Vacuum-Deposited Halide Perovskites And Broadband Transparent Conducting Oxides For Photovoltaics

Pierre-Alexis Repecaud   Yury Smirnov   Nathan Rodkey   Tatiana Soto-Montero

Dominic Post   Adem Mirza   Yorick Birkhölzer   Wiria Soltanpoor   Monica Morales-Masis

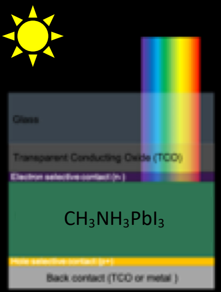
Dr. Monica Morales-Masis
Associate Professor
M^3 Optoelectronic Materials Group @ IMS

4TU Meeting Materials– December 2020

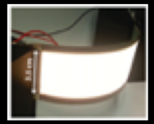
Optoelectronic Thin Film Materials

Solar cells

Photonics



Light emitting devices



Apply and enable functionalities in devices

Synthesize and fabricate

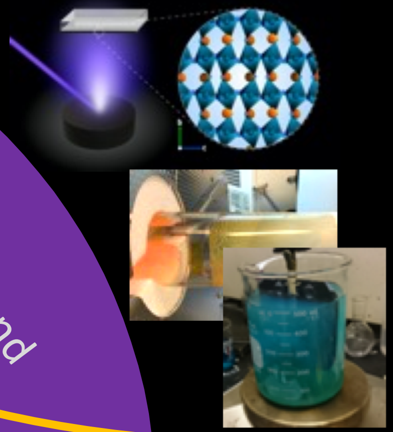
Materials

Transparent Conducting Materials (n- and p-type)

Inorganic and Hybrid Halide Perovskites

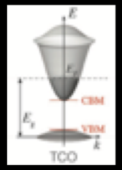
Understand and Design

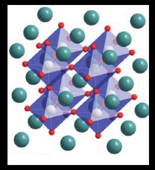
Characterize and Improve

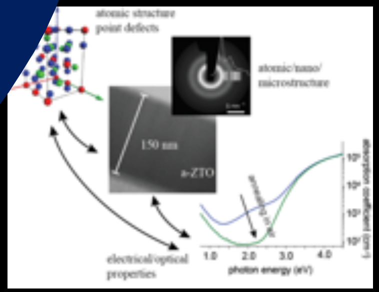


Physical & chemical deposition techniques

Structural and defect analysis.
Material modeling







Structural, electrical, optical property relations

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Reviews

Morales-Masis M., et al. Adv. Electron Mat. Vol.3 (2017)
Fioretti A., Morales-Masis M. J. Phot. Energy (2020)
Soto-Montero T., Soltanpoor W., M.MM. Invited APL Mat (under review)

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UNIVERSITY OF TWENTE.

Pulsed Laser Deposition (PLD)

Known for playing LEGO on atomic scale with complex oxides …

Prof. Mark Huijben
Prof. Gertjan Koster
Prof. Guus Rijnders
Prof. Dave Blank

IMS seminal work on superlattices, in-situ monitoring, PZT and more

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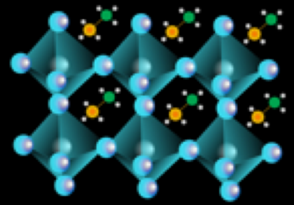
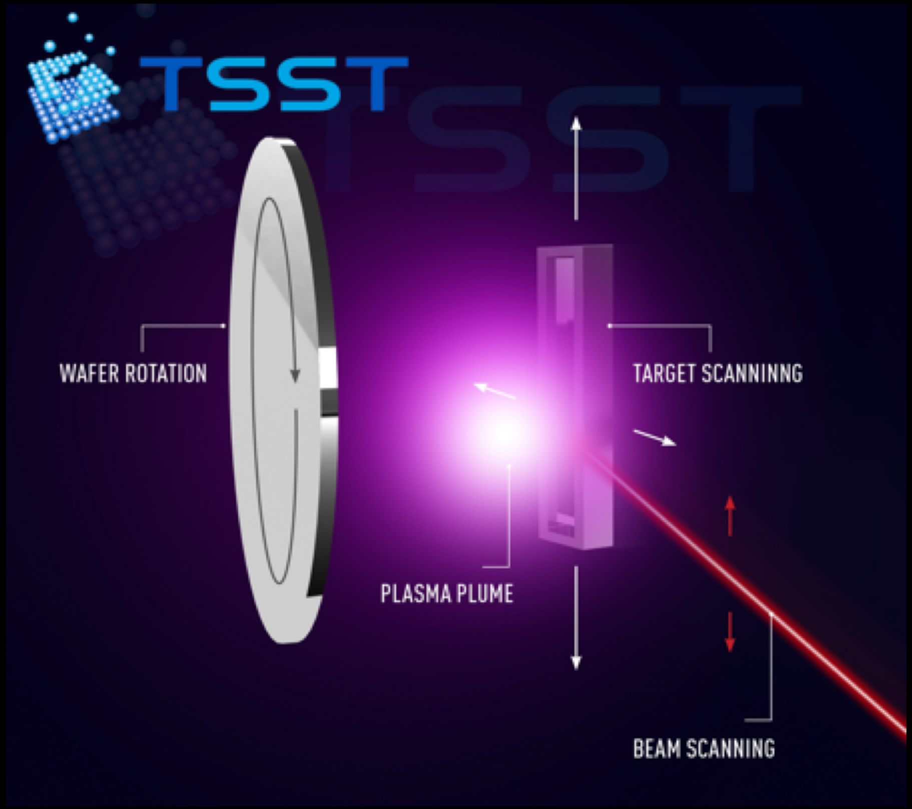
Complex optoelectronic materials for solar cells with PLD?

PLD properties	Interesting for ..
Near stoichiometric transfer of multi-compounds.	Halide Perovskites ABX_3, X = I, Br, Cl 
Volatility insensitive.	
Low-damage deposition of thin films on sensitive substrates.	Transparent Conducting Oxides (TCOs) 

But absolute requirement for PV …

Scalability (deposition on wafer-size substrates)

Scalable (wafer-based) Pulsed Laser Deposition



4 inch wafers

4 – 12 inch wafers

Scalable Pulsed Laser Deposition for TCOs in Solar Cells
Smirnov, Kuik, Schmengler, Repecaud, … Morales-Masis M.
Adv. Mat. Technologies, 2020

TCOs for passivated contacts
Featured in PV Magazine

SOLAR-ERA.NET

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Pulsed Laser Deposition (PLD)

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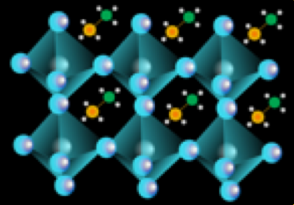
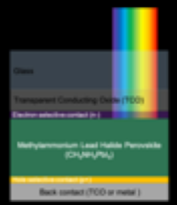
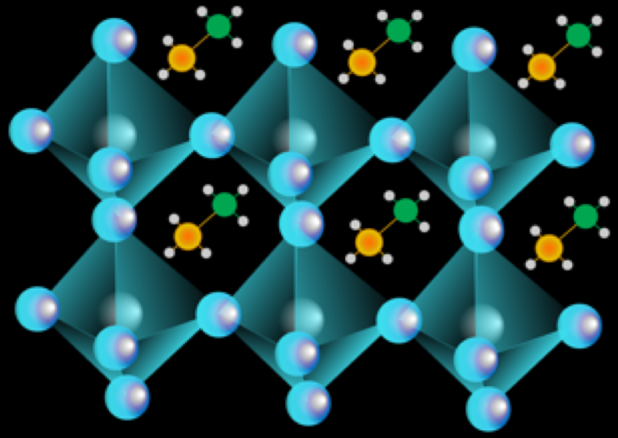
Near stoichiometric transfer of multi-compounds. Volatility insensitive.	Halide Perovskites ABX_3, X = I, Br, Cl 
Low-damage deposition of thin films on sensitive substrates.	Transparent Conducting Oxides (TCOs) 

But absolute requirement for PV …

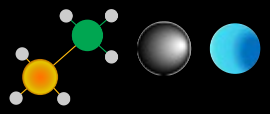
Scalability (deposition on wafer-size substrates)

PLD for halide perovskite growth?

Hybrid and Inorganic Halide Perovskites



ABX_3



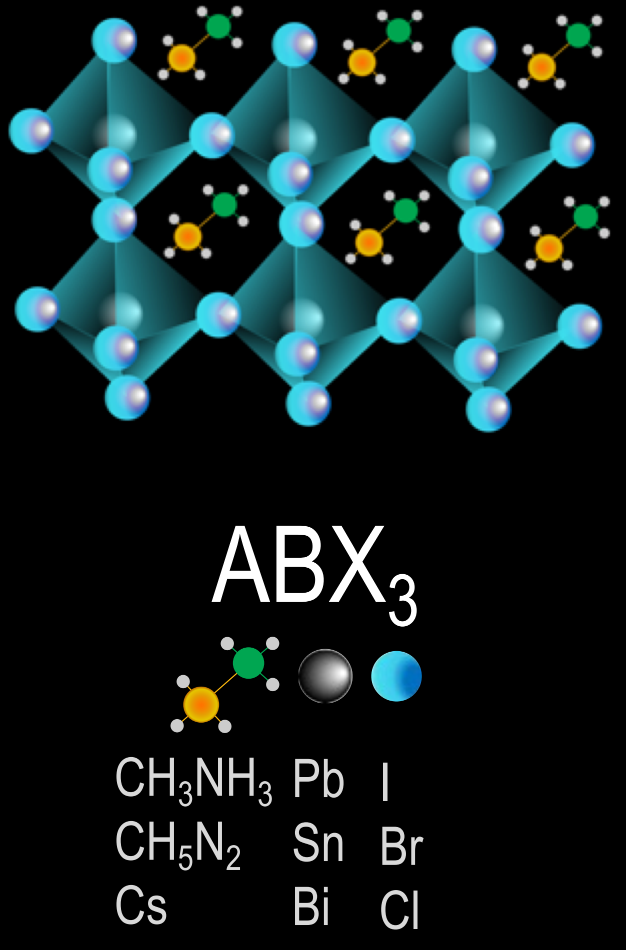
A	B	X
CH_3NH_3	Pb	I
CH_5N_2	Sn	Br
Cs	Bi	Cl

Record solar cell efficiencies
High and tunable luminescence
Defect tolerance
Simple fabrication

But
Unstable (thermal, environmental)
Pb-based
Lack of controlled growth

PLD for halide perovskite growth?

Hybrid and Inorganic Halide Perovskites



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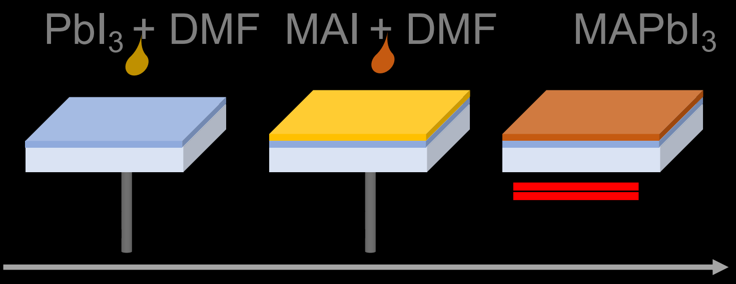
Current deposition methods

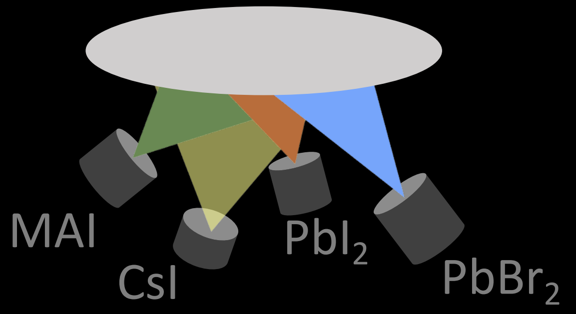
Solution Process

Solubility dependent



Thermal Co-Evaporation

Volatility dependent



PLD for halide perovskite growth?

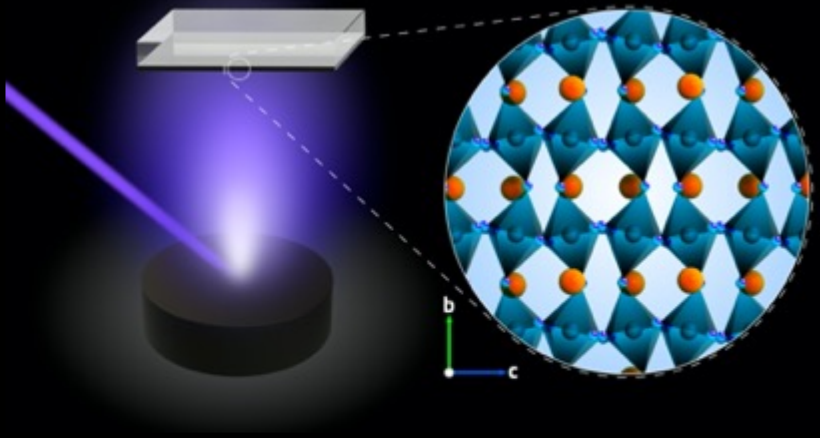
New Laser-Based Methods

European Research Council

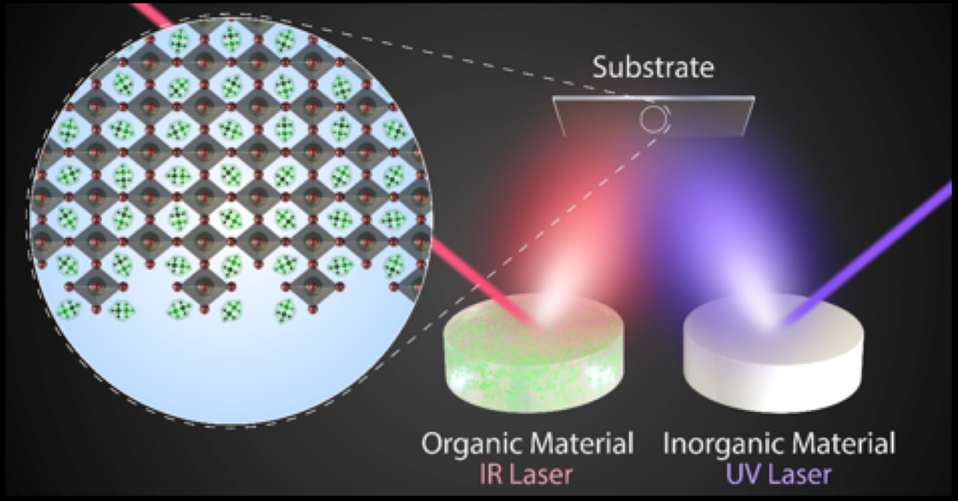
Established by the European Commission

CREATE

Single-source



Dual-laser deposition



Current deposition methods

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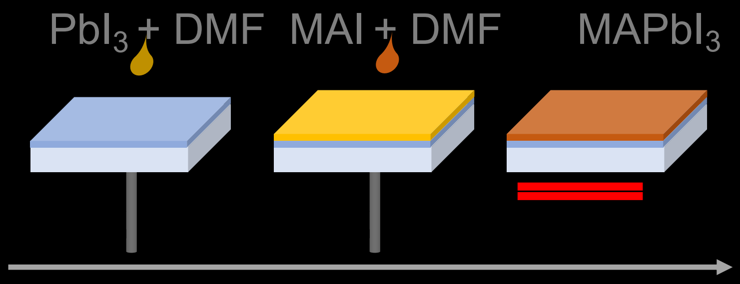
Solubility dependent



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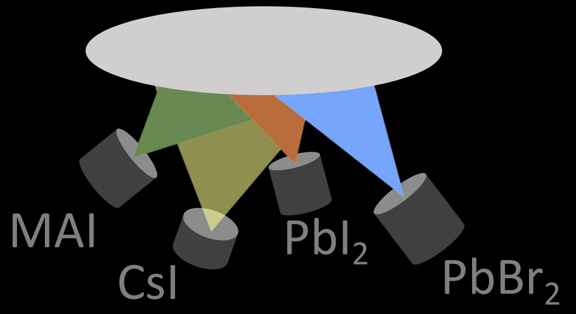
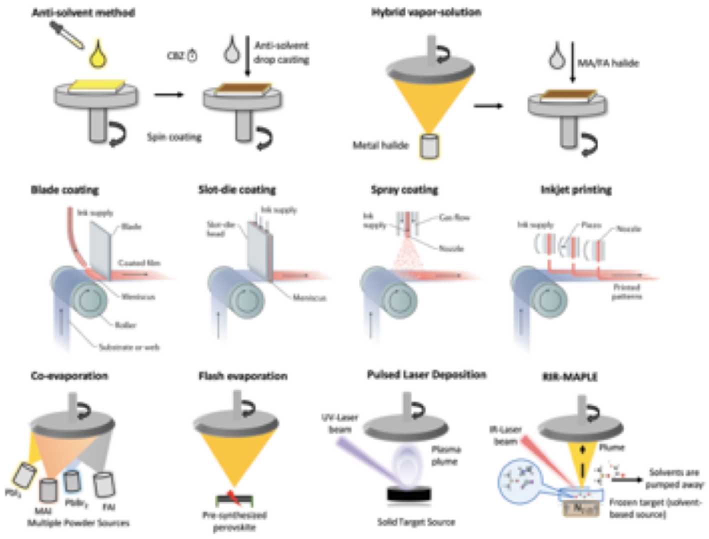


APL Materials

scitation.org/journal/apm



Volume 8, Issue 11, Nov. 2020

Pressing challenges of halide perovskite thin film growth

APL Mater. **8**, 110903 (2020); doi.org/10.1063/5.0027573

Tatiana Soto-Montero, Wiria Soltanpoor, and Monica Morales-Masis

AIP Publishing

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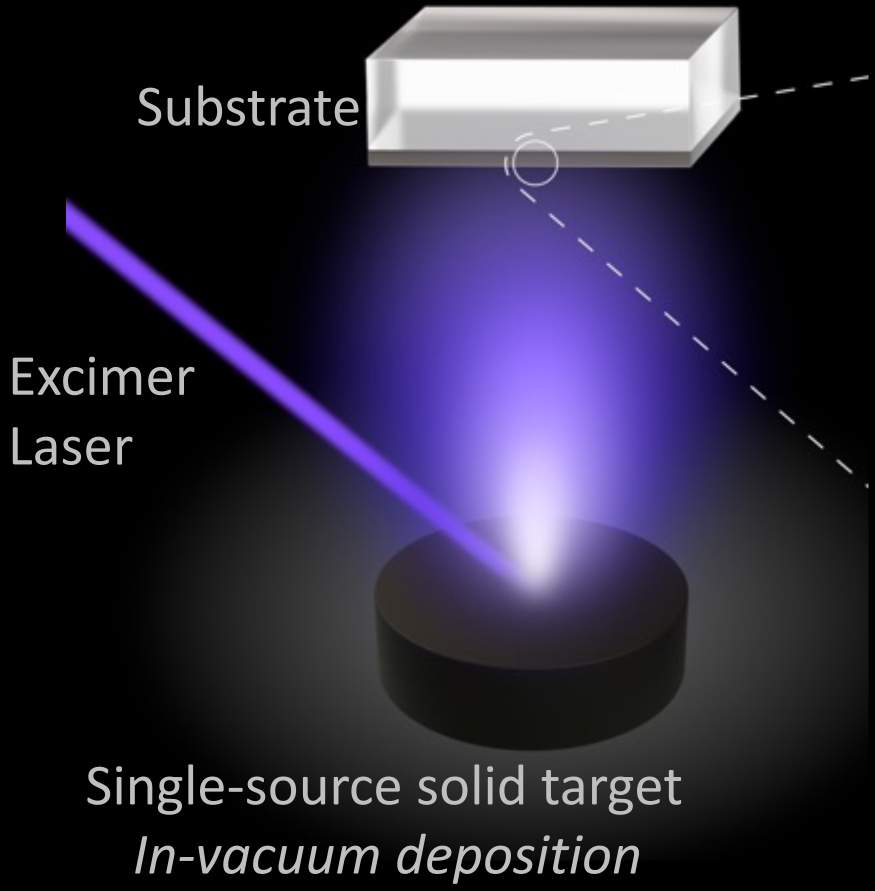
Single Source PLD of Inorganic Halide Perovskites

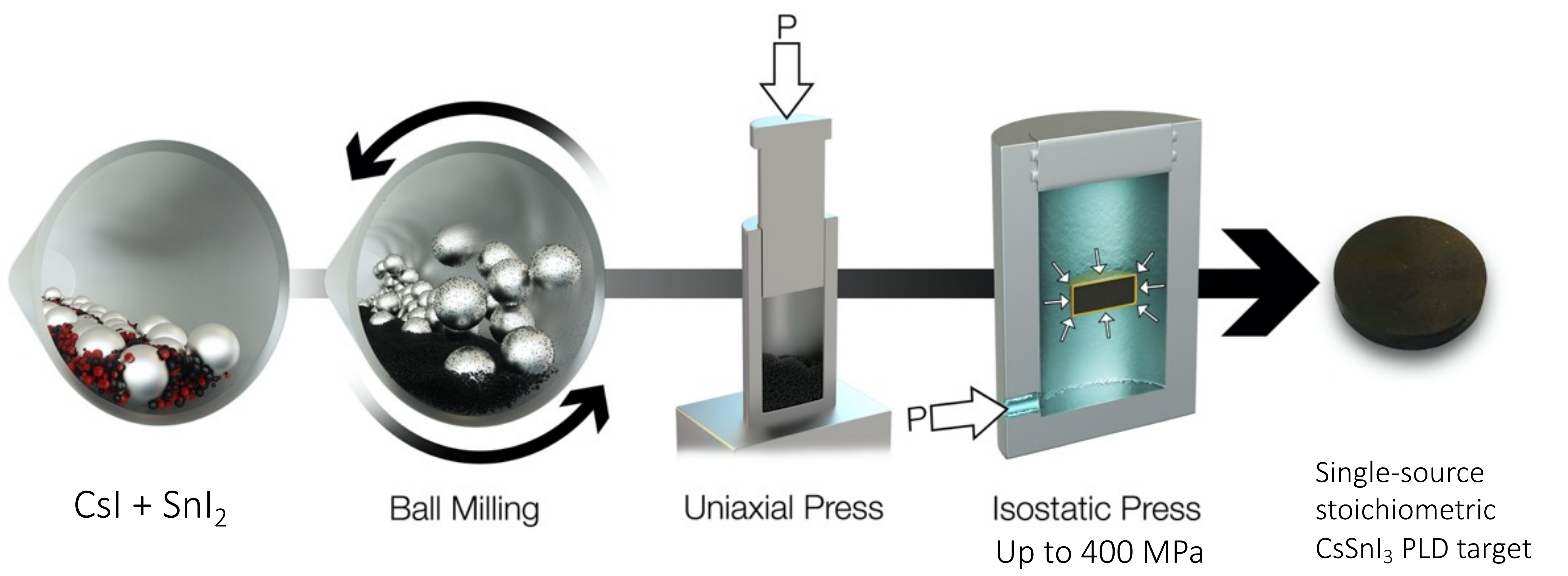


$CsSnI_3$

Challenging material:

- Oxidation of Sn ($Sn^{2+} - 2e^{-} \rightarrow Sn^{4+}$)
- Two independent stable polymorphs at RT :
  - Optically active black-phase (orthorhombic B-γ)
  - Non-optically active yellow-phase

Single Source Halide PLD Target Fabrication



V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

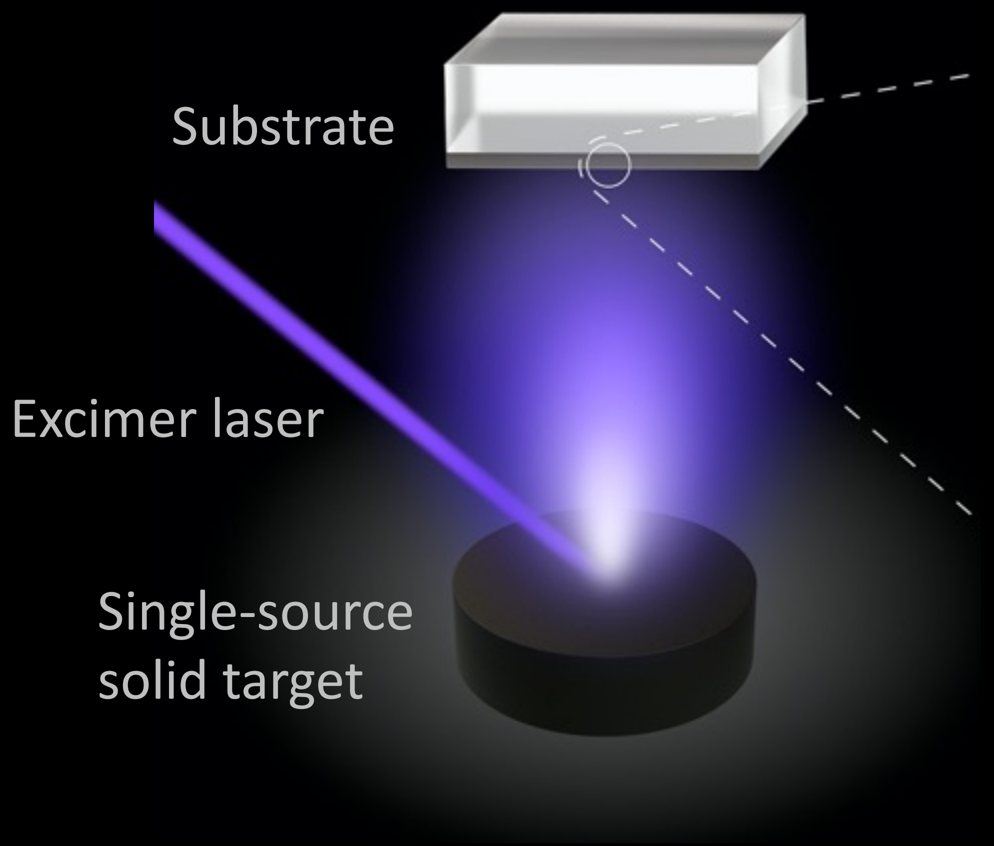
Single Source PLD of Inorganic Halide Perovskites

Vacuum

Deposition under inert Ar atmosphere

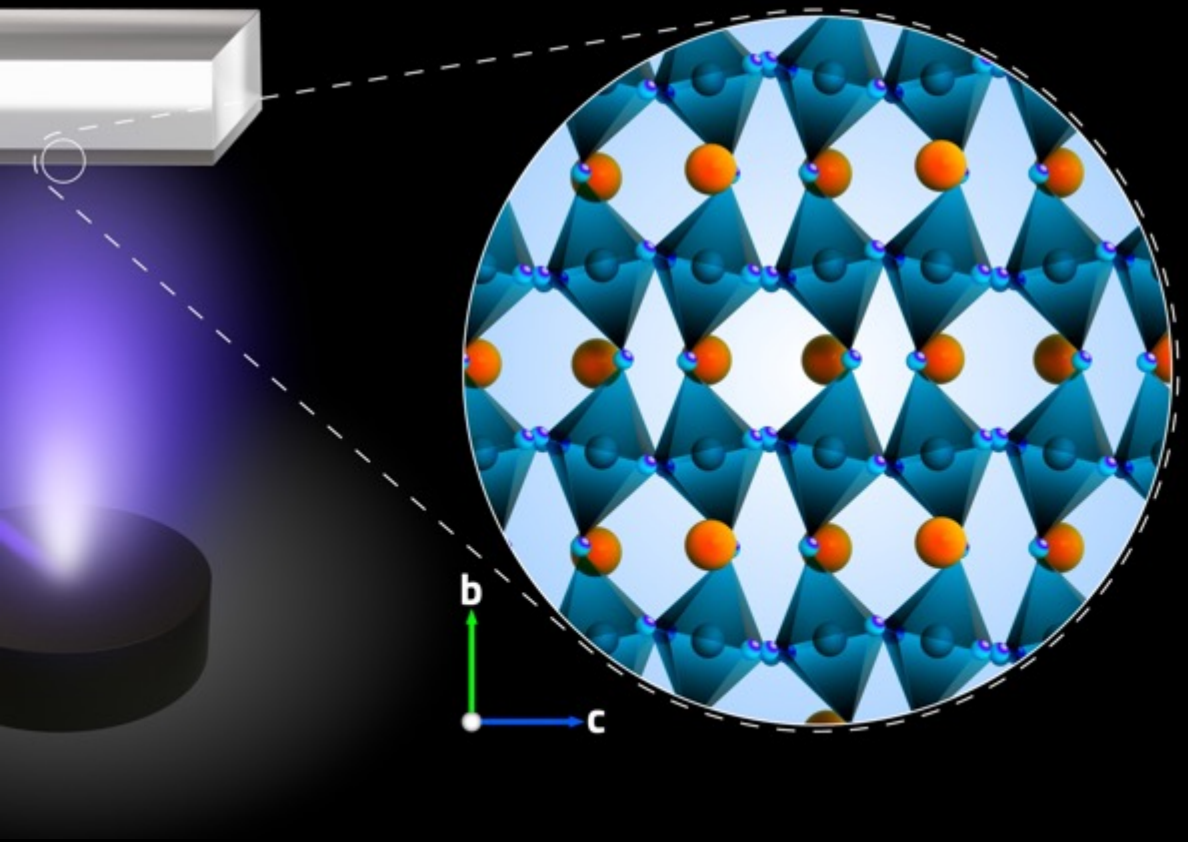
Substrate at RT:
Si/native SiOx
Fused silica
Glass

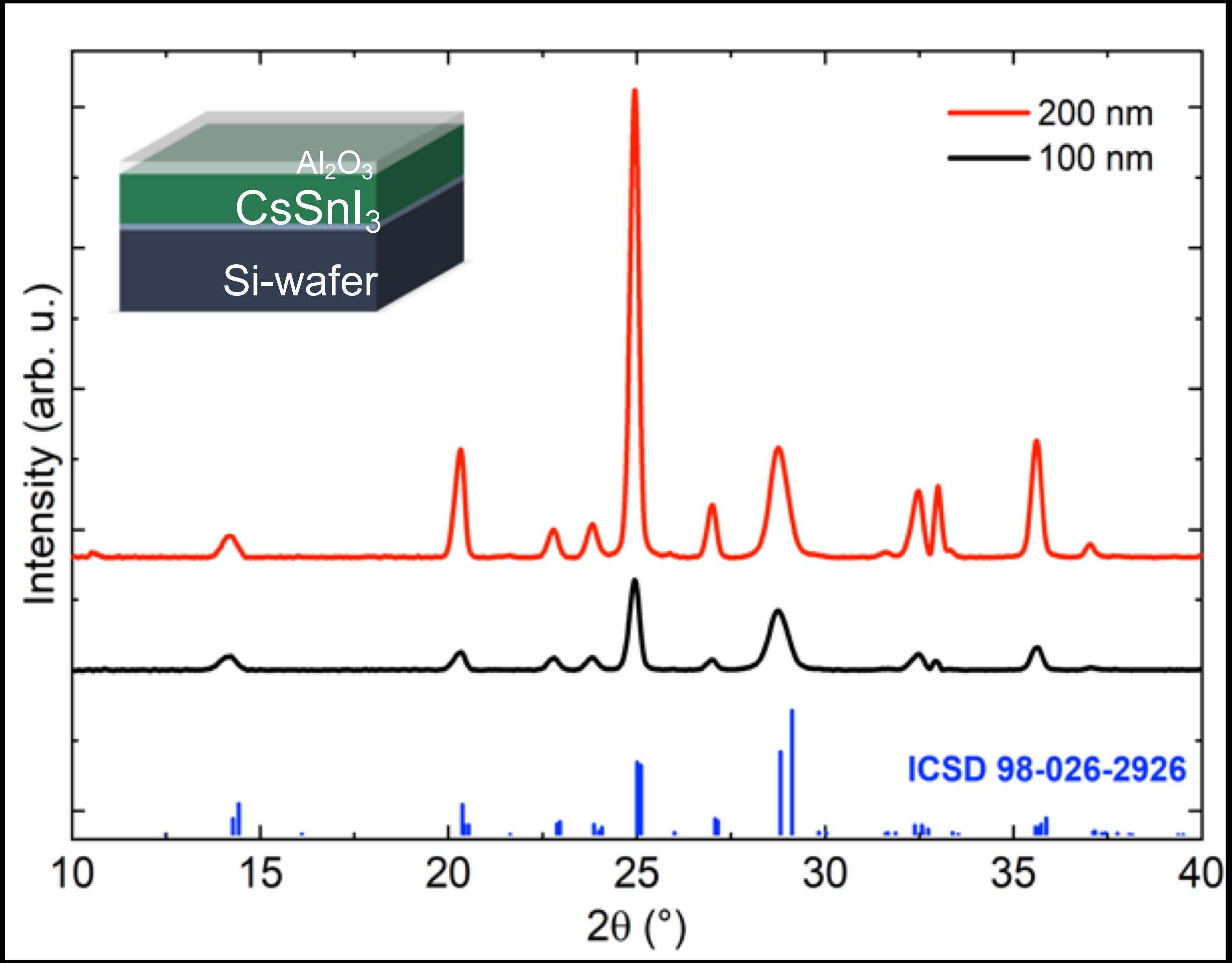
Al_2O_3 capping layer



V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

Confirmation of Black-γ-phase $CsSnI_3$ films





X-ray diffraction

V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

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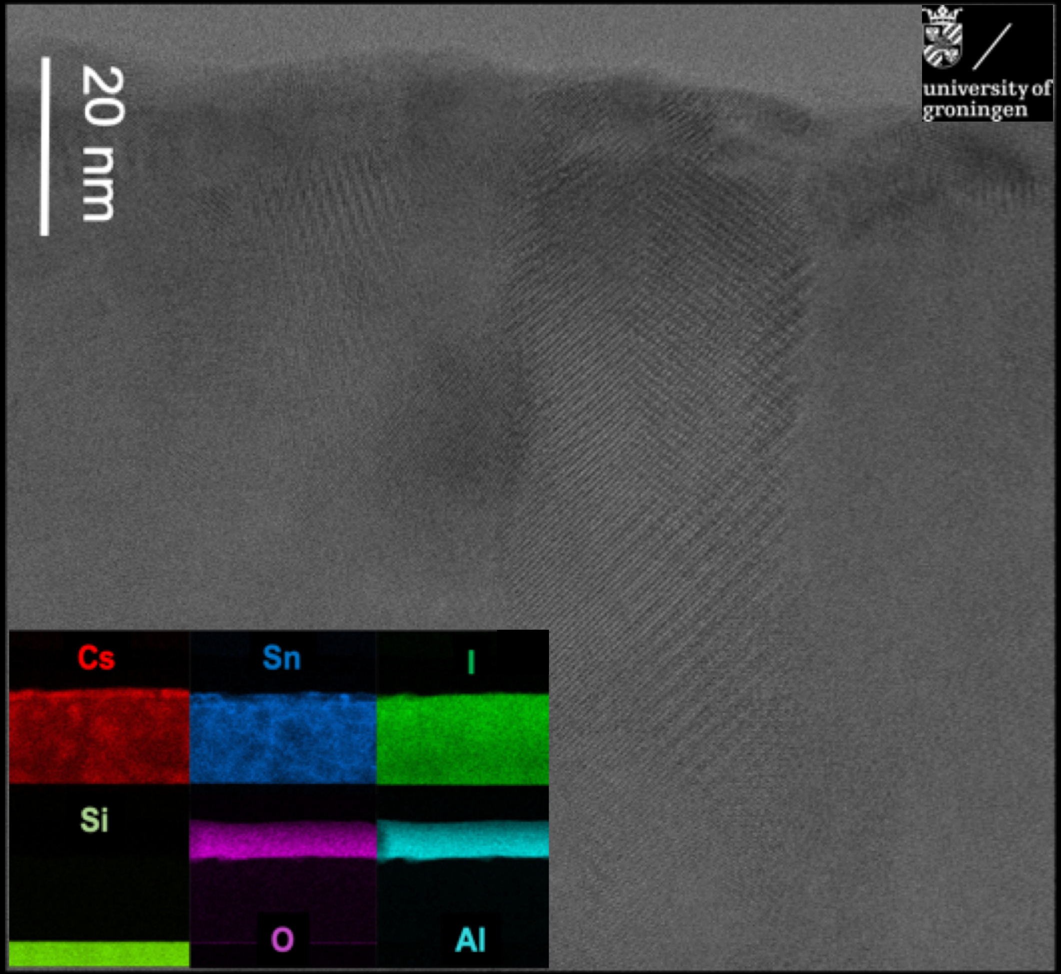
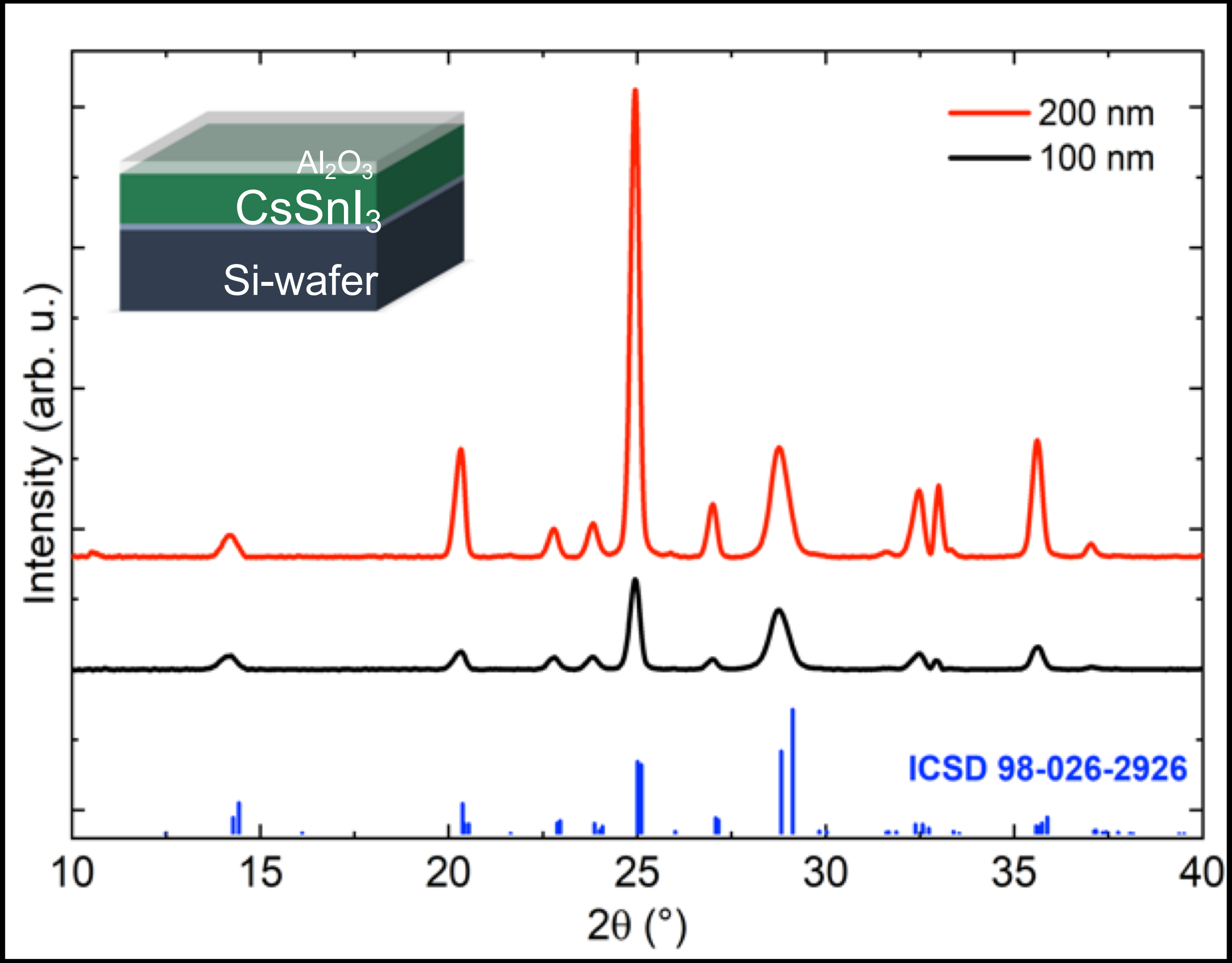


TEM - EDX



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PLD $CsSnI_3$: high absorption coefficient and optimum band gap for PV

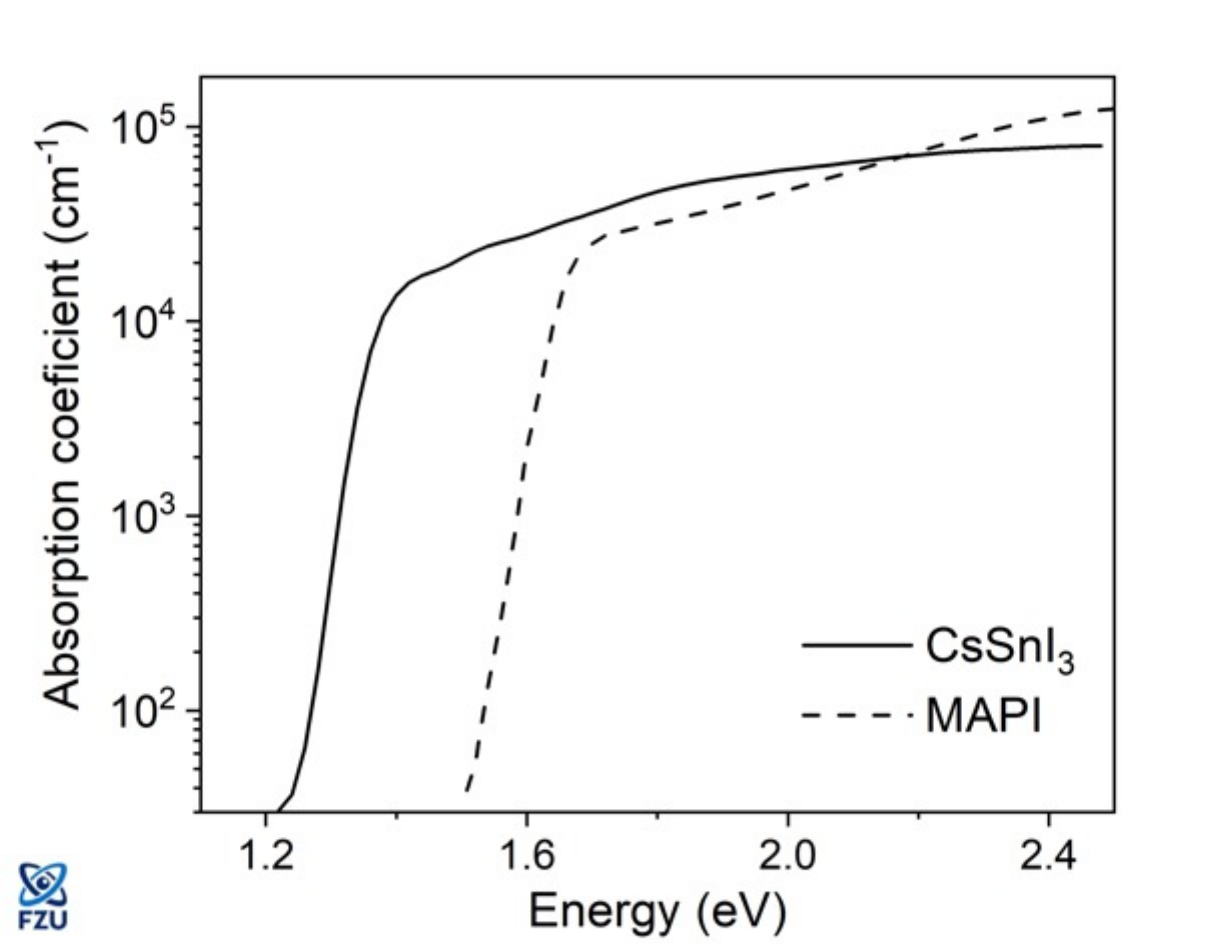
Band Gap of 1.32 eV

Sharp Absorption Edge

High quality film quantified by Urbach energy (E_U)

$$\alpha \propto \exp(-h\nu/E_U)$$

E_U - $CsSnI_3$: 12.9 meV
E_U – $MAPbI_3$: 12.5 meV



V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

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PLD $CsSnI_3$: Higher absorption coefficient than c-Si

Band Gap of 1.32 eV

Sharp Absorption Edge

High quality film quantified by Urbach energy (E_U)

$$\alpha \propto \exp(-h\nu/E_U)$$

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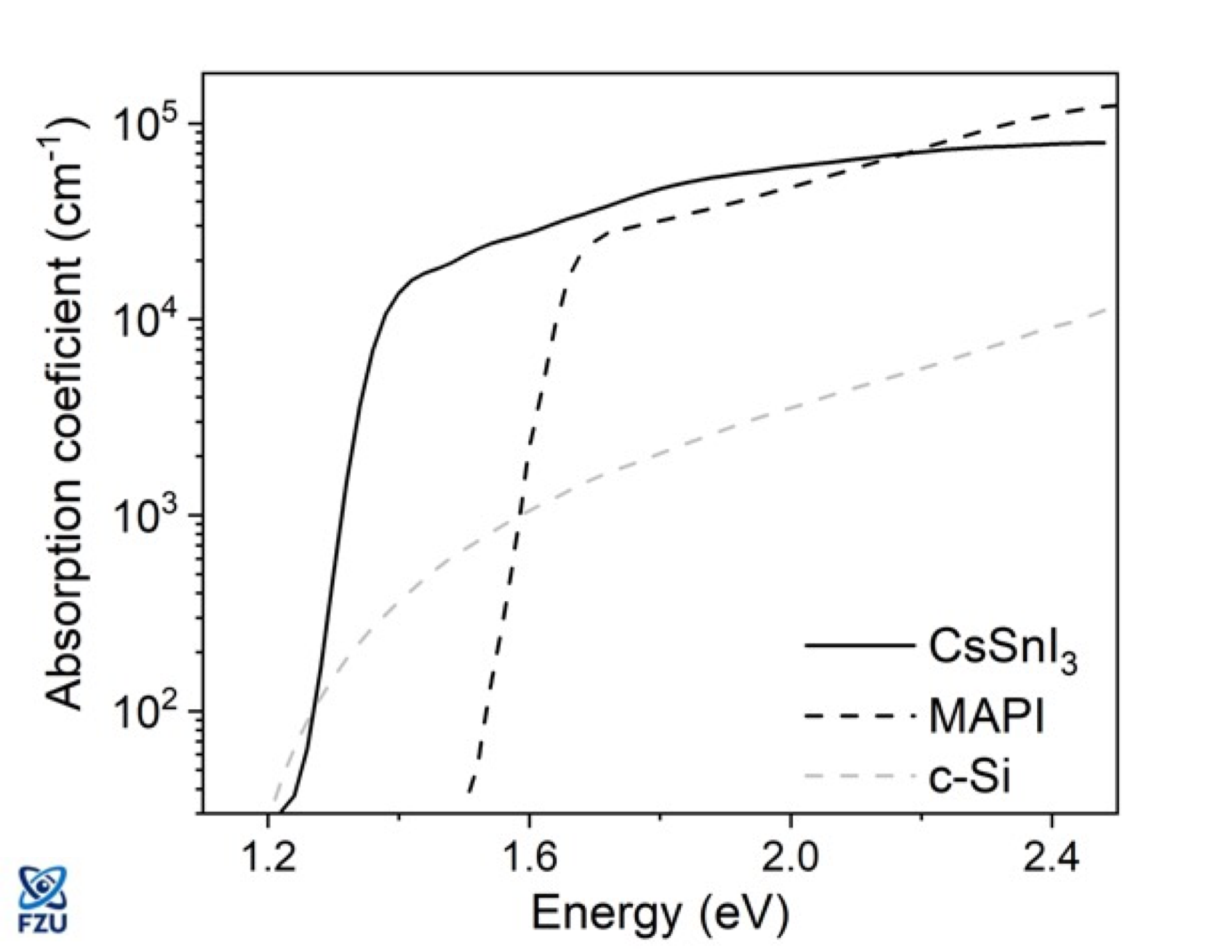

V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

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PLD $CsSnI_3$: NIR Photoluminescence

Band Gap of 1.32 eV

Sharp Absorption Edge

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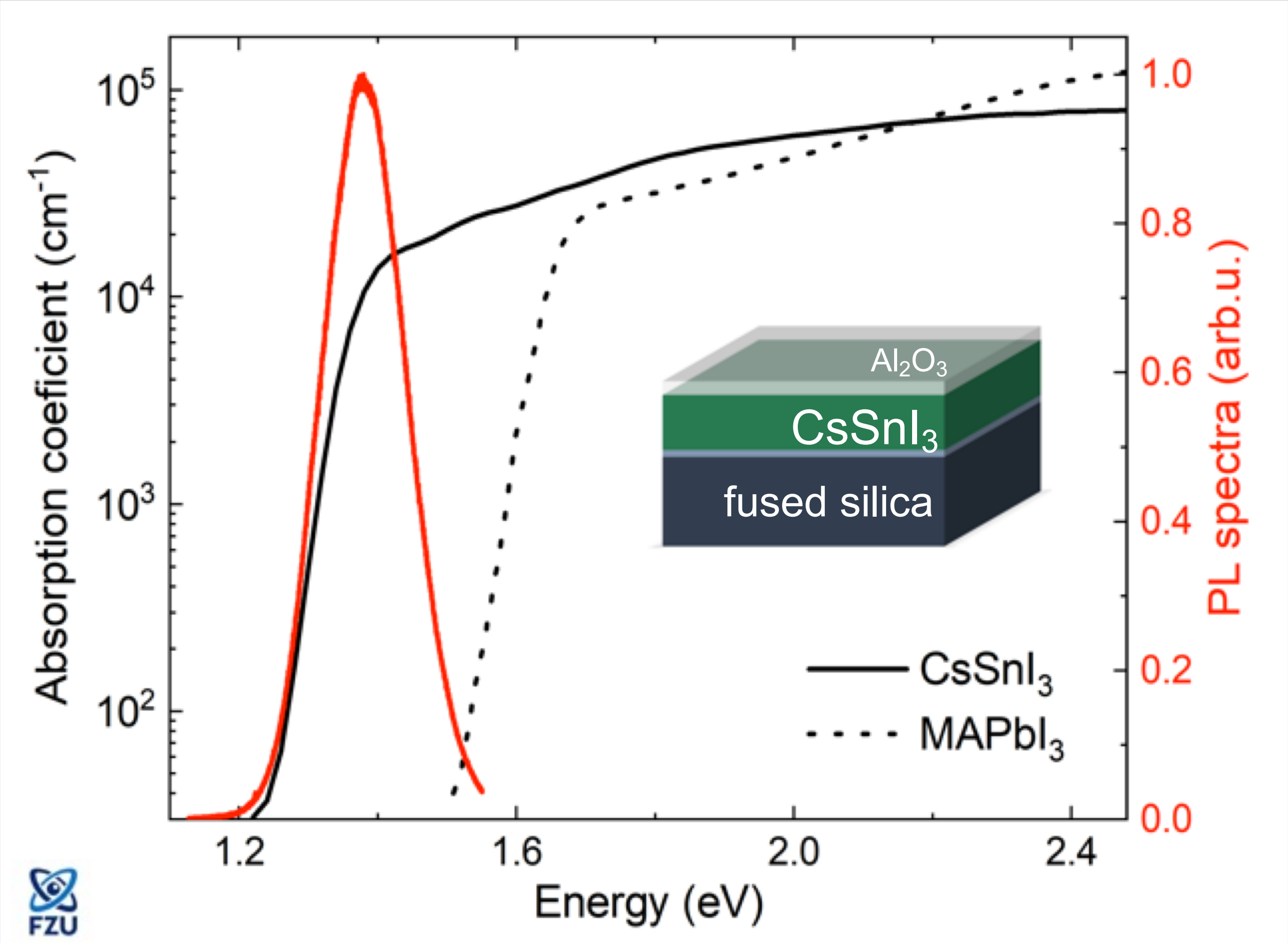


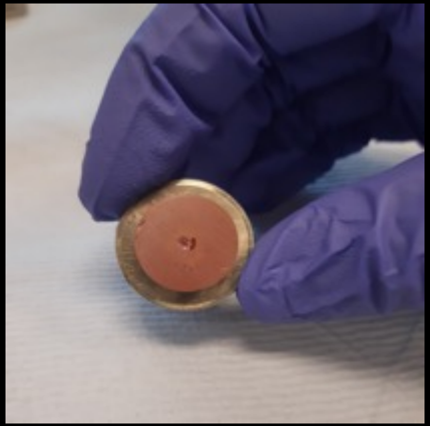
Direct Band Gap

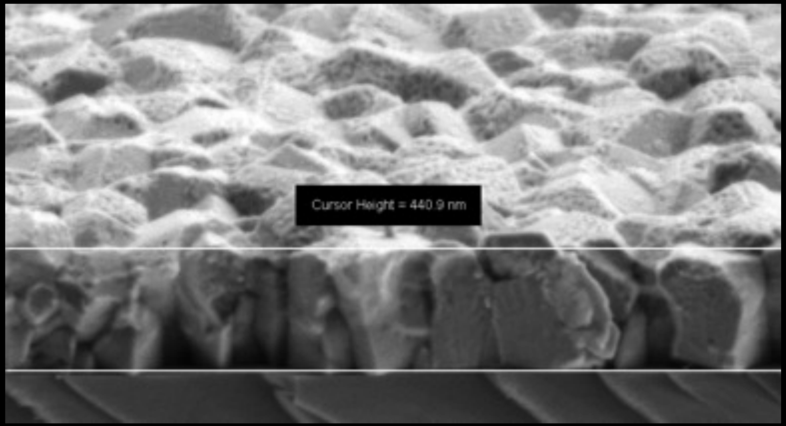
High PL

V. M. Kiyek, Y. A. Birkhölzer, Y. Smirnov, …, G. Koster, G. Rijnders, M. Morales-Masis. *Adv. Mat. Interfaces, 2020*

Other halide perovskite compositions?

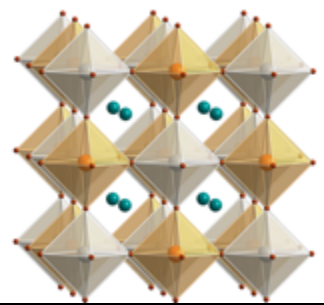
$Cs_2AgBiBr_6$





$CsBr + AgBr + Bi(III)Br \rightarrow CsAgBiBr_6$

Mechanochemical synthesis



Nathan Rodkey, Stan Kaal, et al unpublished results

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Solar Cells?

Collaboration with solar cell groups:

Pulsed Laser Deposition (PLD)

Known for playing LEGO on atomic scale with complex oxides …

Prof. Mark Huijben
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Complex optoelectronic materials for solar cells with PLD?

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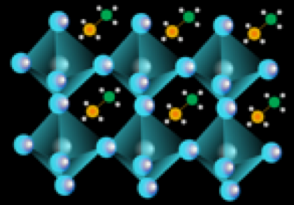
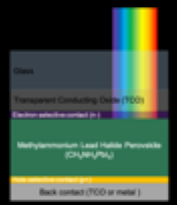
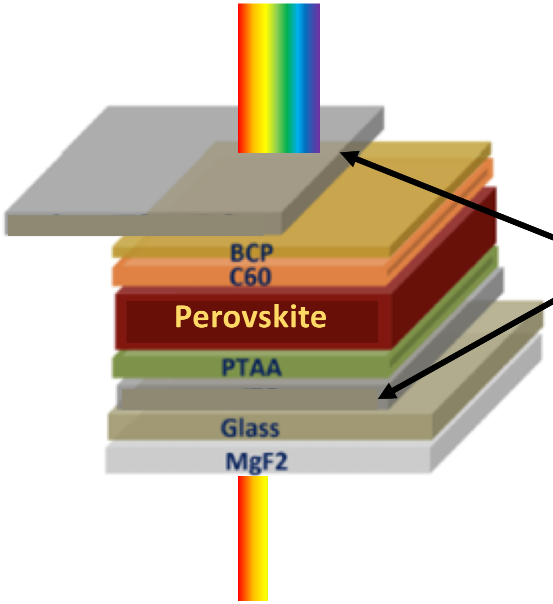
Near stoichiometric transfer of multi-compounds. Volatility insensitive.	Halide Perovskites ABX_3, X = I, Br, Cl	
Low-damage deposition of thin films on sensitive substrates.	Transparent Conducting Oxides (TCOs)	

But absolute requirement for PV …

Scalability (deposition on wafer-size substrates)

Scalable PLD of Transparent Conducting Oxides for Solar Cells

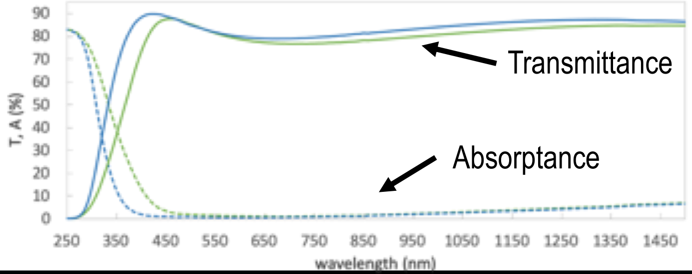
Zr-doped In_2O_3 (IZrO) as Vis-NIR transparent and conductive material



Transparent Conducting Electrodes

↓

Zr-doped In_2O_3



σ = 1500 $\Omega^{-1}cm^{-1}$ (amorphous)

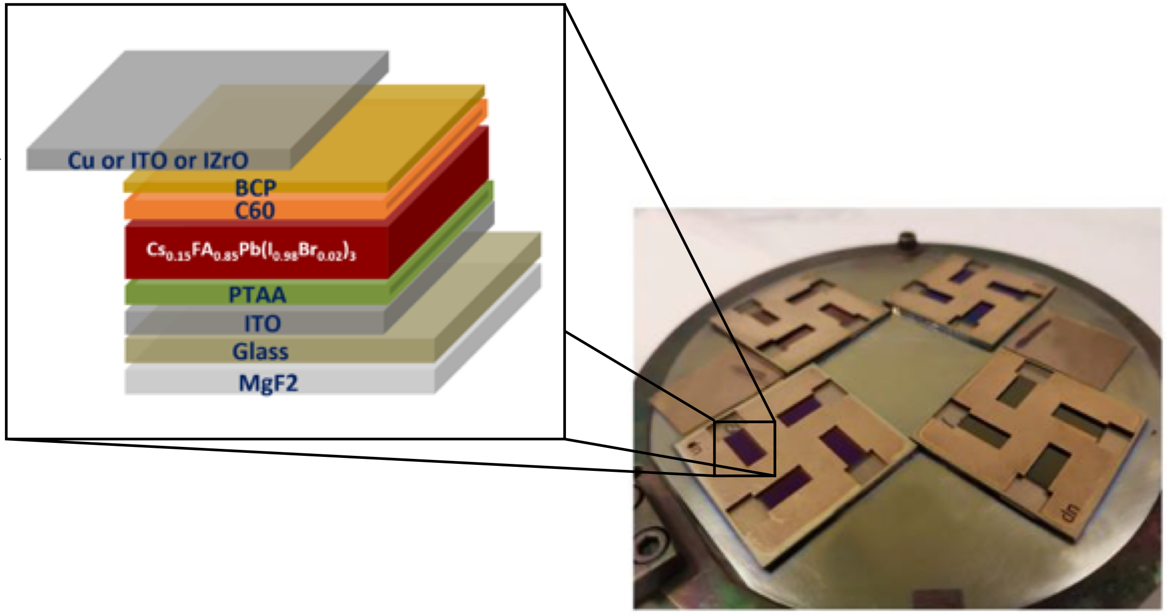
σ = 4200 $\Omega^{-1}cm^{-1}$ (polycrystalline)

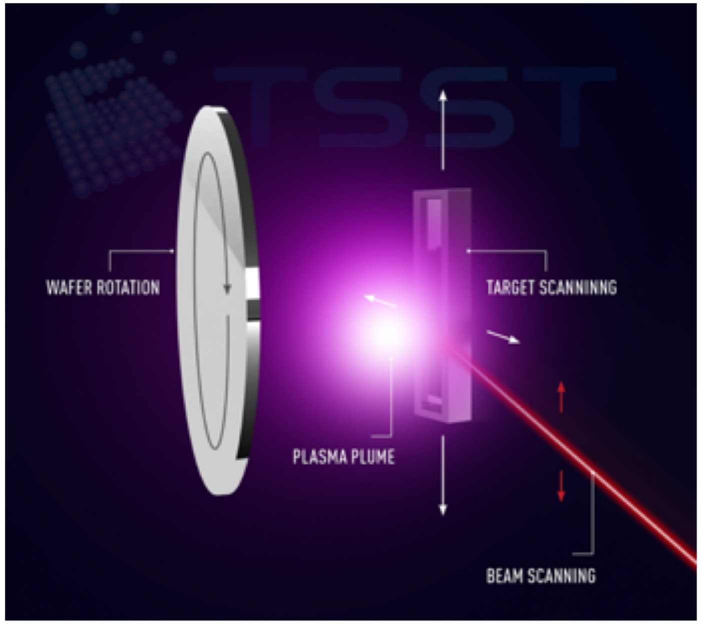
M. Morales-Masis, et al. IEEE JPV, Vol.8, 2018

E. Aydin , …Y. Smirnov, M. Morales-Masis,..S. De Wolf et al. Adv. Funct. Mater. 2019

PLD of IZrO as Rear Electrode for Semitransparent Perovskite Solar Cells

Transparent
Conducting
Rear Electrode





SOLAR RESEARCH
SOLLIANCE

Wafer scale PLD of IZrO:

- 4 substrates (30 x 30 mm) with 4 cells (0.09 cm2) per deposition;
- RT deposition (50 Ohm/sq)

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Ref.
Smirnov, Schmengler, Kuik,... Morales-Masis – In-Press, Adv. Mater. Technol. 2020

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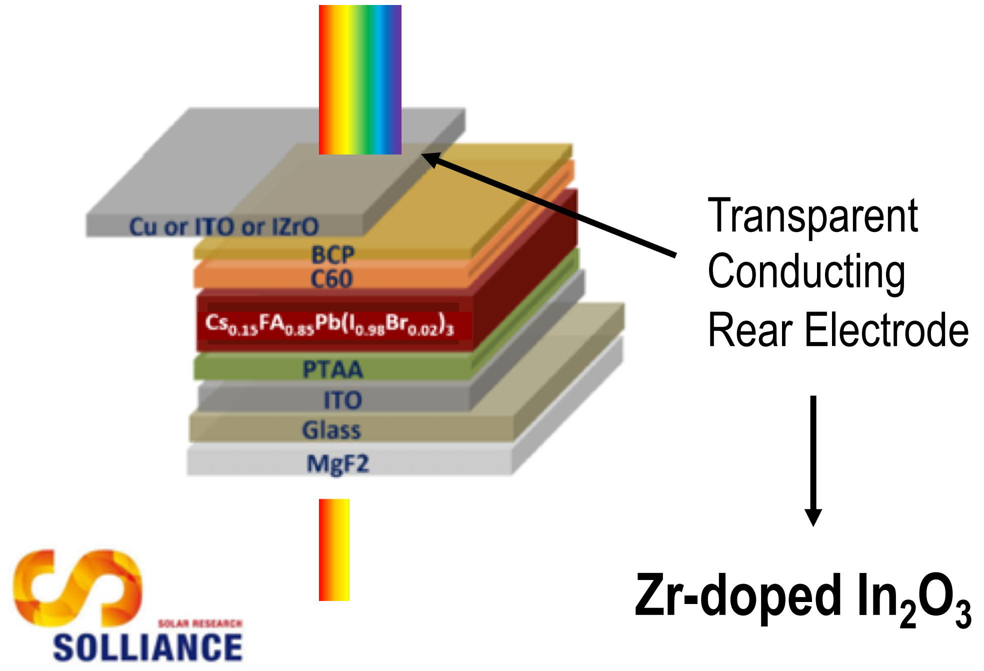
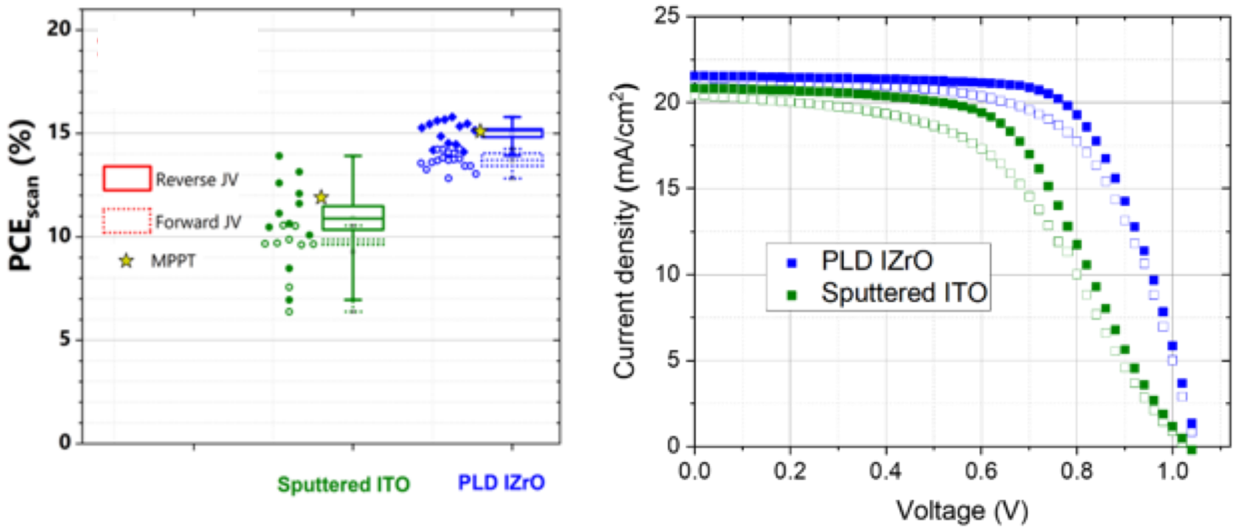
PLD of IZrO as Rear Electrode for Semitransparent Perovskite Solar Cells





Cells with PLD IZrO:

- No S-shape IV (R_{sh} of ITO and IZrO ˜ 50 Ohm/sq)
- Improved FF and V_{oc} compared to sputtered ITO

Ref.
Smirnov, Schmengler, Kuik,... Morales-Masis – In-Press, Adv. Mater. Technol. 2020

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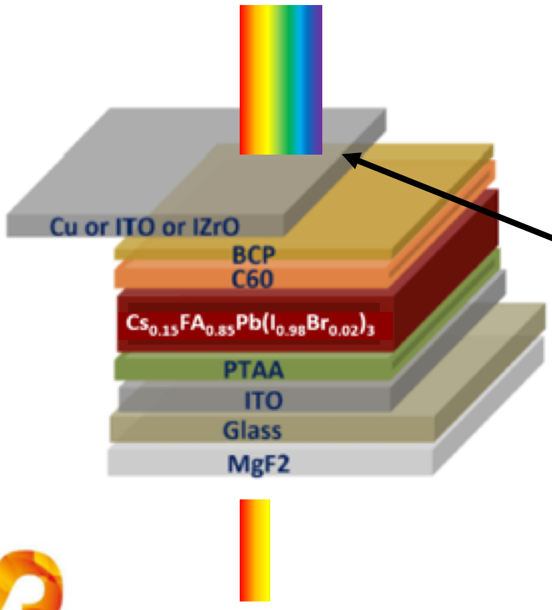
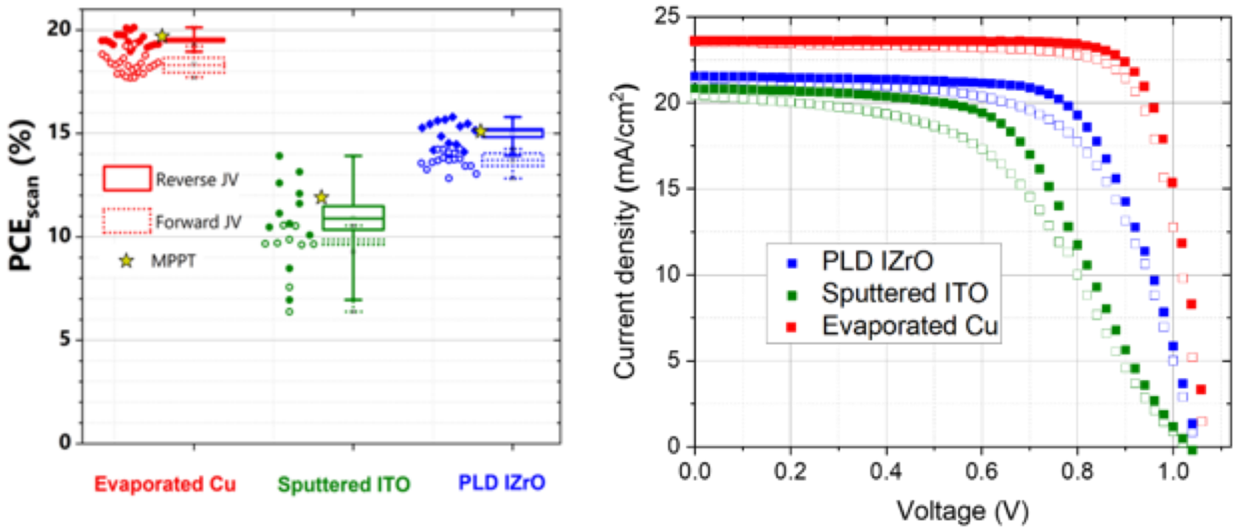


Transparent
Conducting
Rear Electrode

↓

Zr-doped In_2O_3

SOLLIANCE SOLAR RESEARCH



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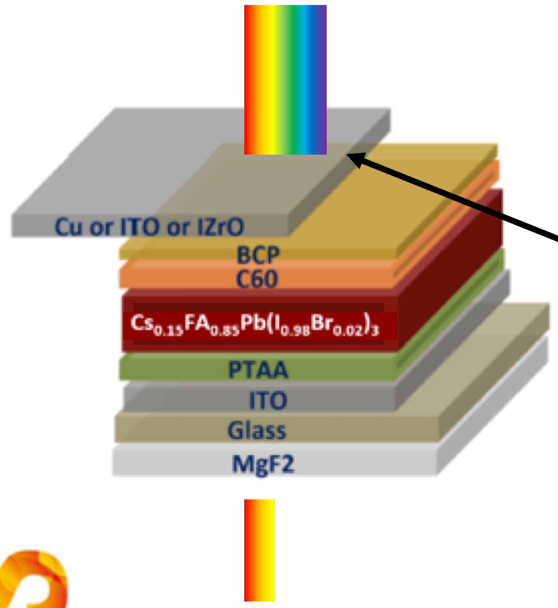
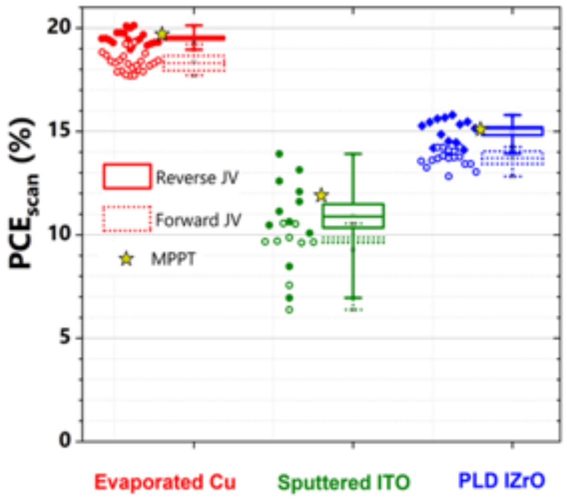
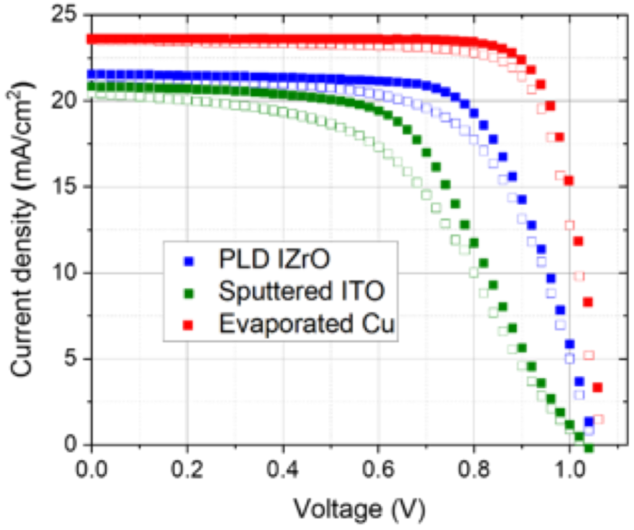
PLD of IZrO as Rear Electrode for Semitransparent Perovskite Solar Cells



Transparent
Conducting
Rear Electrode

Zr-doped In_2O_3





Cells with PLD IZrO:

- Cu baseline = 20% (high quality absorber)
- Improved FF and V_{oc} compared to sputtered ITO

Ref.
Smirnov, Schmengler, Kuik,... Morales-Masis – In-Press, Adv. Mater. Technol. 2020

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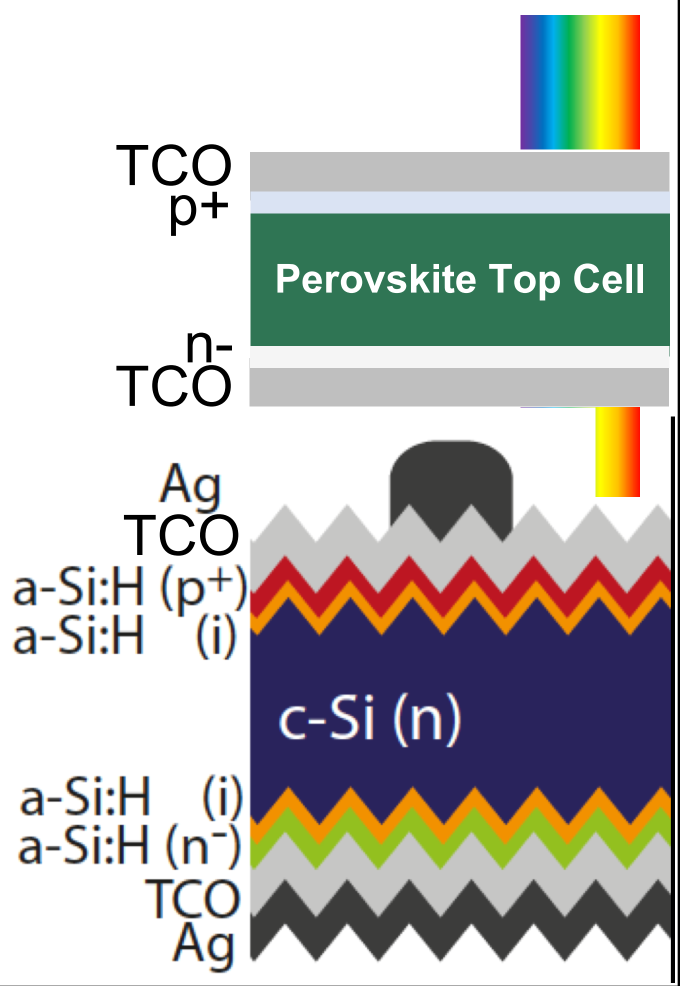
Outlook

Tandems: potential for >30% efficiency

Hybrid perovskite top cell
Excellent blue-Vis response
Low subgap absorption

SHJ solar cell
Excellent red response
Excellent surface passivation
(V_{oc} up to 750 mV)

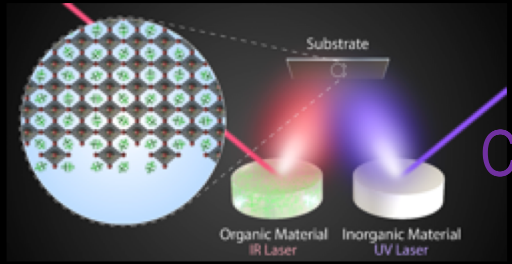


PLD

1. Monolithic integration of halide perovskites on textured silicon bottom cells

2. Soft deposition of the contacts on top of sensitive device layers.

3. Exploration of new stable and Pb-free perovskite compositions



CREATE

M³ Lab

MESA+ UNIVERSITY OF TWENTE.

Thank you

Team members, IMS group, NEM cluster and MESA+

Collaborators

SOLAR RESEARCH SOLLIANCE

FZU

VNIVERSITAT DE VALÈNCIA

Fraunhofer ISE

KAUST

SOLMATES THIN FILM EQUIPMENT

TSST

Funding

European Research Council
Established by the European Commission

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NWO

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