Summer 2021

Surface Energy and Microstructure: The Effect of the Underlying Substrate on Perovskite Film Formation for Solar Cell Absorbers

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Recommended Citation

Rasmussen, Mirra M.; Crowley, Kyle M.; and Martin, Ina T., "Surface Energy and Microstructure: The Effect of the Underlying Substrate on Perovskite Film Formation for Solar Cell Absorbers" (2021). *Student Scholarship*. 12.
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Surface Energy and Microstructure: The effect of the underlying substrate on perovskite film formation for solar cell absorbers

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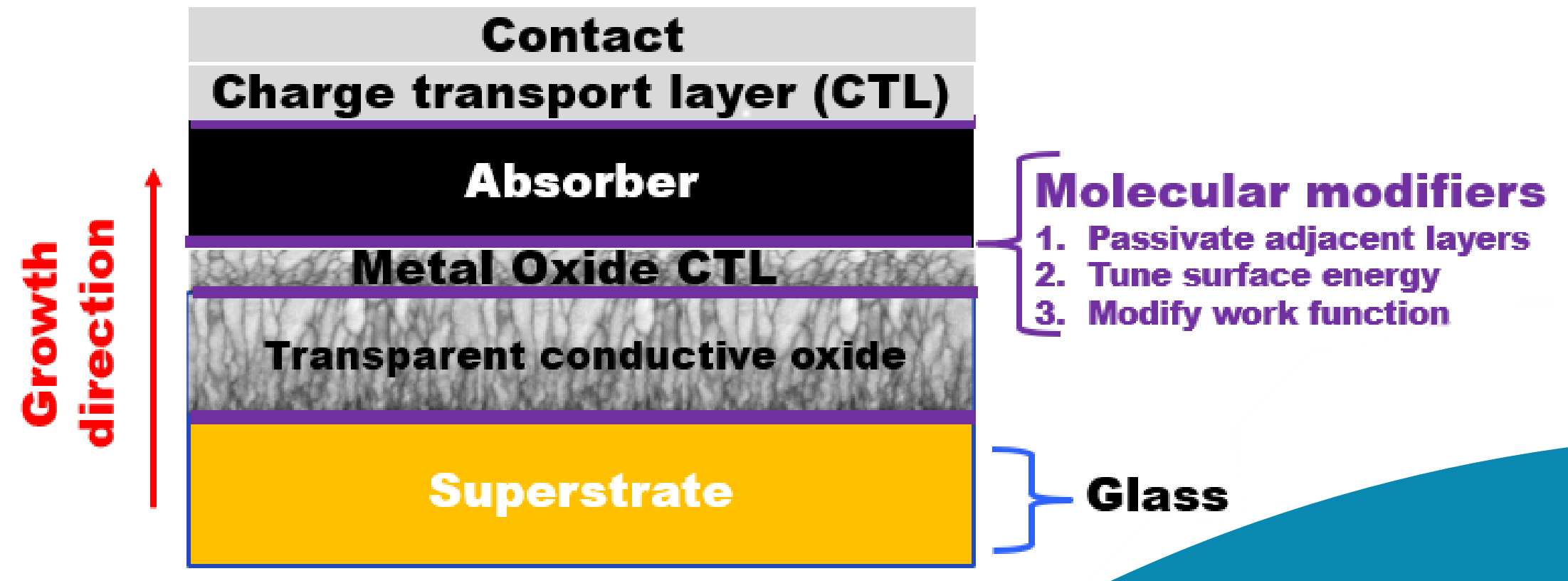
Introduction & Background

Pb-Based Perovskite Films as an Emerging PV Absorber

Record devices are over 20% efficient but there are materials problems that need to be solved [1].

Interfacial modification affects:

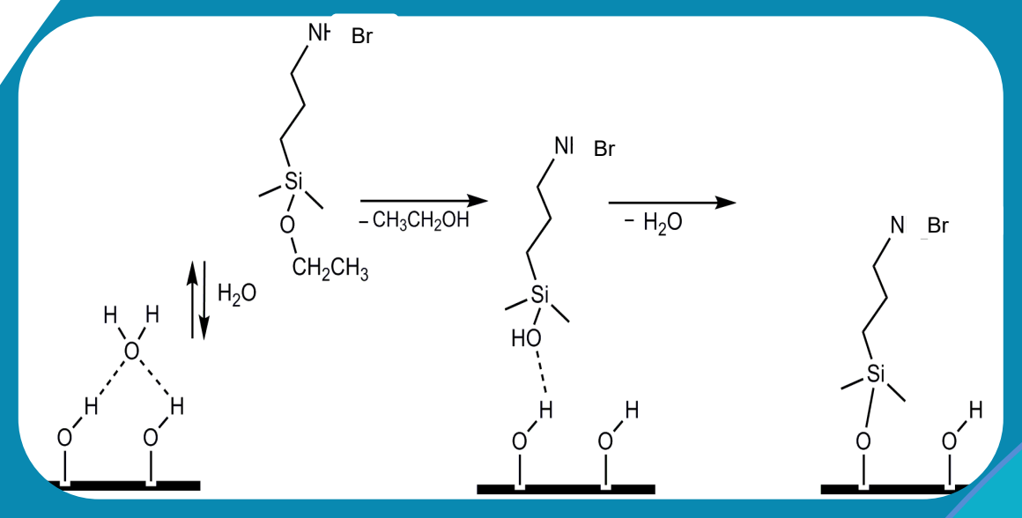
- Film uniformity
- Crystallinity
- Grain size
- Defect density



Small molecule modifiers and their positive effects on device performance. Data from references [2] and [4].

Modifier	Stack Structure	V_{oc} [V]	J_{sc} [mA cm^{-2}]	PCE [%]
Bromobenzoic Acid *(Br-BA)* [2]	ITO/NiO_x/ $MAPbI_3$/PCBM /bis-C_{60}/Ag	1.07	19.1	15.3
	ITO/NiO_x/ **Br-BA**/ $MAPbI_3$/PCBM /bis-C_{60}/Ag	1.11	21.7	18.4
(3-Aminopropyl) triethoxysilane *(APTES)* [4]	FTO/SnO_2/ $MAPbI_3$/ Spiro-OMeTAD/Au	1.065	20.84	14.69
	FTO/SnO_2/ **APTES**/ $MAPbI_3$/ Spiro-OMeTAD/Au	1.16	21.23	17.03

Goal: Improve stability of perovskite absorbers through small molecule modification of perovskite-TCO interface.



Chemical process of small molecule modification of a metal oxide.

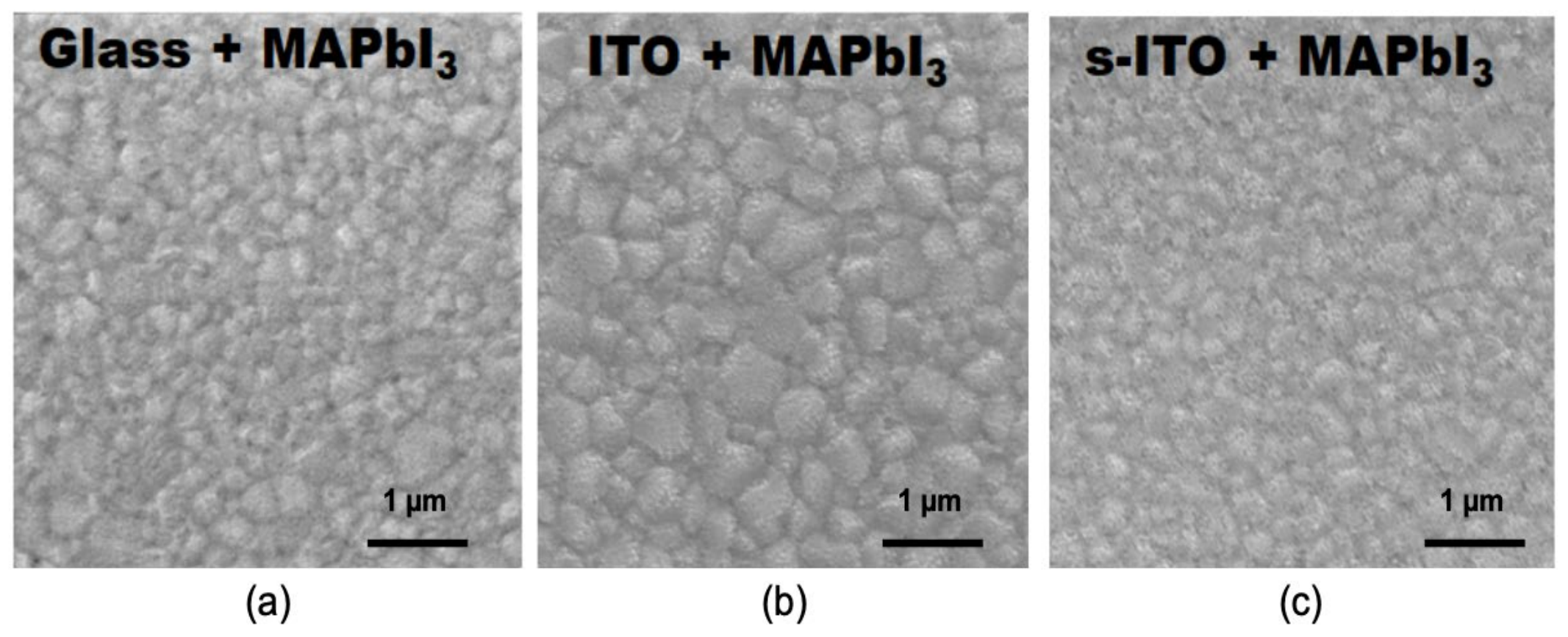
Device properties and performance are directly tied to perovskite film properties [3].

Interfacial Modification and Stability

BPTMS and $MAPbI_3$ Grain Growth

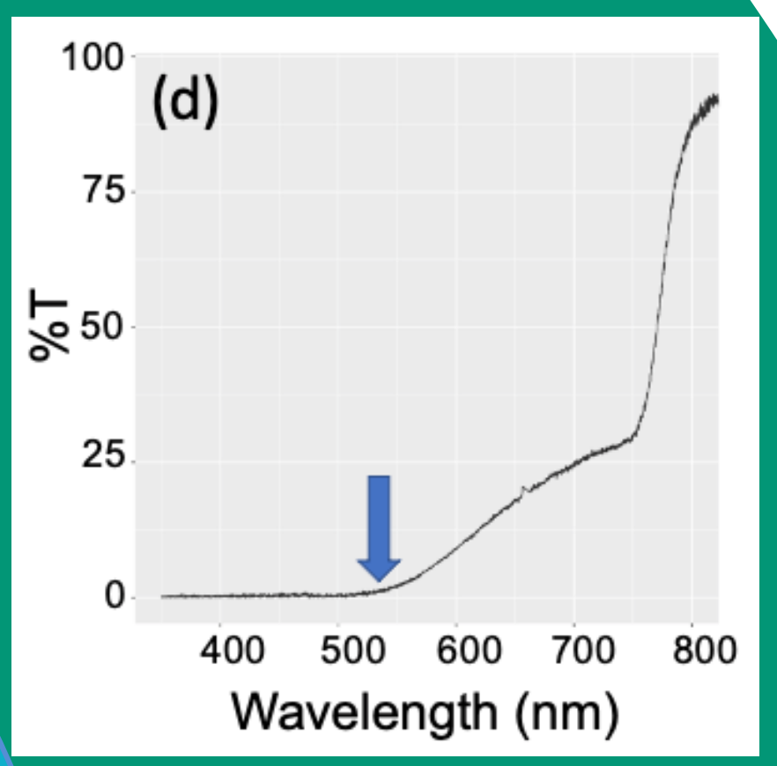
"s-" denotes inclusion of BPTMS interlayer

- BPTMS leads to growth of smaller grains on ITO
- $MAPbI_3$ grains on s-ITO comparable in size to those grown on glass



(a) (b) (c)

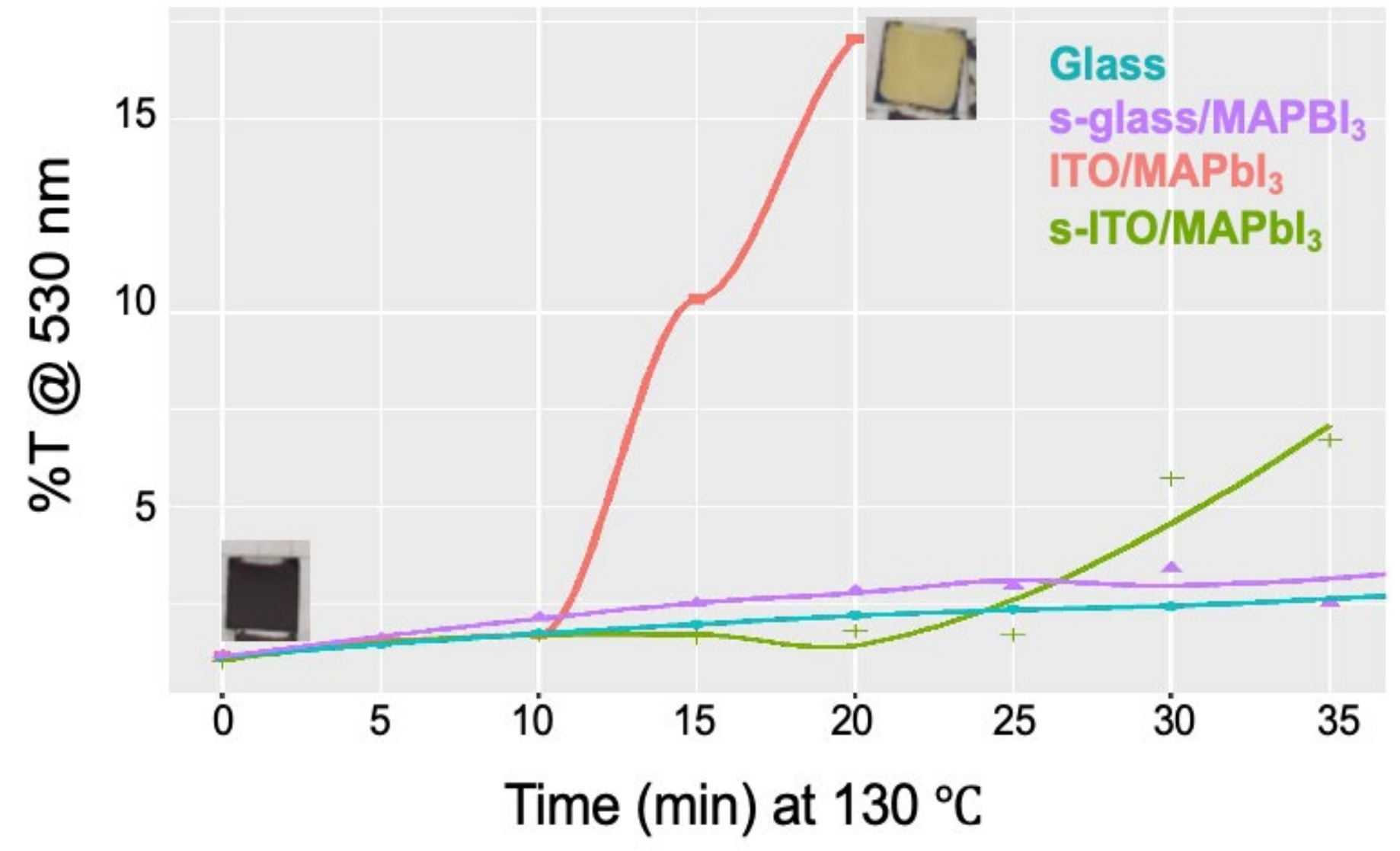
Results: BPTMS passivates the perovskite-TCO interface, affecting both the film morphology and degradation profile of the perovskite.



UV-Vis spectrum of $MAPbI_3$ on s-ITO.

BPTMS and $MAPbI_3$ Degradation

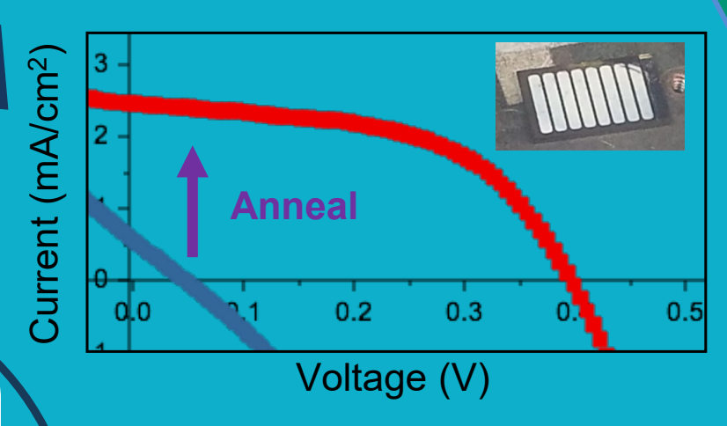
- BPTMS mitigates $MAPbI_3$ degradation on ITO (in green) compared to the unmodified control (in red)
- Decouples effects of grain size from interfacial chemistry in terms of stability

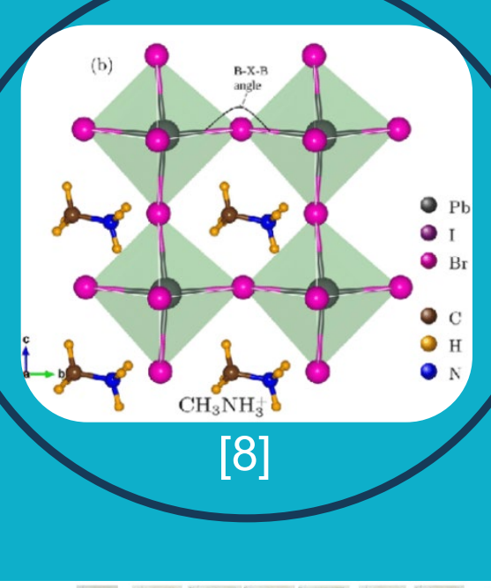


Materials Design for Reliability

Materials Synthesis & Characterization

Device Fabrication & Optimization





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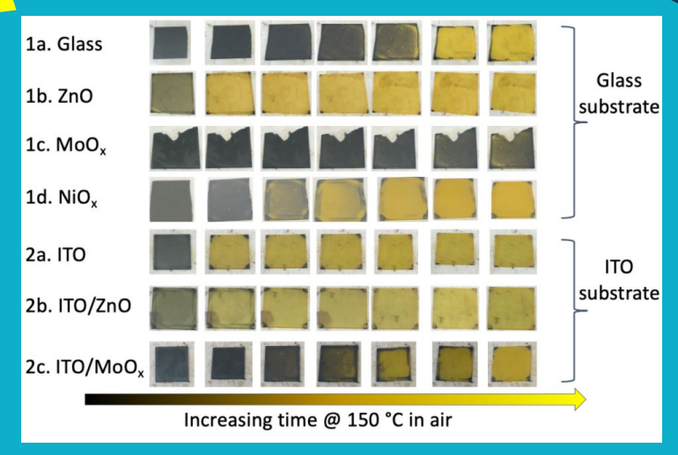


Lifetime Enhancement

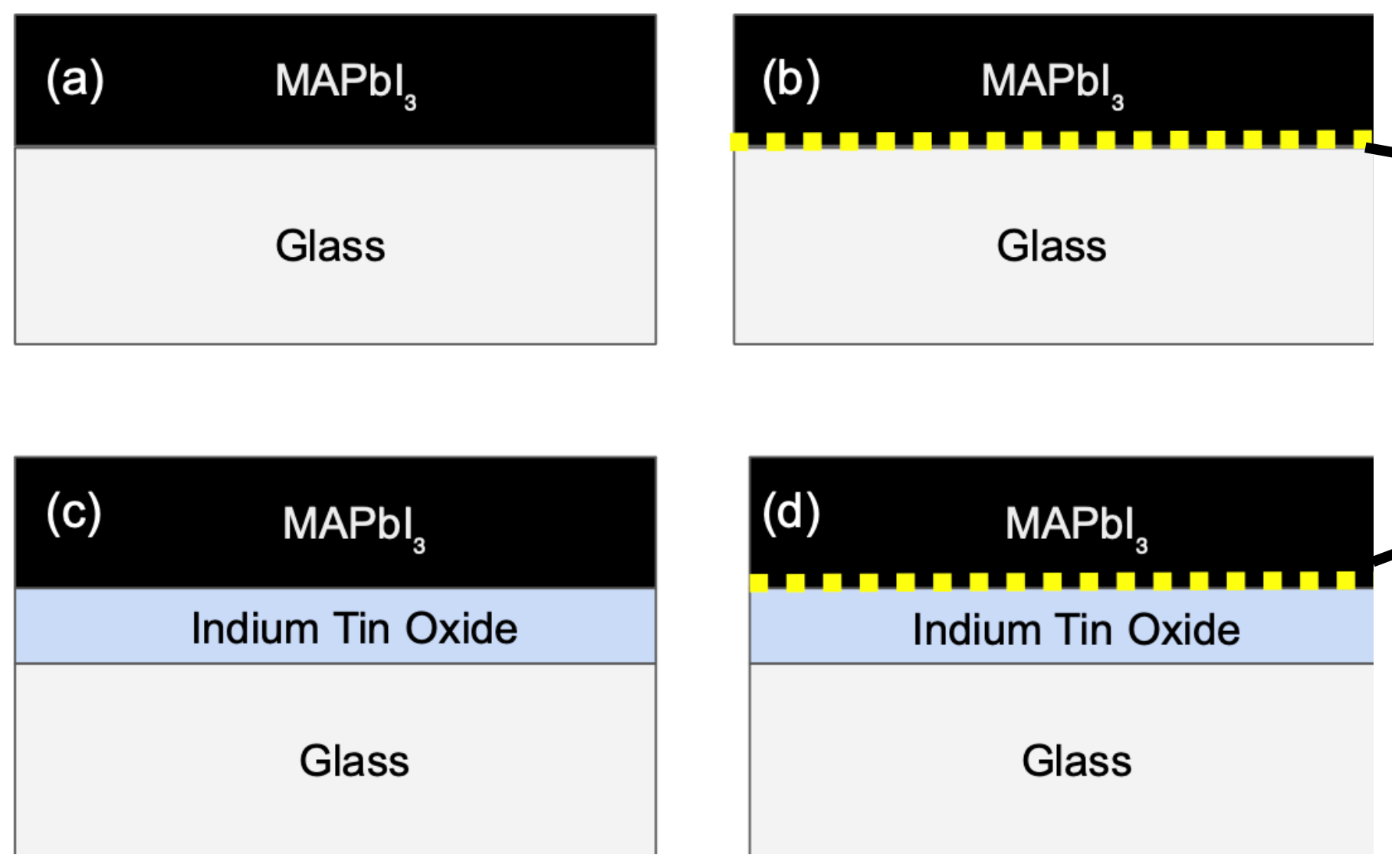
Silane and Perovskite Deposition

Experimental Flow

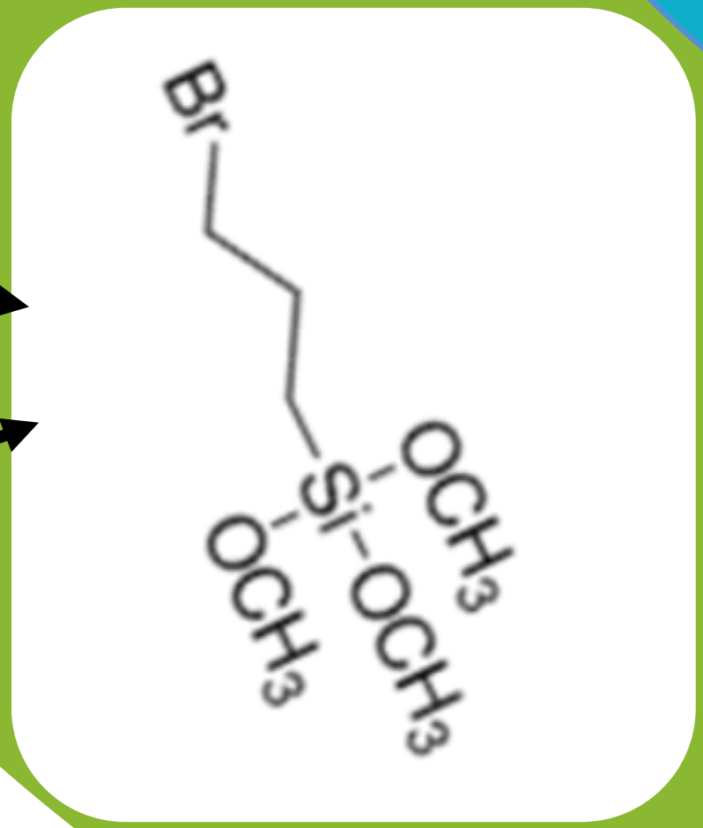
1. Clean substrates
2. Deposit organofunctional silane [6,7]
3. Spin coat $MAPbI_3$ and anneal [5]
4. Characterization and degradation

Approach: Deposition of $MAPbI_3$ on bare and silane-modified substrates to systematically investigate effects of a BPTMS interlayer on perovskite degradation.

Schematic overview of film stacks



Dashed line indicates organofunctional silane layer.

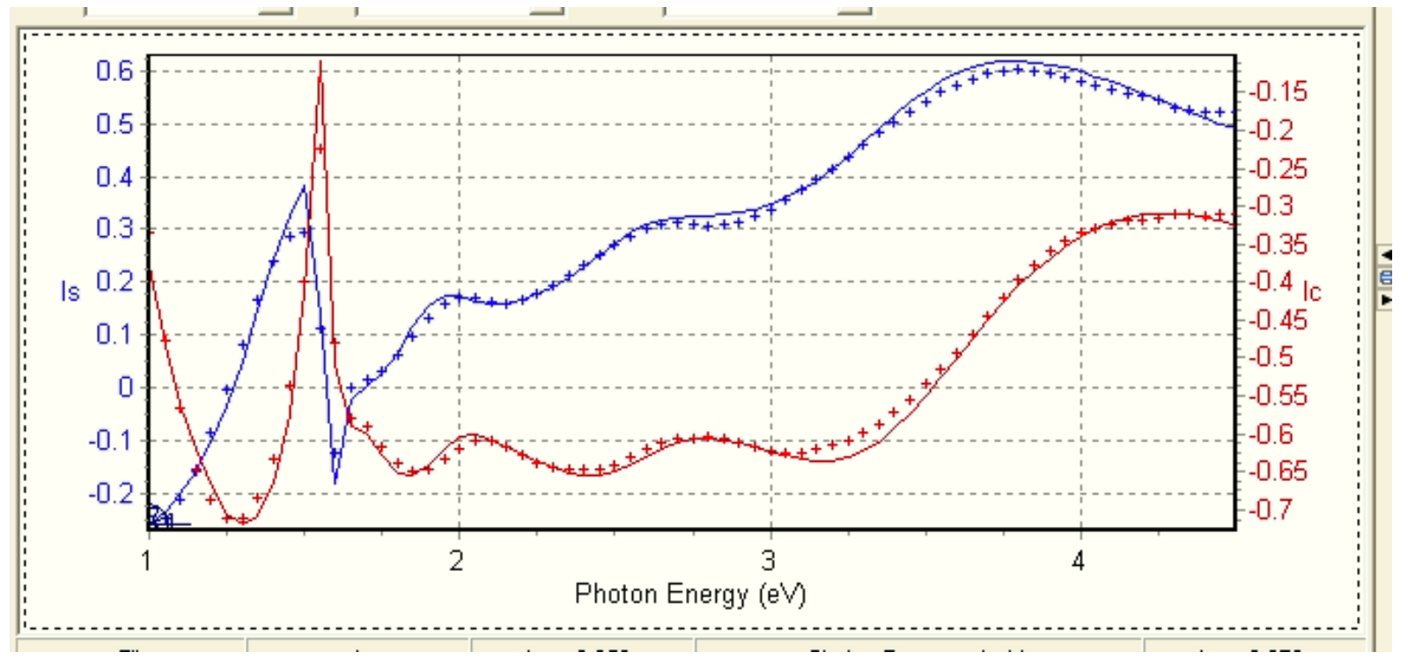


Molecular structure of 3-Bromopropyl trimethoxysilane [BPTMS]

Substrate	Thickness, Å	Contact Angle, degrees
Silicon	11 ± 1	62 ± 3
	24 ± 1	81 ± 2
	34 ± 2	84 ± 1
ITO	6 ± 1	72 ± 2

Left: Characteristics of BPTMS modified ITO and silicon. Silane thickness is modelled from spectroscopic ellipsometry measurements.

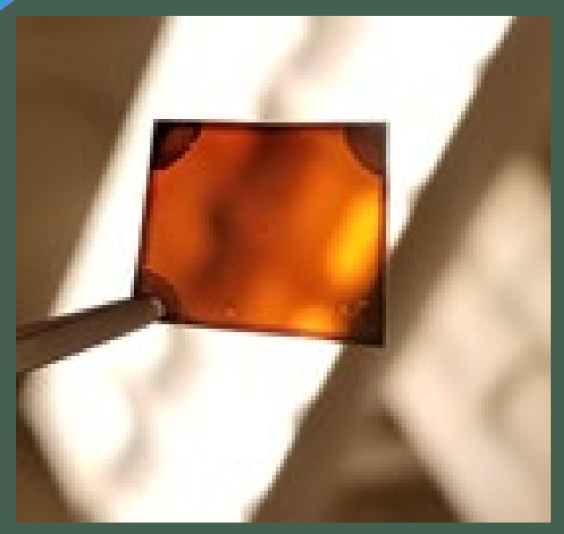
Right: SE characterization of perovskite films



Conclusions and Future Directions

Future Directions:

- Apply silanes to MOs (Metal Oxides), commonly used as PV charge transport layers
- Investigate systematically varied TCO/MO/silane combinations in half-stack degradation studies



- Further investigate silane-MO interface and its effects on the perovskite film with SE and XPS

Conclusions

- ❖ Results highlight importance of film studies under device-relevant conditions
- ❖ Organofunctional silanes used as molecular modifiers can passivate a TCO/perovskite interface
- ❖ Interfacial modifiers have multifaceted effects on perovskite film morphology and lifetime

Acknowledgements

We acknowledge the Case Western Reserve University School of Engineering Faculty Investment Fund for funding the bulk of this work ("Fundamental Materials Studies of a Novel Lead-Free Perovskite"). We also acknowledge the CWRU Flora Stone Mather Center for Women for funding Mirra Rasmussen via a 2021 Women in STEM SOURCE grant. Experimental work was performed in the CWRU Materials for Opto/electronics Research and Education (MORE) Center, a core facility est. 2011 by Ohio Third Frontier grant TECH 09-021.

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