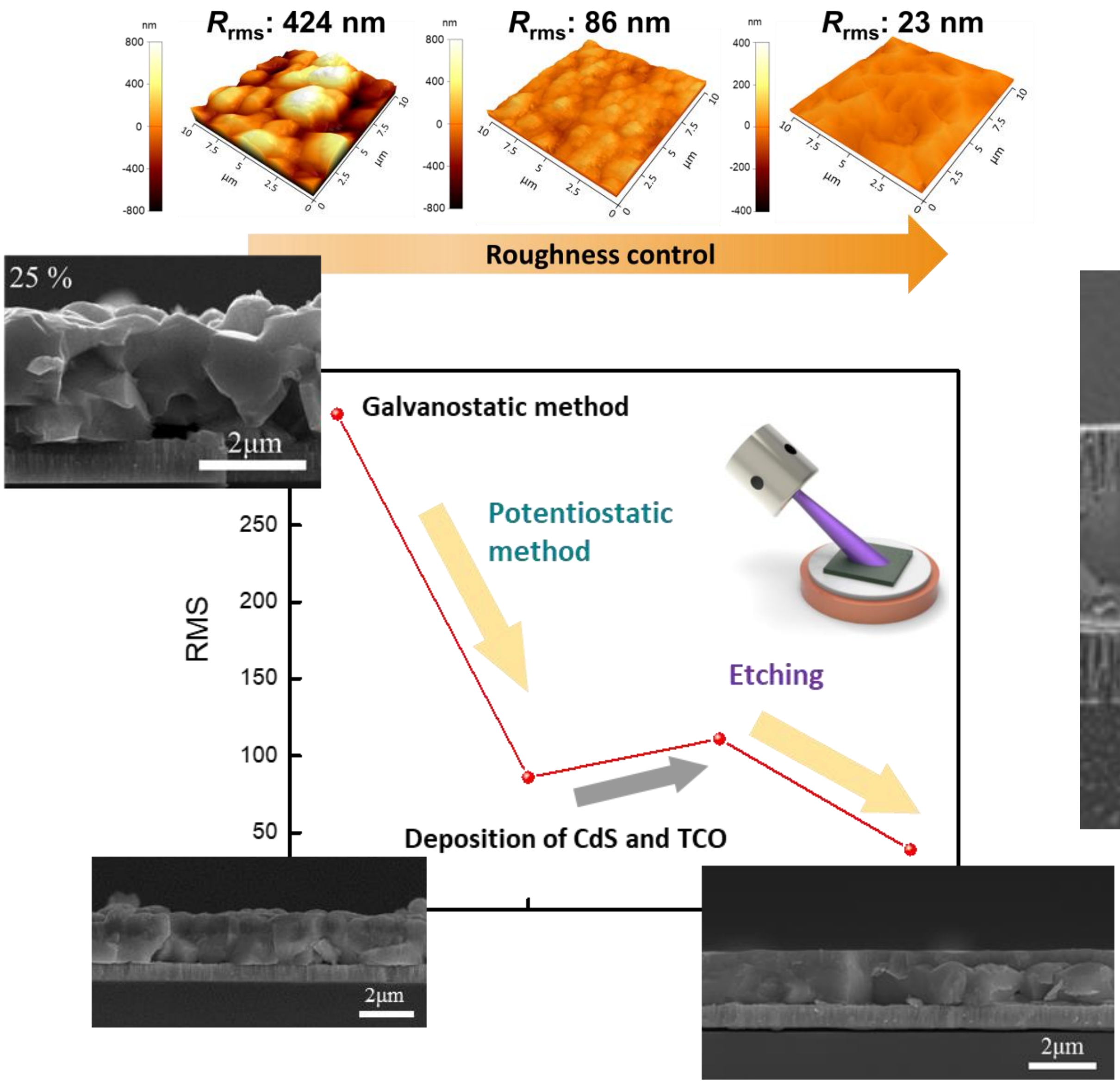
Effect of bottom cell roughness

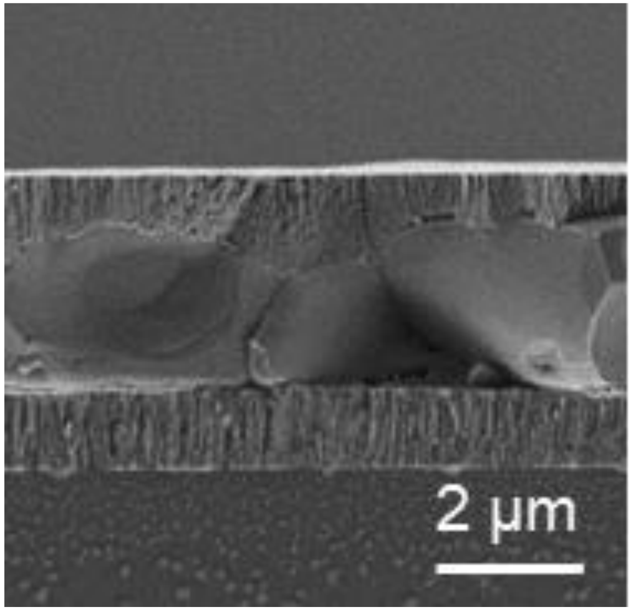


- CZTSSe bottom cell should have extremely flat surface in order to fabricate the perovskite tandems

Hwang et al., Energy Environ. Mater., e12489 (2024)

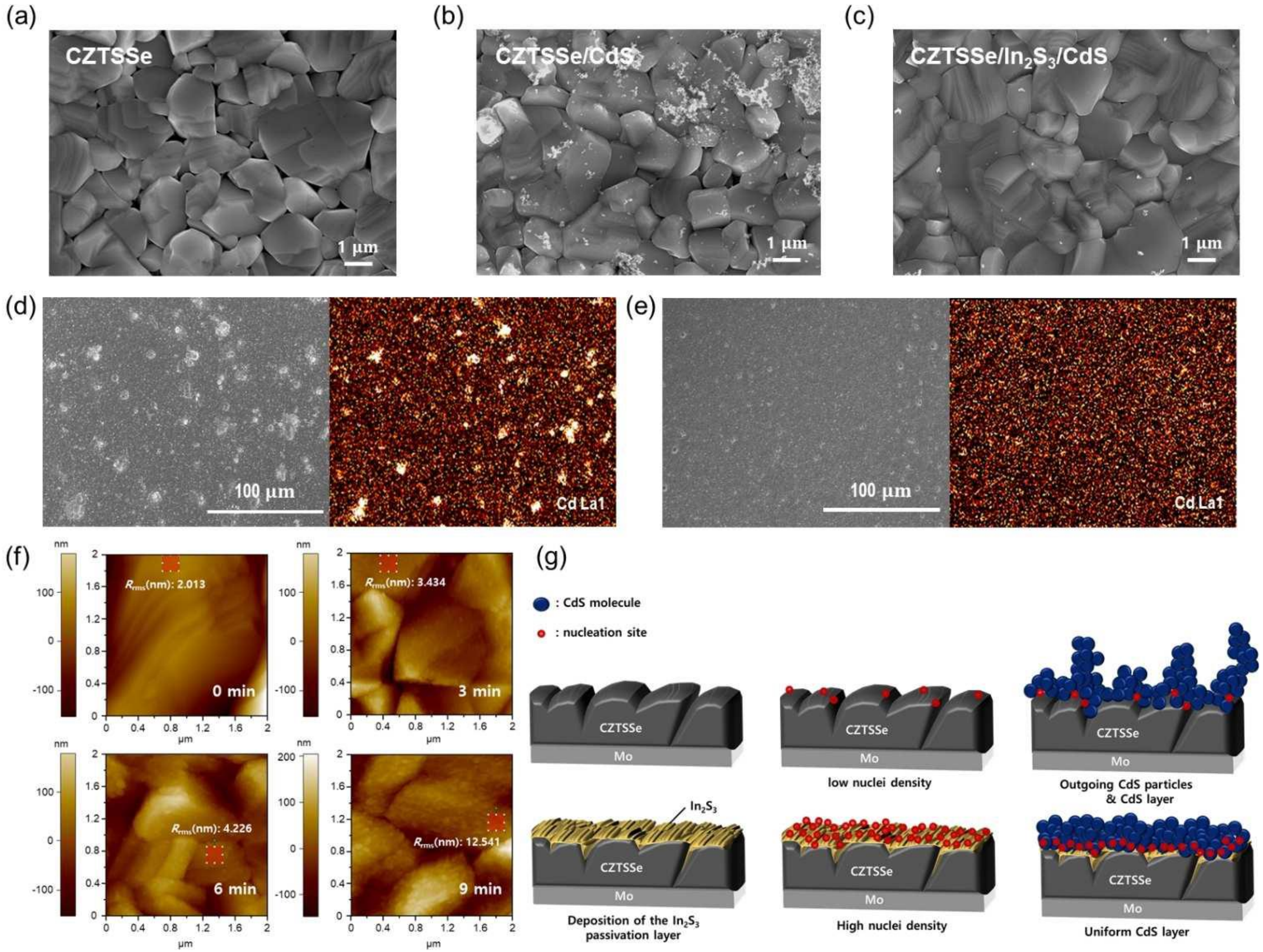
Strategy for the roughness control





Hwang et al., Energy Environ. Mater., 7, e12489 (2024)

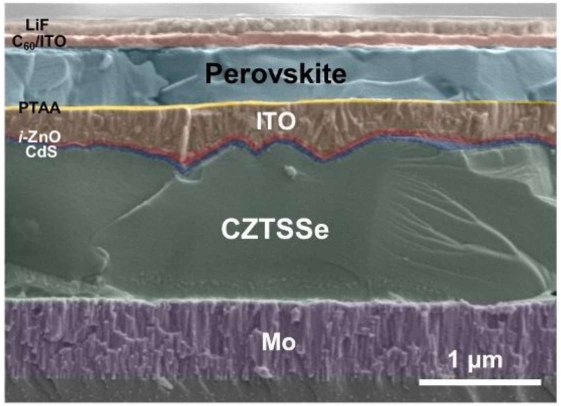
Strategy for the roughness control

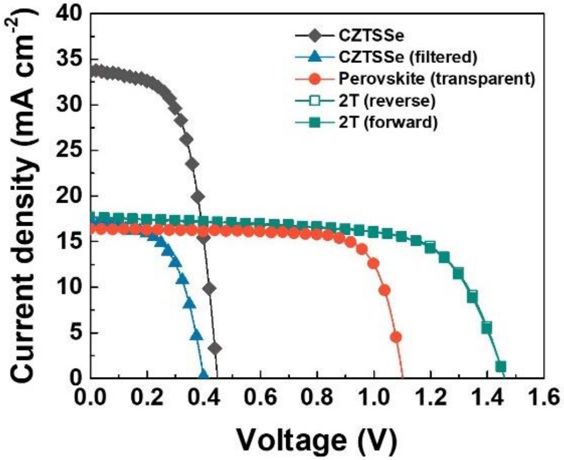


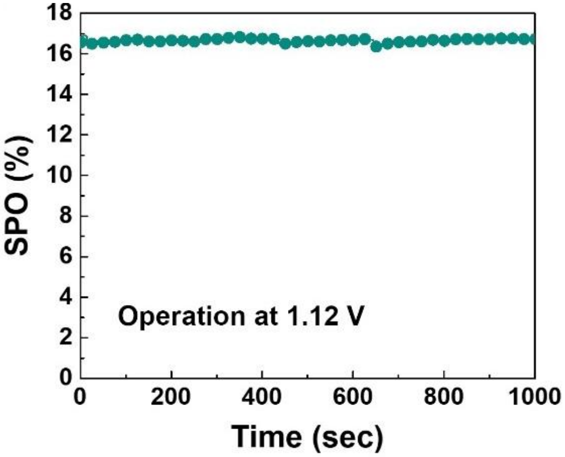
- Introducing additional In_2S_3 layer between CZTSSe and CdS prevents the agglomeration of the CdS clusters during the CBD process

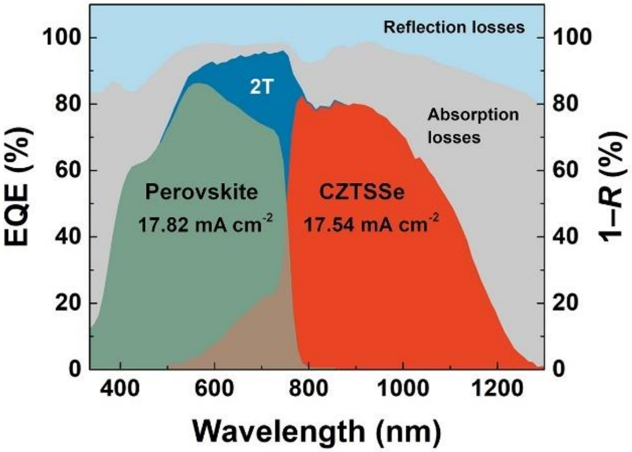
Song et al.,ChemSusChem, 15, e202102350 (2022)

Perovskite/CZTSSe tandems





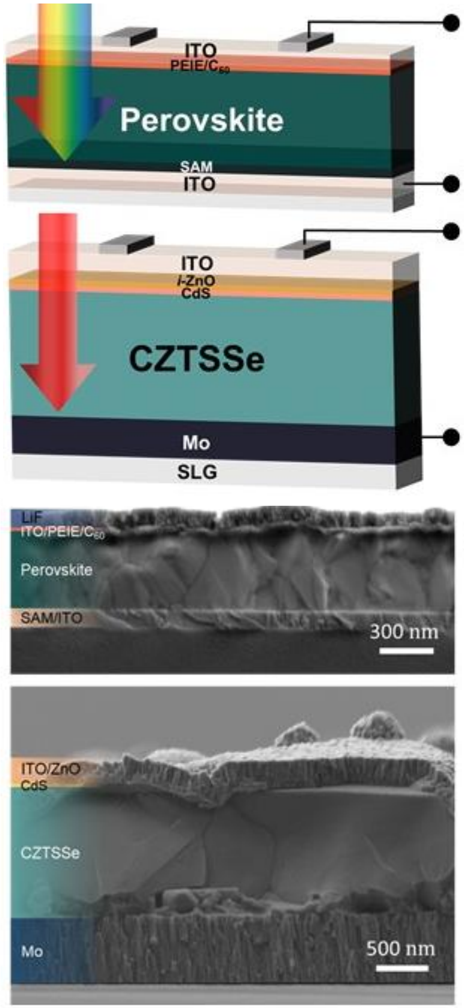


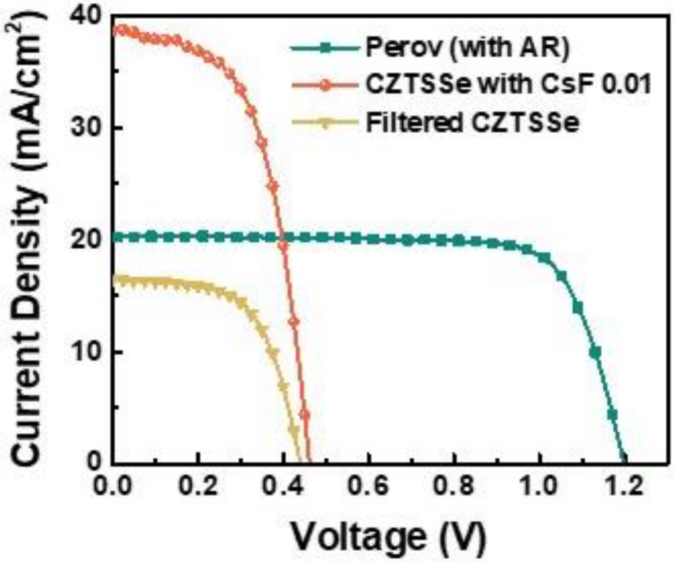


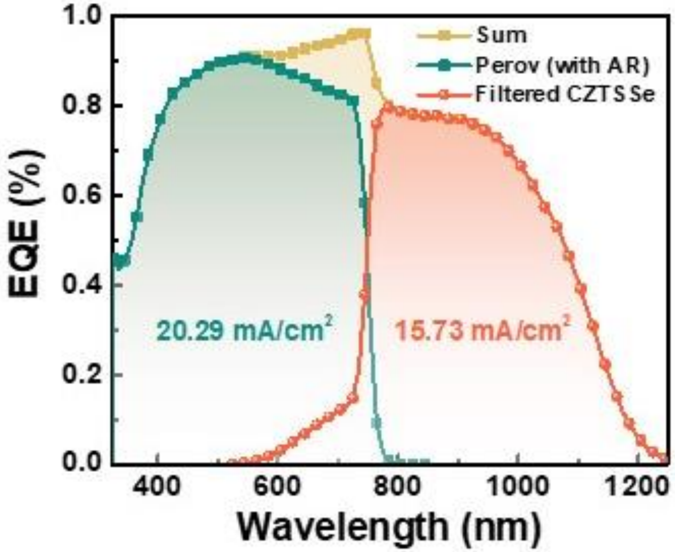
- Perovskite/CZTSSe tandem with the world record efficiency (**17.5%**) can be prepared with the flat CZTSSe bottom cell and perovskite top cell (*cf*. previous/current record: **4.5% for tandem** - previous, **14.9% for CZTSSe single cell** - current)

Hwang et al., Energy Environ. Mater., e12489 (2024)

4T PVSK/CZTSSe tandem





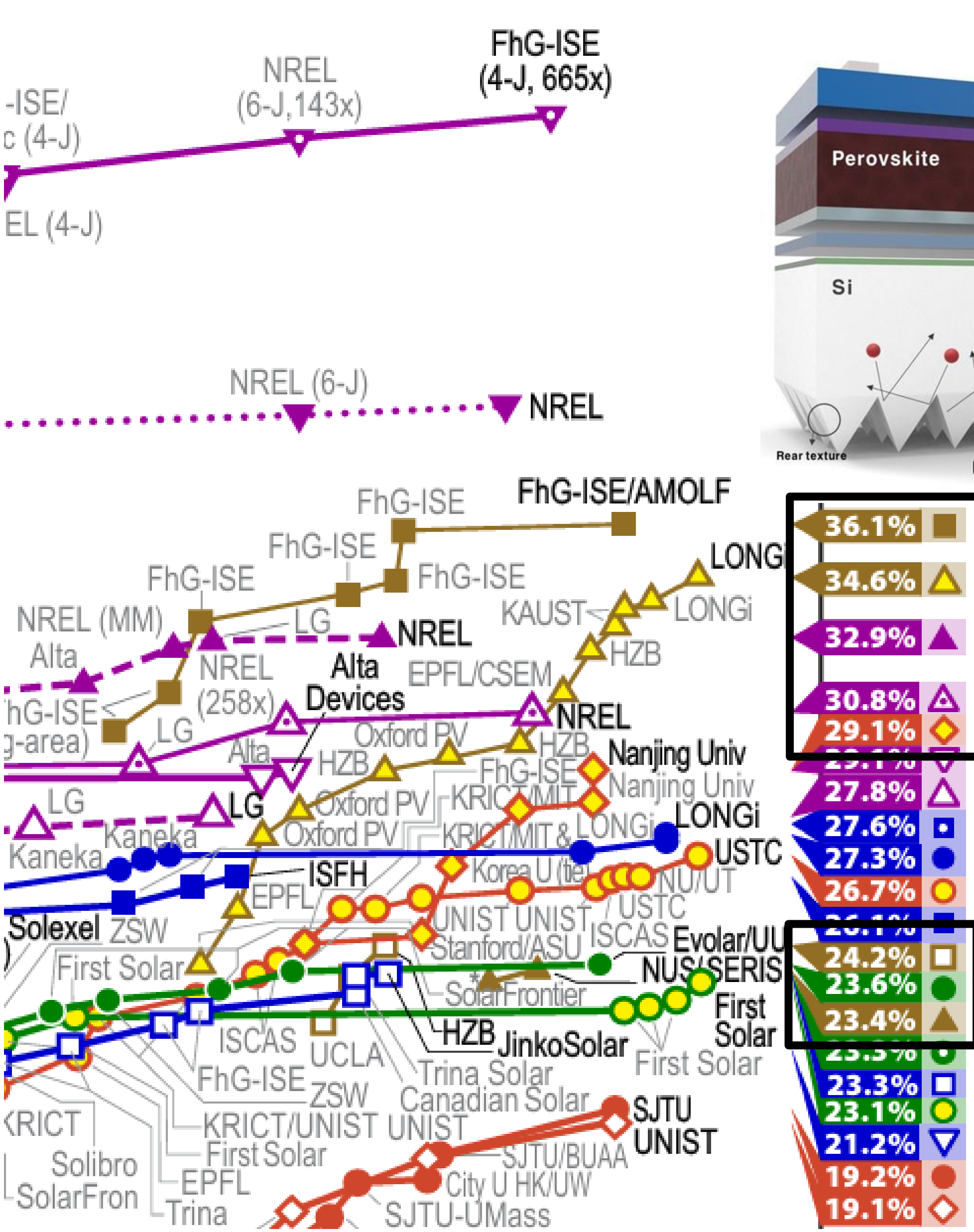


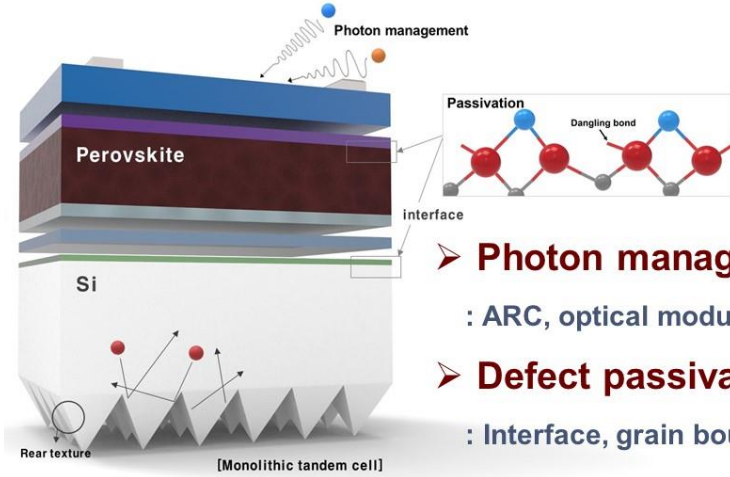
J-V	Jsc (mA/cm^2)	Voc (V)	PCE (%)	FF
Perovskite	20.21	1.19	18.63	0.78
CZTSSe	38.55	0.46	10.20	0.58
Filtered CZTSSe	16.42	0.44	4.38	0.61
Sum			**23.01**	

- Highest reported 4T perovskite/CZTSSe tandem efficiency of ~ 23% could be achieved.

Hwang et al., Small, 20, 2307175 (2024)

Tandem PV: A realistic future





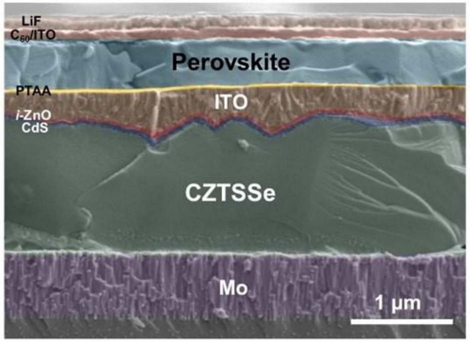
➢ **Photon management**

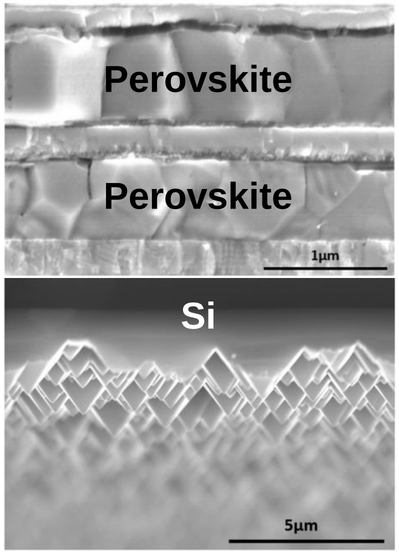
: ARC, optical modulation, texturing etc.

➢ **Defect passivation**

: Interface, grain boundary, etc.

Emerging tandems





Thank you!!

NRF 한국연구재단

KETEP 한국에너지기술평가원

<u>Contact</u>

Jin Young Kim

Professor

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Interface control for perovskite solar cells

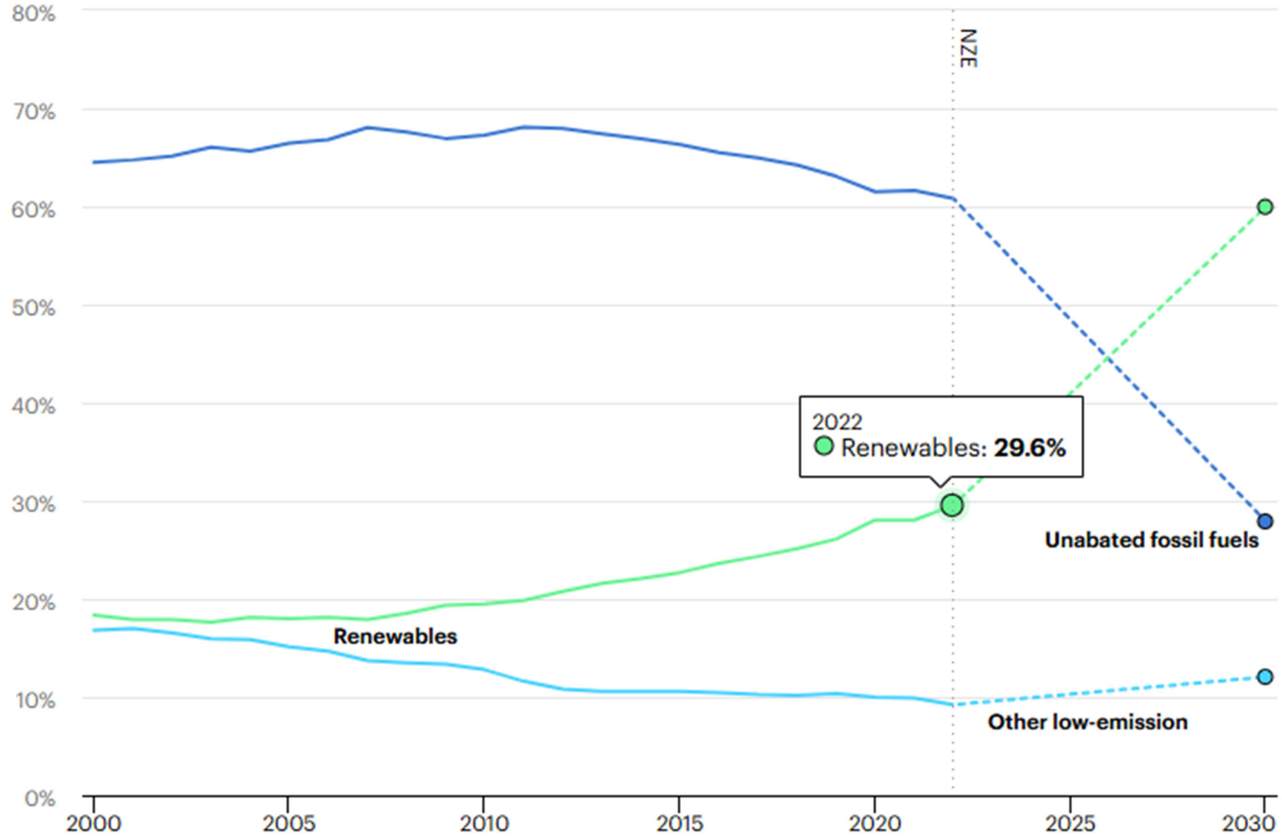
Hui-Seon Kim

Department of Chemistry, Inha University

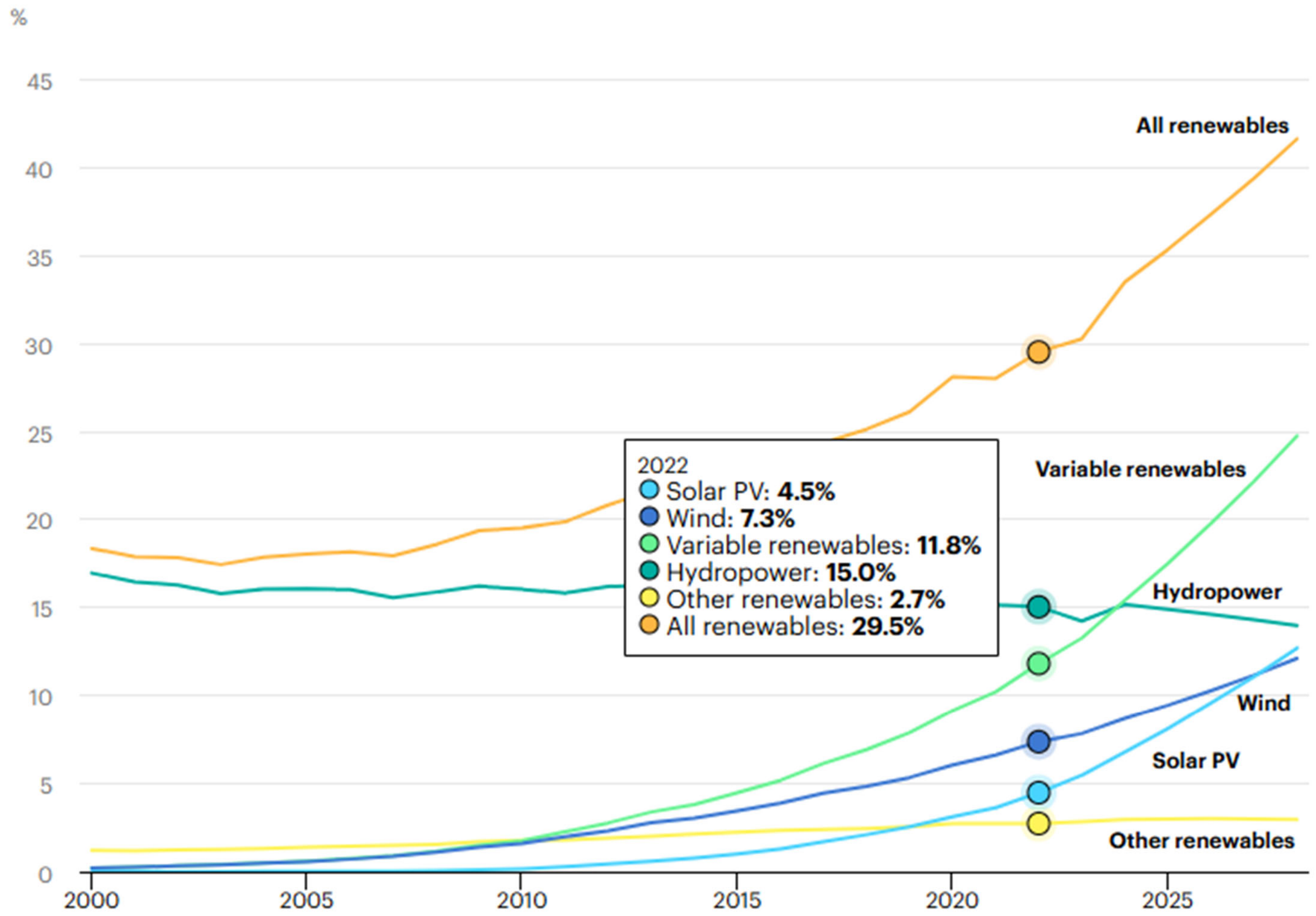
e-mail: hui-seon.kim@inha.ac.kr

Shares of global electricity generation by source

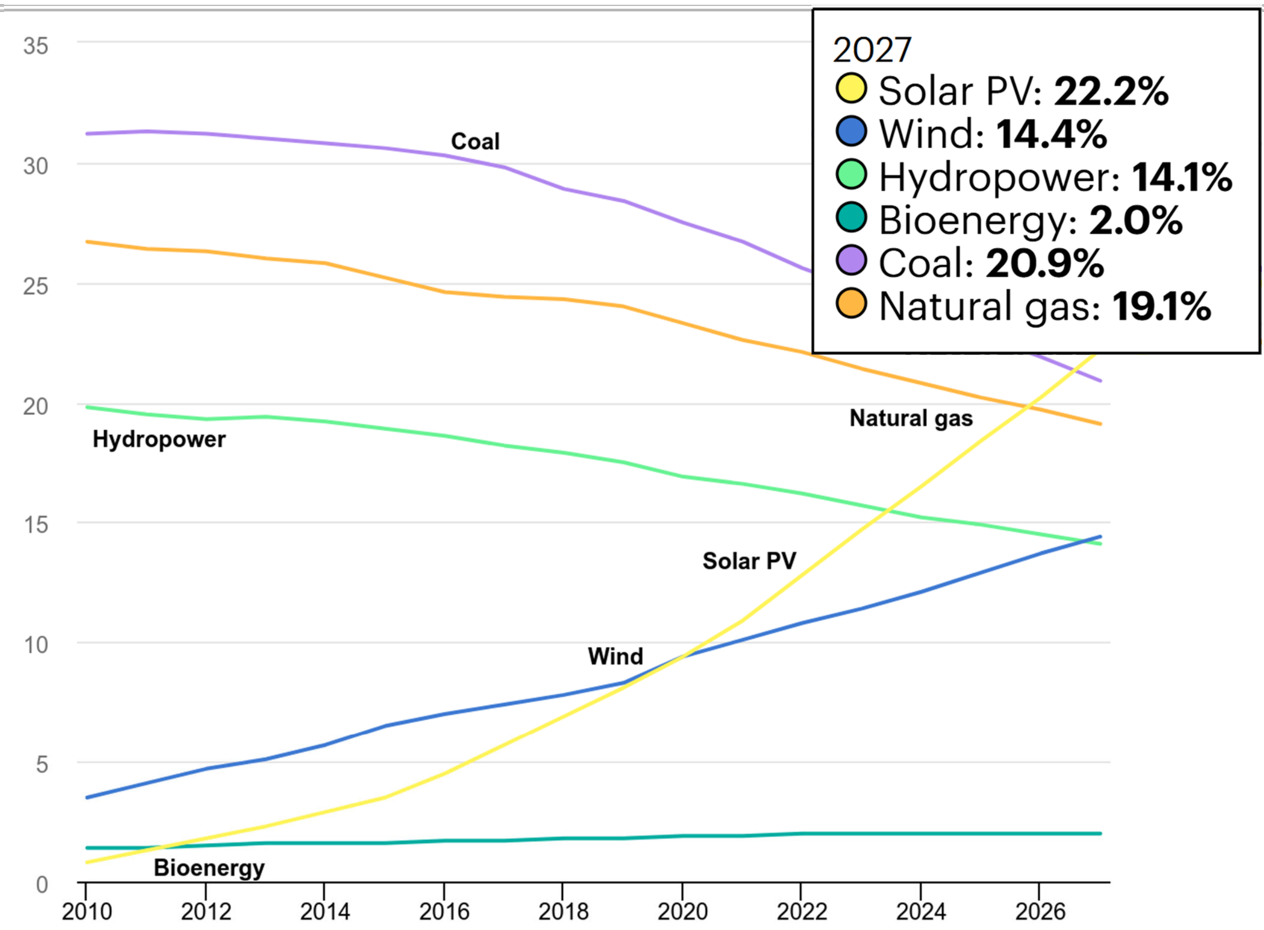
Source: IEA



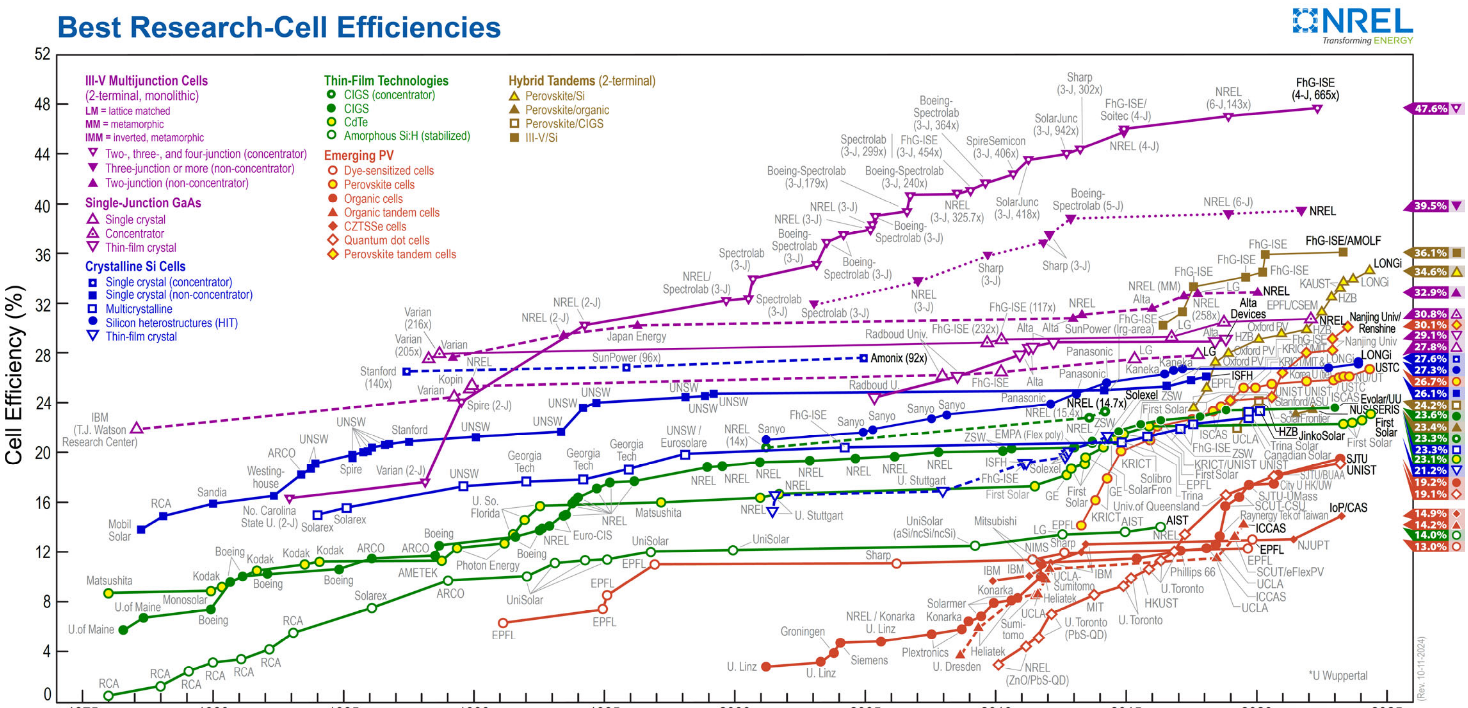
Shares of renewable electricity generation



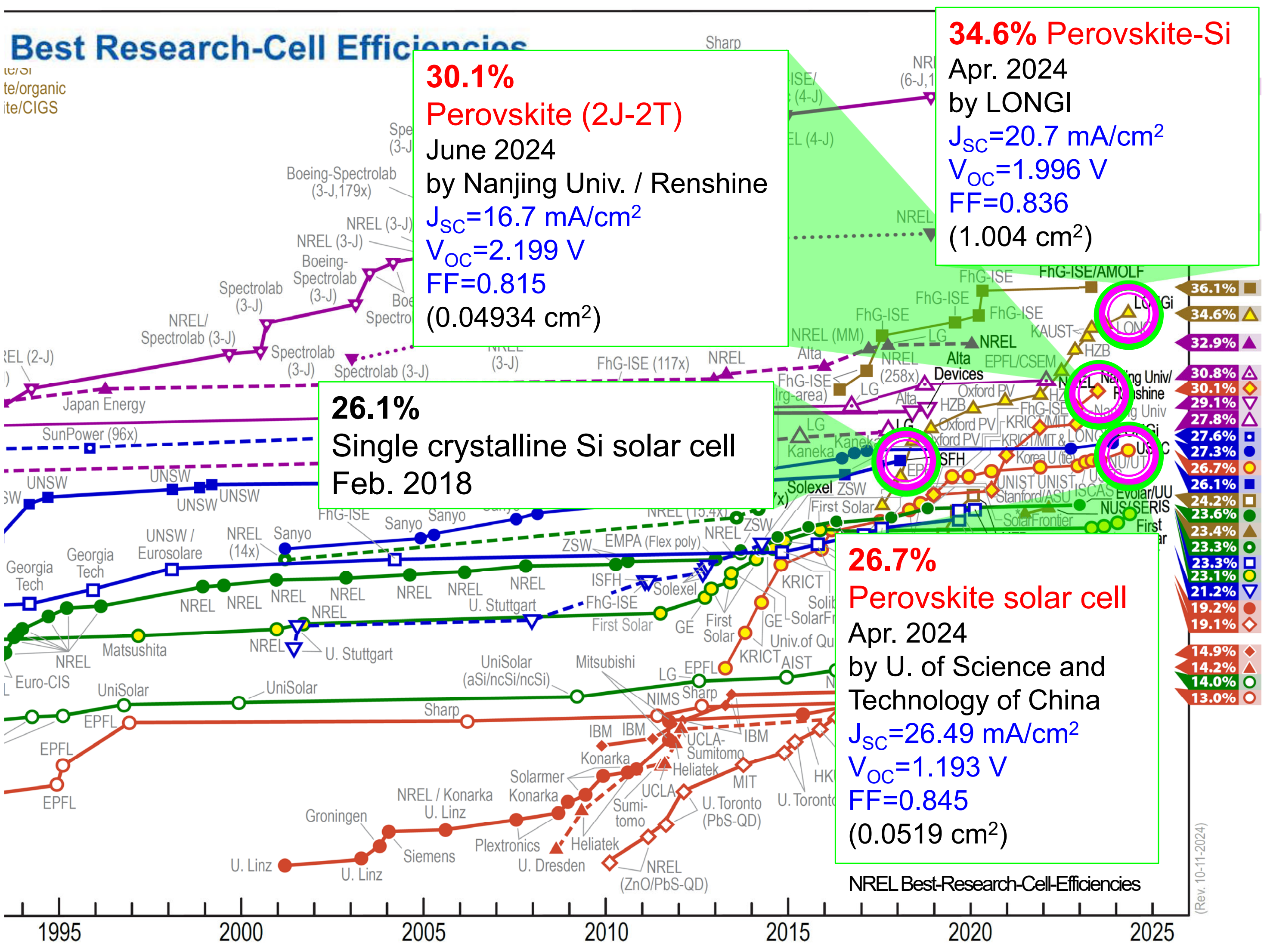
Share of cumulative power capacity



accessed: 14-01-2025

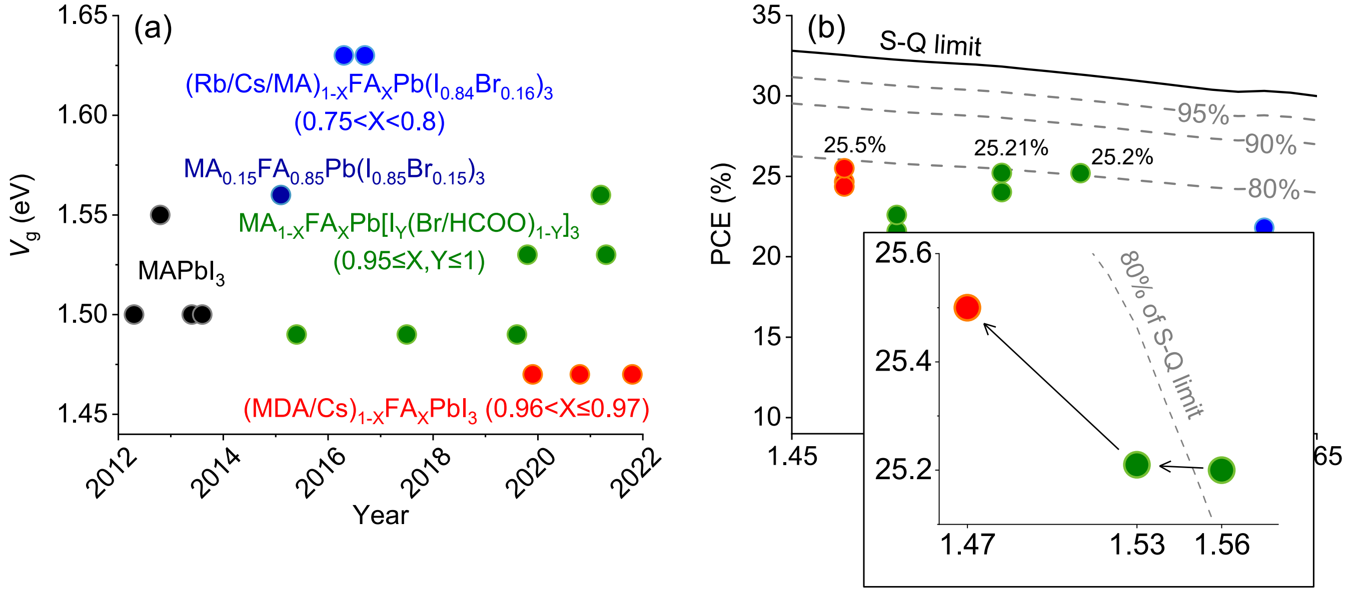


The 8th KAST-Leopoldina Bilateral Symposium



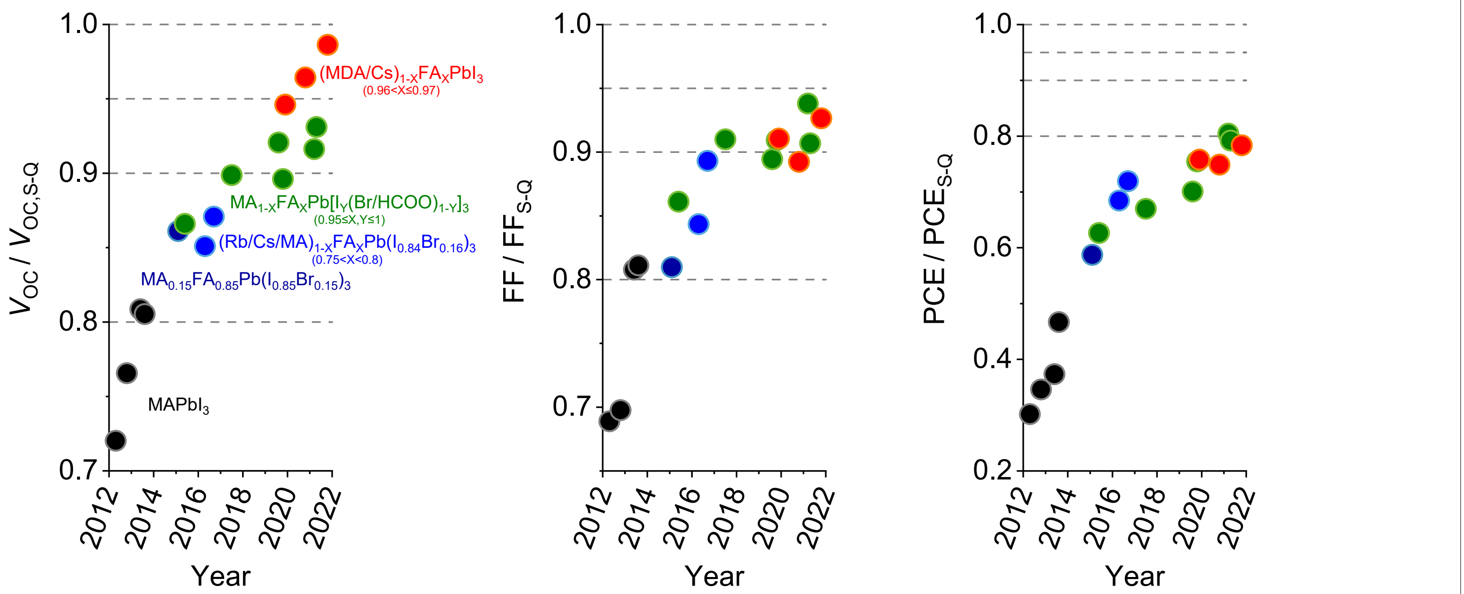
Records of PSCs

Adv. Mater. **2023**, 202204807



Toward the S-Q limit

Adv. Mater. **2023**, 202204807

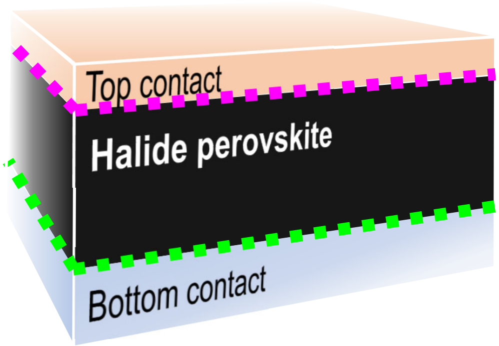


$$qV_{OC} = qV_{OC,S\text{-}Q} + kT\ln(\eta_{ext})$$

$$\eta_{ext} = \frac{P_{esc}B_{rad}n^2}{A_{SRH}n + P_{esc}B_{rad}n^2\left(1+{n_r}^2(1-R)\right) + C_{Aug}n^3}$$

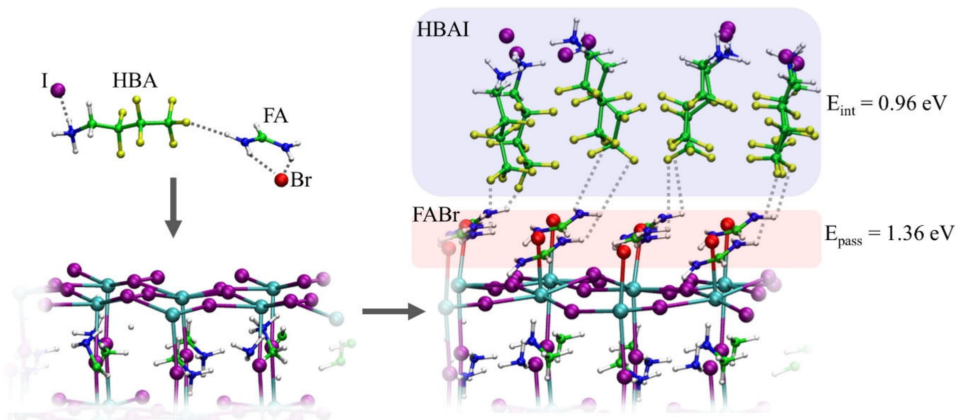


B Yang J Suo H-S Choi



- ***Top*** **interface: surface reconstruction**
- ***Bulk*** grain boundary: crystal growth
- ***Bottom*** interface: strain control

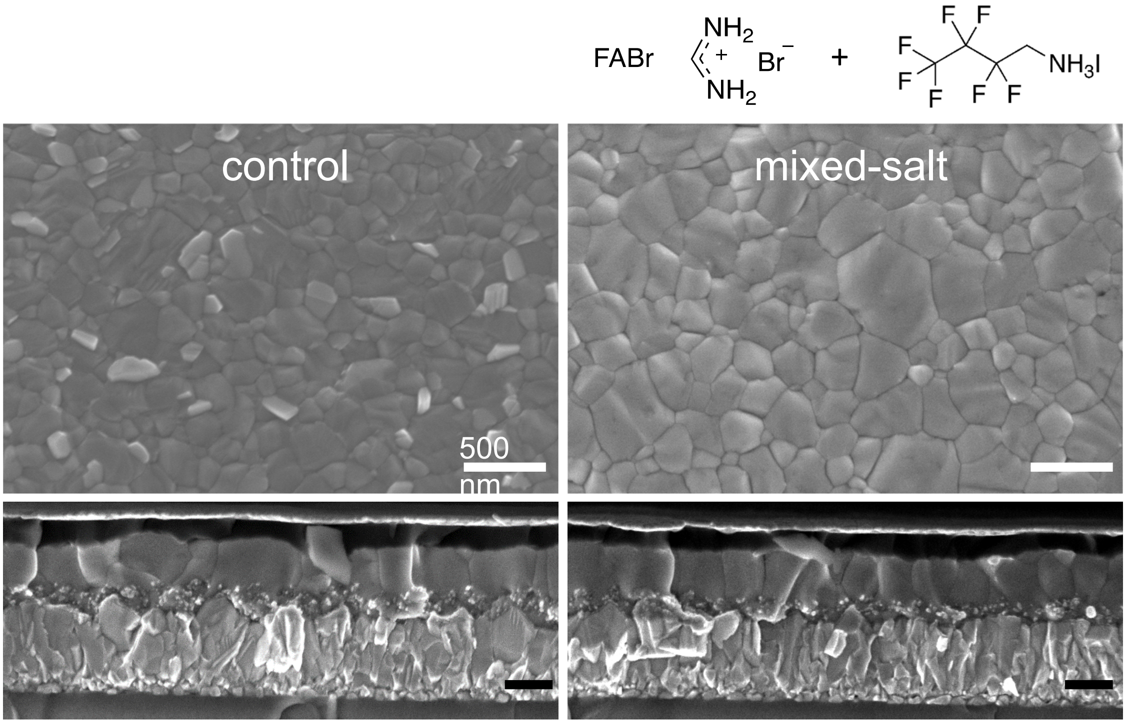
Formation of passivation layer



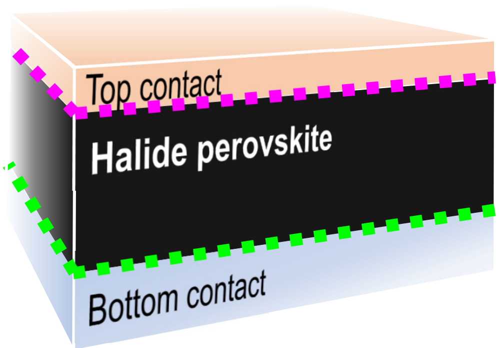
	CPD (mV)	Work function
Control	123.477	5.11
HBAI-FABr	249.181	4.98

Adv. Funct. Mater. **2021**, 2102902

Reconstructed morphology by the mixed-salt



Y-N Lee J-H Choi



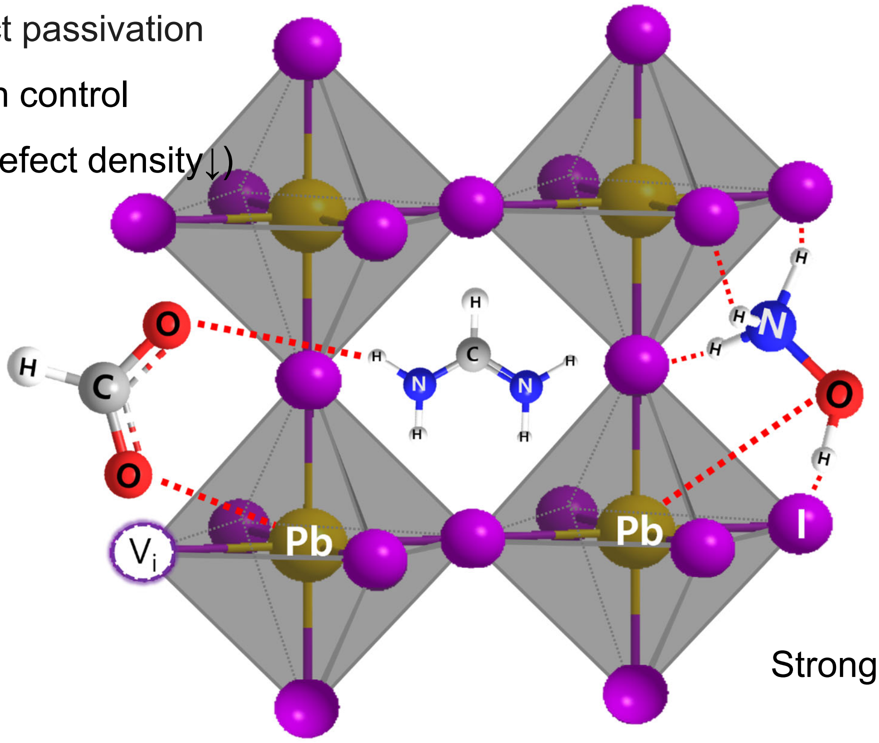
- ***Top*** interface: surface reconstruction
- ***Bulk*** grain boundary: crystal growth
- ***Bottom*** interface: strain control

Additive-assisted structural stability

$HCOO^-$

- Surface defect passivation
- Crystal growth control

  (grain size↑, defect density↓)

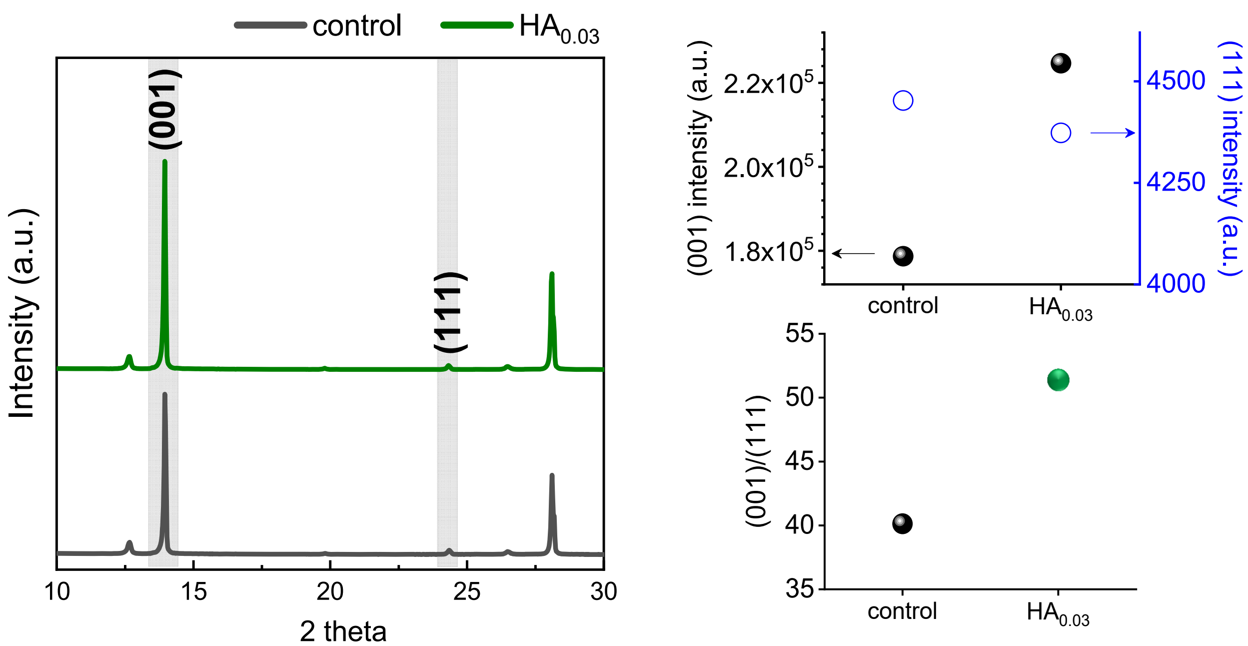


HA^+

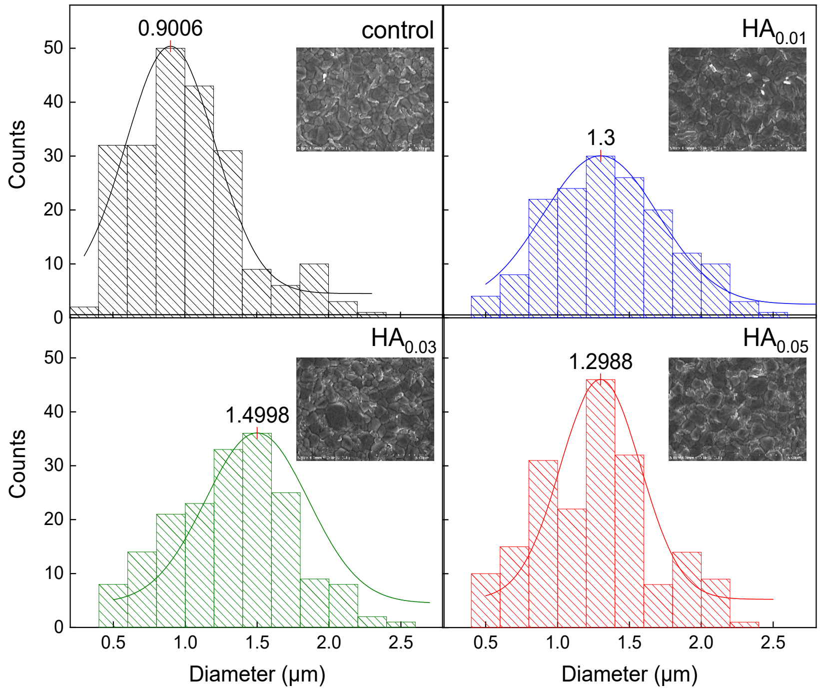
Strong hydrogen bond to PbI_6 cage

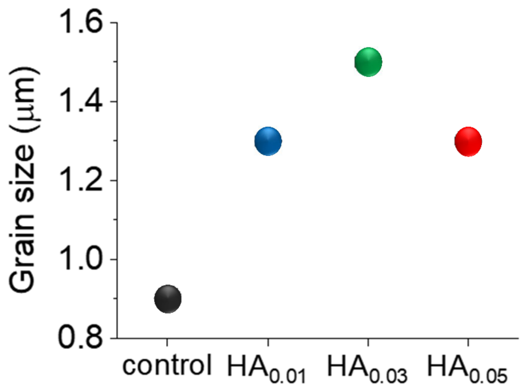
→ Increasing lattice stability

Additive effect on crystal growth

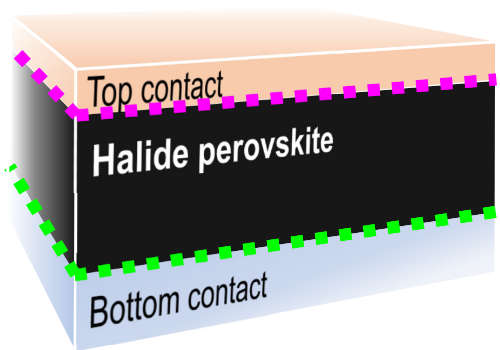


Additive effect on grain size



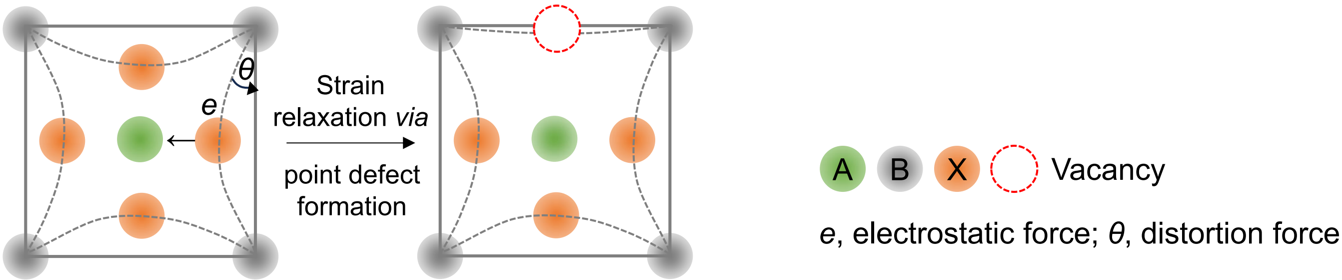


S-Y Ju Y-K Hong

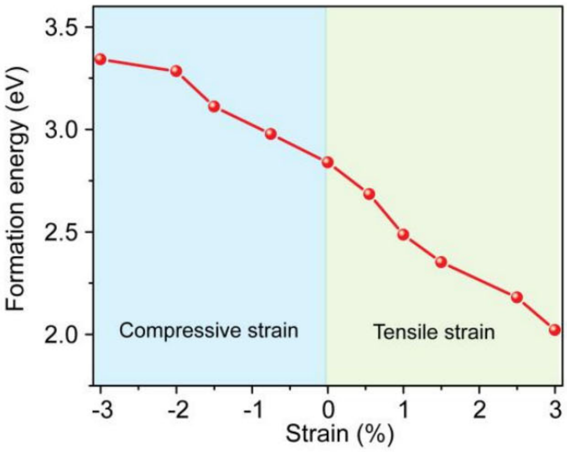


- ***Top*** interface: surface reconstruction
- ***Bulk*** grain boundary: crystal growth
- ***Bottom*** interface: strain control

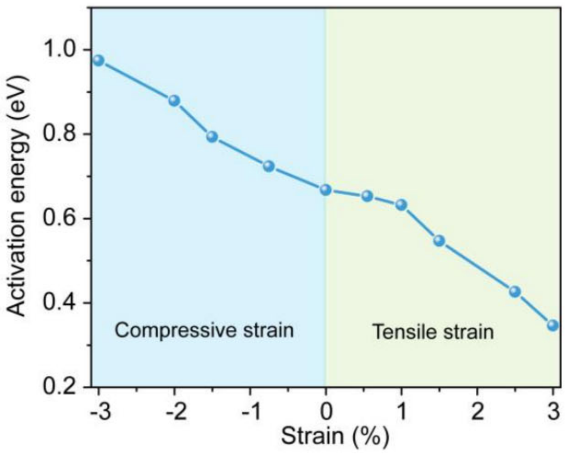
Tensile strain : facile vacancy formation



Halide vacancies formation energy

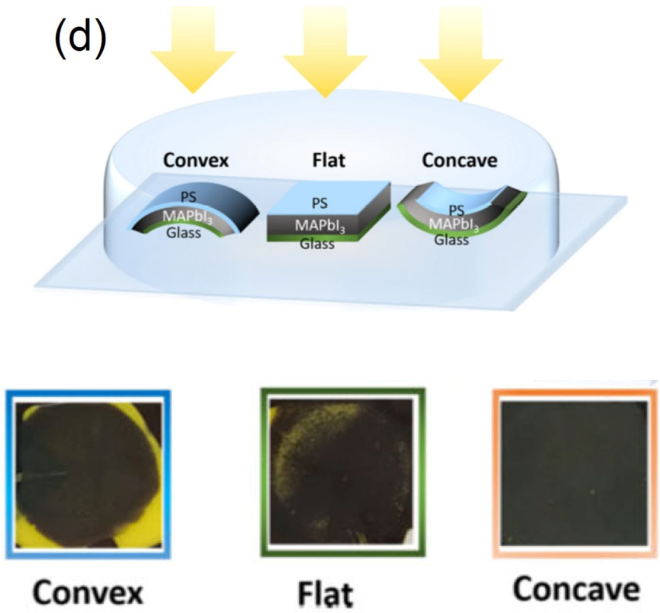


Halide ion migration activation energy

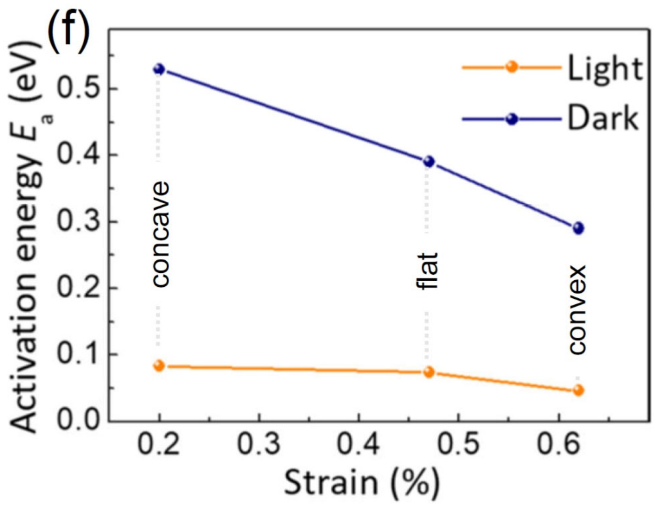


Nature communications, 2020, 11, 1514

Tensile strain : low phase stability



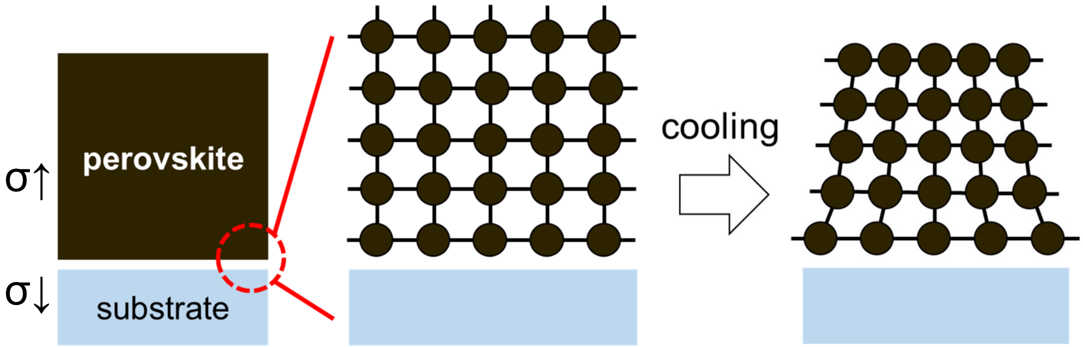
Zhao et al., Sci. Adv. 2017;3: eaao5616



In-plane residual tensile strain

$FAPbI_3$: 0.99~1.00 ×10^{-4} K^{-1}

$MAPbI_3$: 1.57 ×10^{-4} K^{-1}

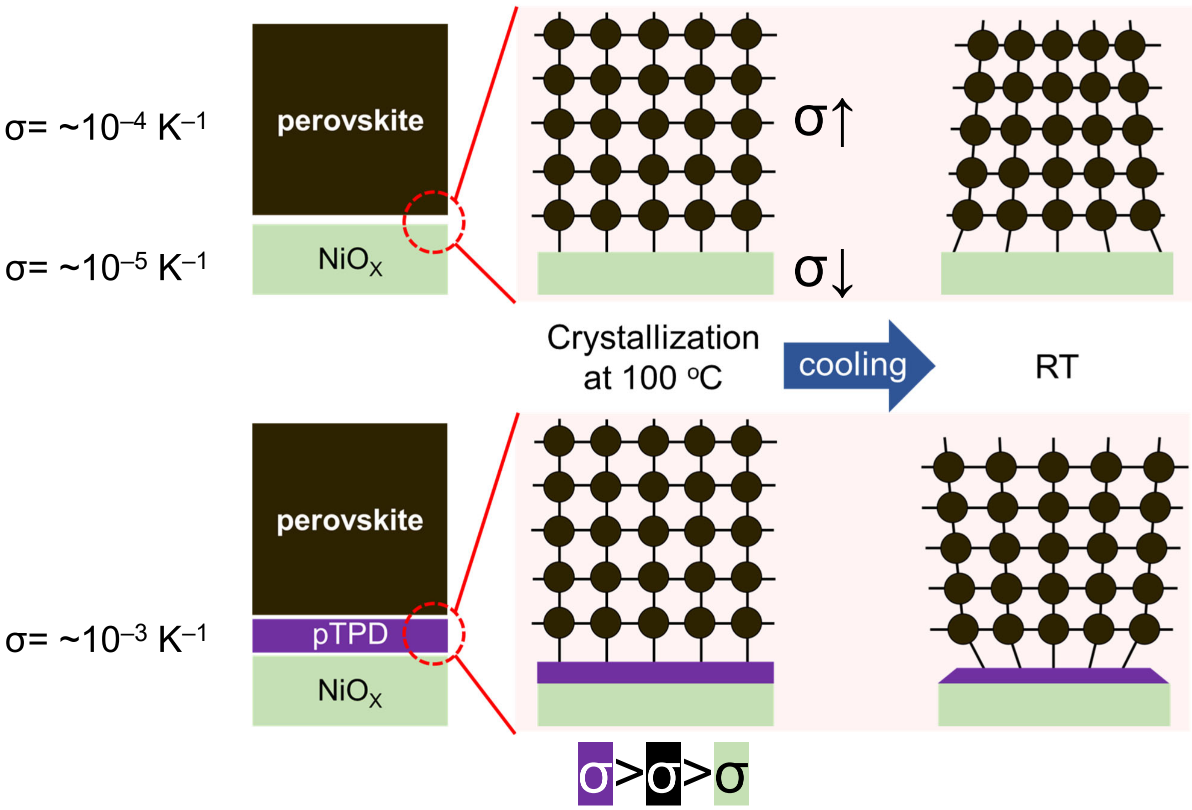


Metal oxide : ~10^{-5} K^{-1}

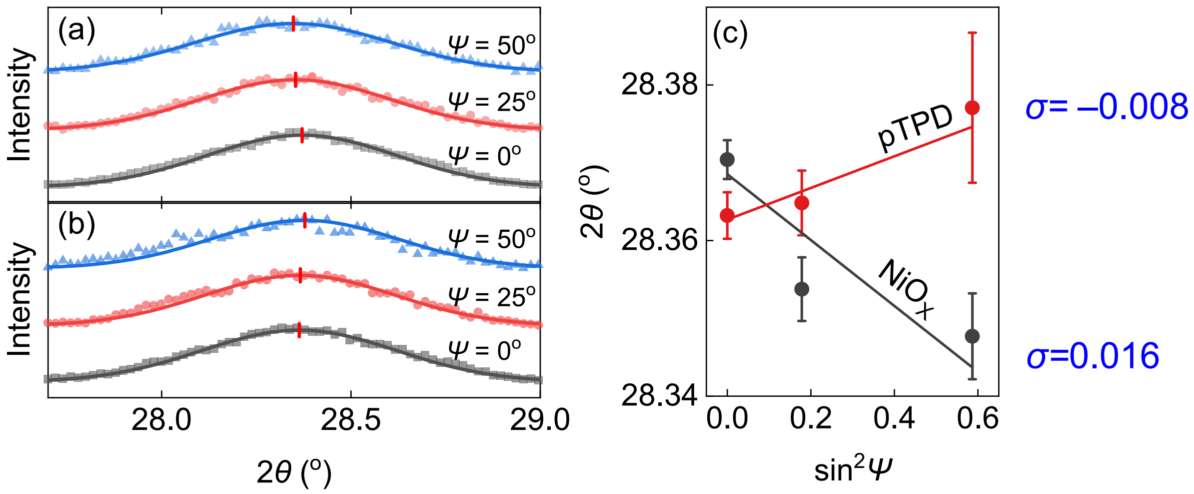
Crystal growth at 150 °C

In-plane tensile strain at RT

Strategy I: thermal expansion

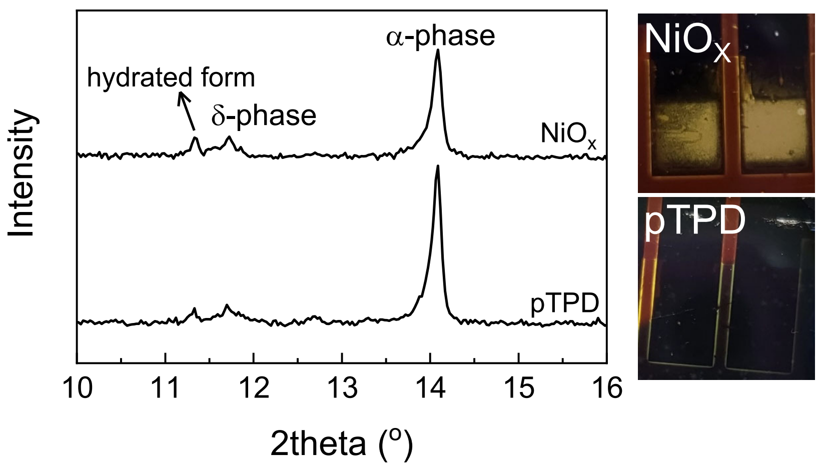


GIXRD: compressive lattice strain



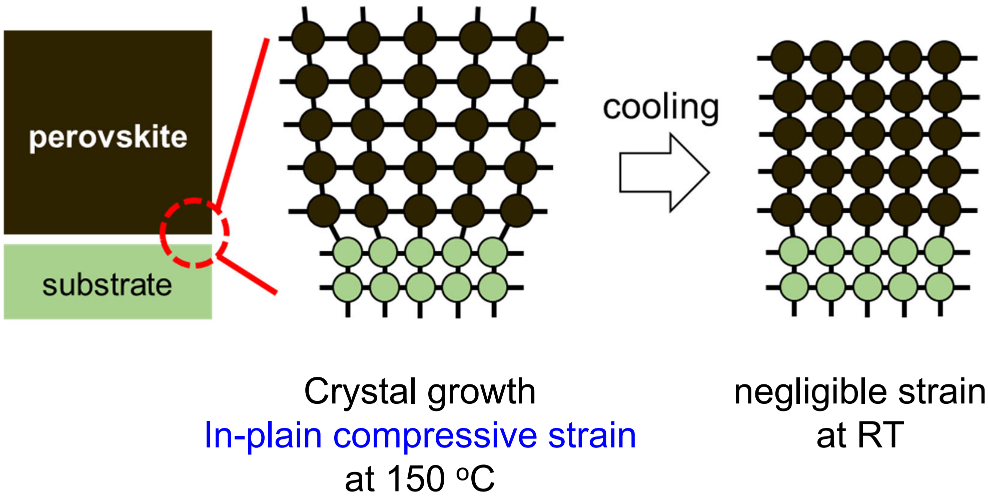
$$\sigma = -\frac{E}{2(1+\nu)}\frac{\pi}{180}cot\theta_0\frac{\partial(2\theta)}{\partial sin^2\psi}$$

Improved crystal phase stability

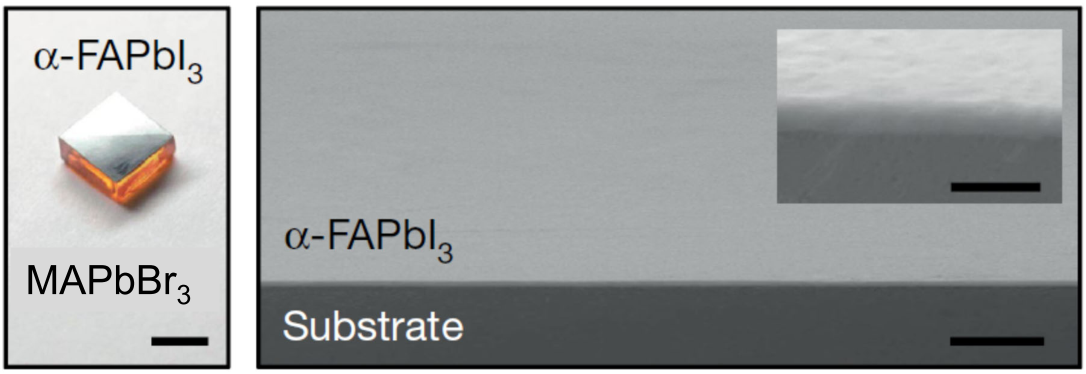


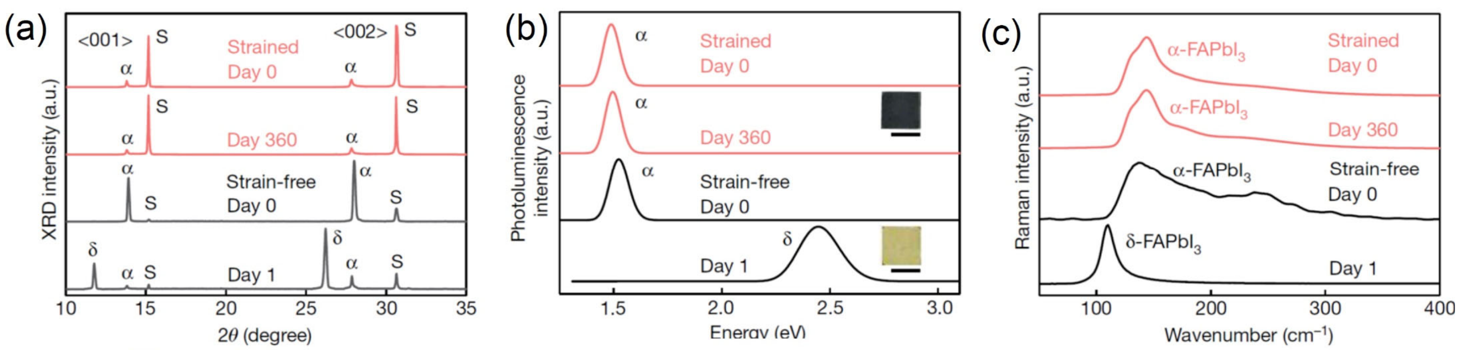
ACS AMI **2022**, *14*, 39996–40004

Strategy II: heteroepitaxial crystal growth

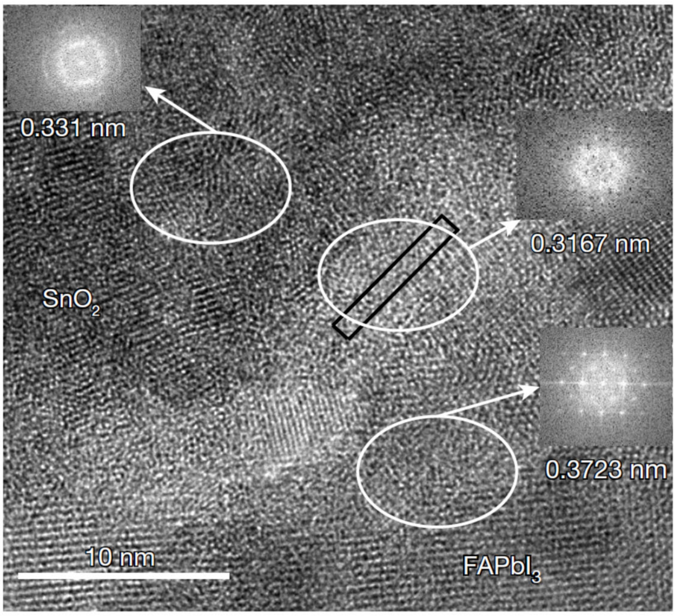


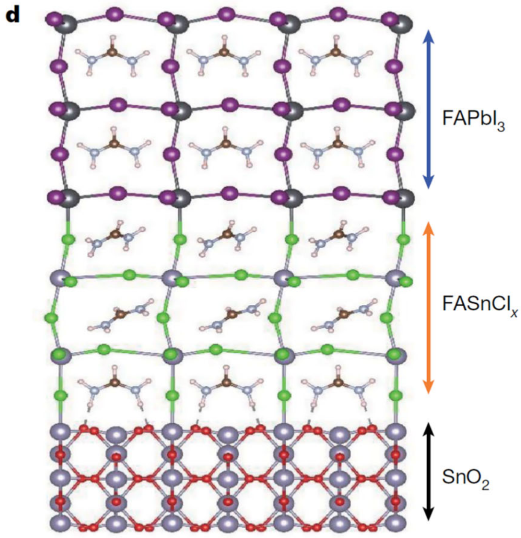
Sheng Xu et al. Nature 2020 577, 209-215



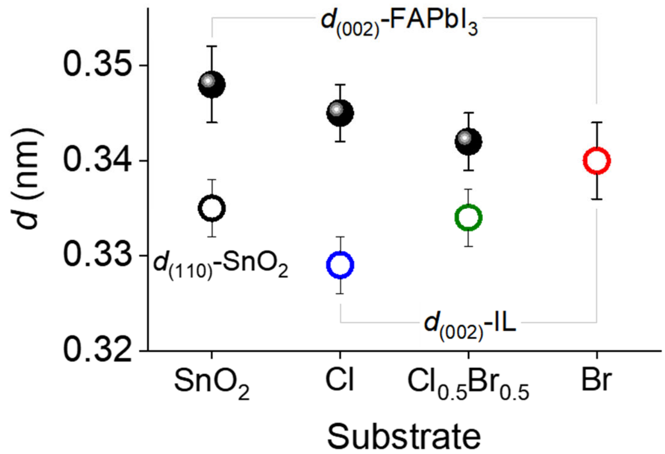


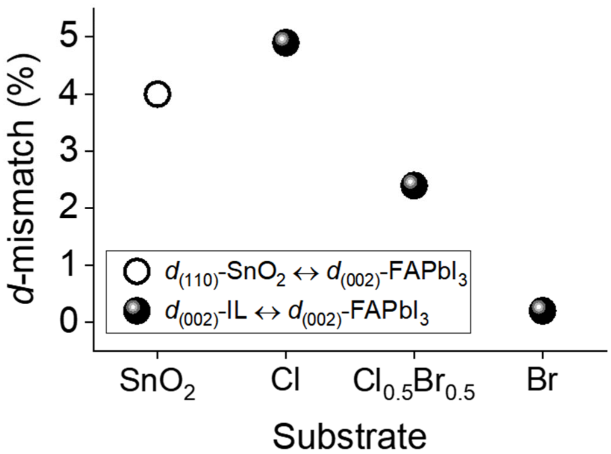
Sang Il Seok *et al.* *Nature* **2021**, 598, 444–450



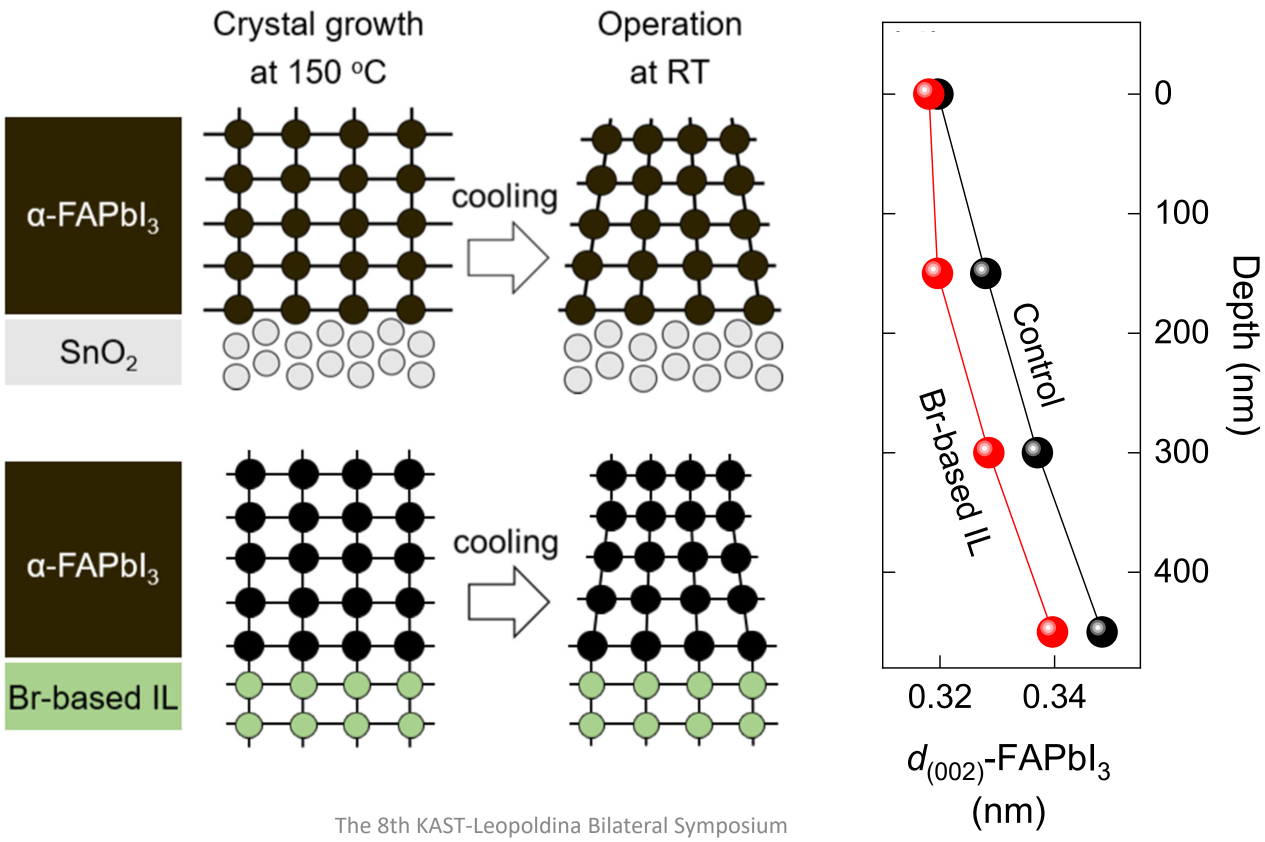


Control of the perovskite lattice distance

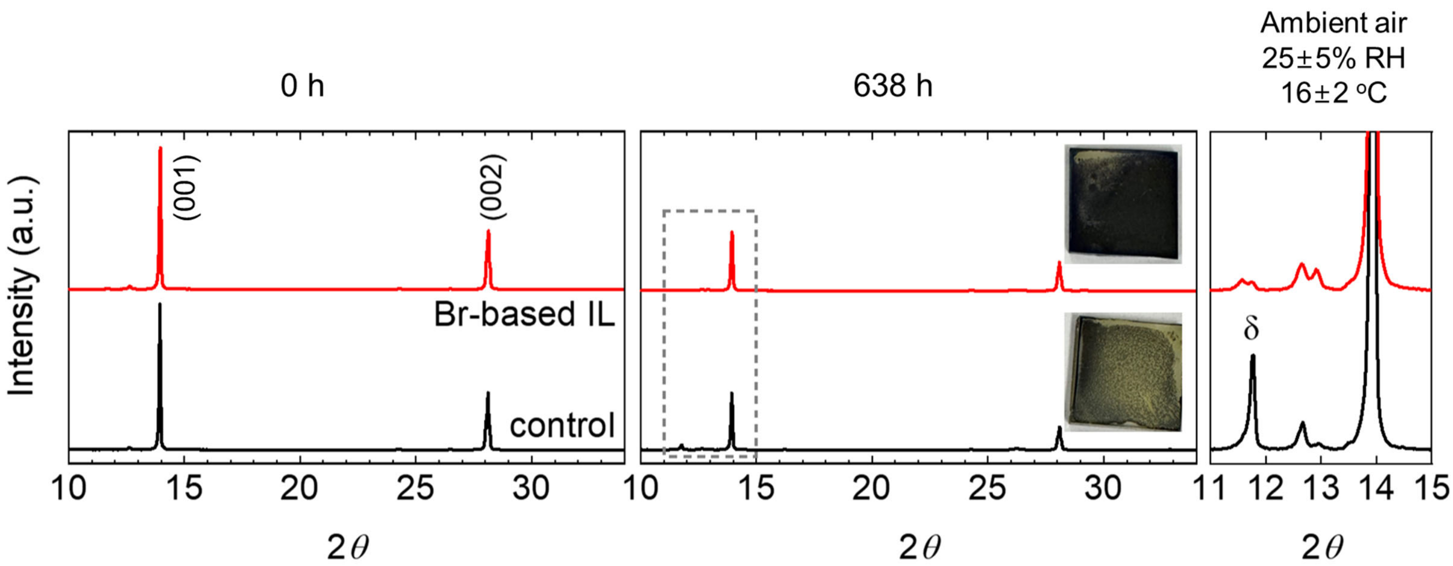




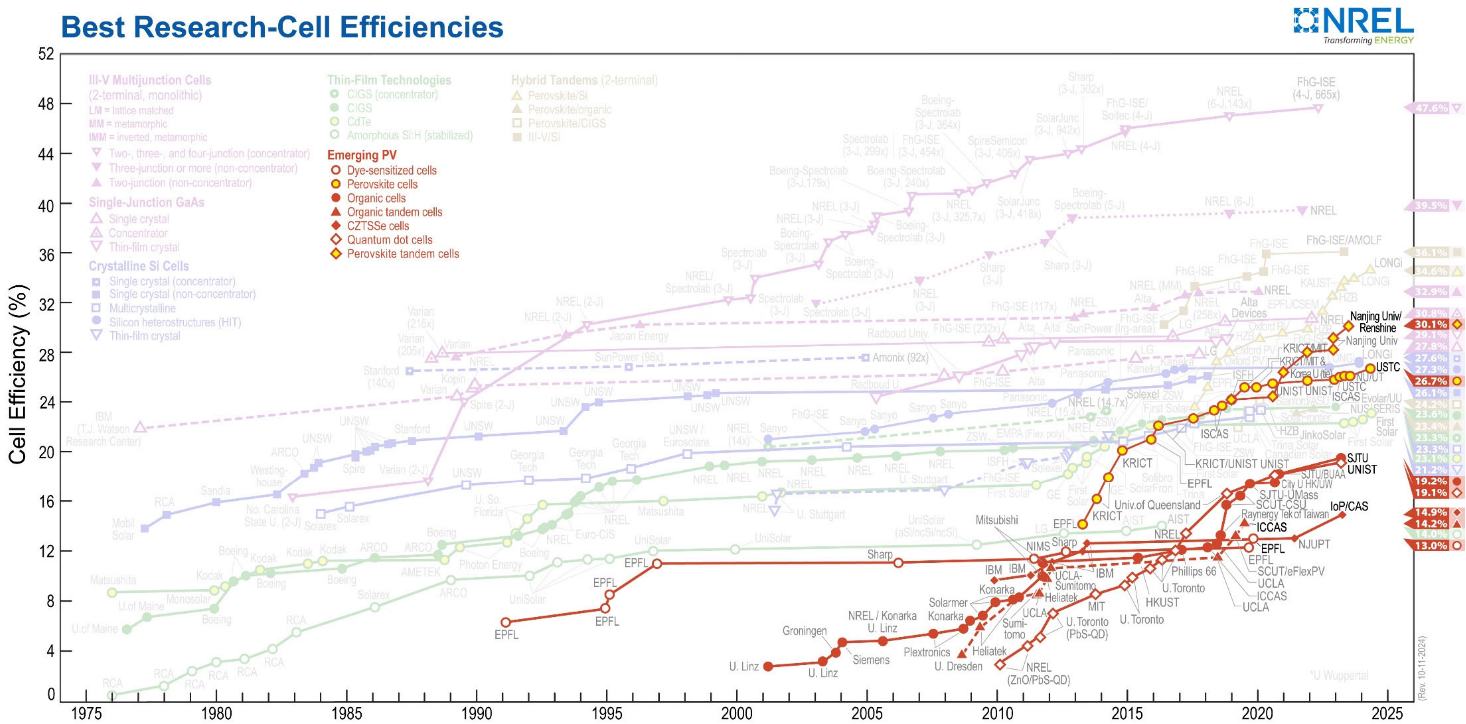
Control of the perovskite lattice distance



Phase stability



Summary



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NEDL

Hyeon-Seo Choi
Yun-Kyeong Hong
So-Yeon Ju
Yu-Na Lee
Yu-Na Kim

NRF National Research Foundation of Korea

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포스코청암재단 POSCO TJ Park Foundation