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Understanding the Role Thin Film Interfaces Play in Solar Cell Performance and Stability

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Understanding the Role Thin Film Interfaces Play in Solar Cell Performance and Stability

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AIM: Improve stability of perovskite and Si solar cells through optimization of the metal oxide/thin film interfaces.

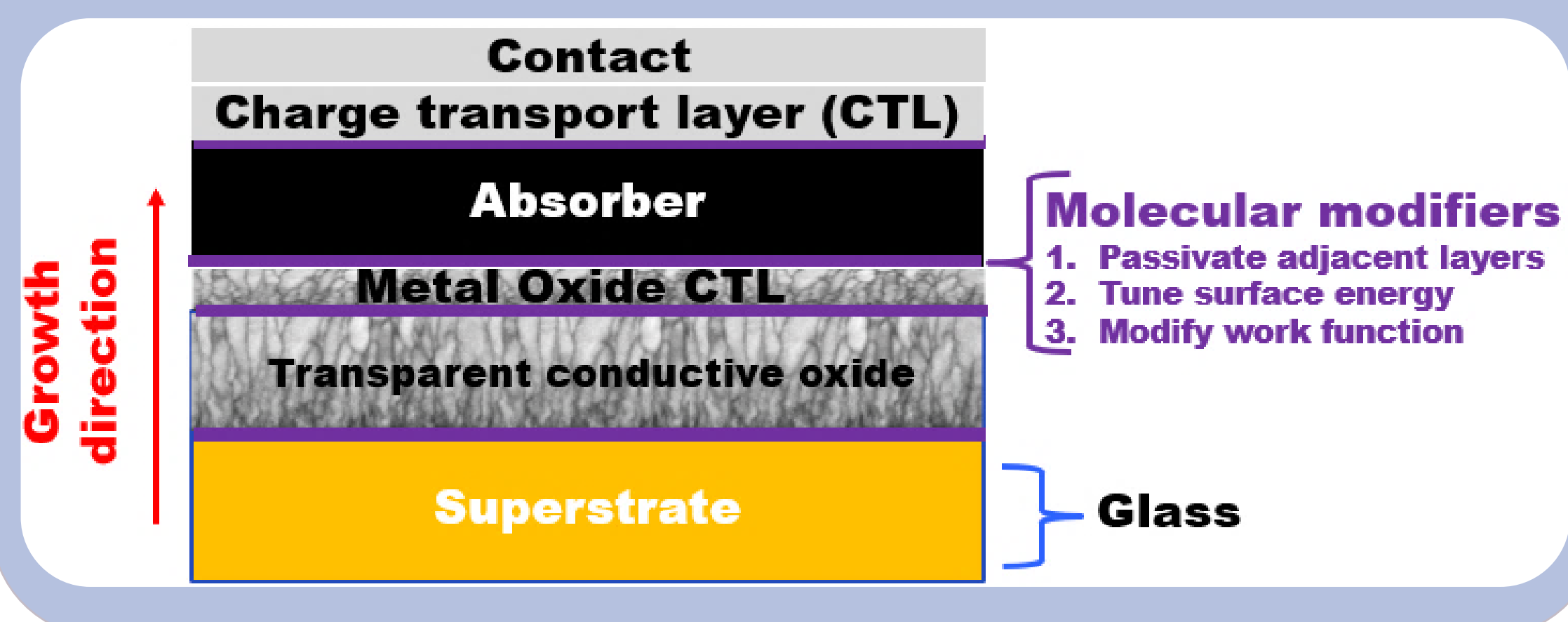
Film Studies and Device Performance

- Interfacial modification/structure affect:
 - Film uniformity
 - Crystallinity
 - Grain size
 - Defect density

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) [3]	FTO/SnO ₂ /MAPbI ₃ /Spiro-OMeTAD/Au	1.07	20.84	14.69
	FTO/SnO ₂ / APTES /MAPbI ₃ /Spiro-OMeTAD/Au	1.16	21.23	17.03
Naphthalene-imide Self-assembled Monolayer (NMI) [4]	ITO/Cs _{0.05} FA _{0.8} MA _{0.15} PbI _{2.5} Br _{0.5} /Spiro-OMeTAD/Au	1.00	18.3	11.5
	ITO/ NMI /Cs _{0.05} FA _{0.8} MA _{0.15} PbI _{2.5} Br _{0.5} /Spiro-OMeTAD/Au	1.03	20.0	12.6

Approach

Deposition of MAPbI₃ on bare and silane-modified substrates to systematically investigate effects of TCO and interlayers on perovskite degradation.



a-Si:H/TCO Films

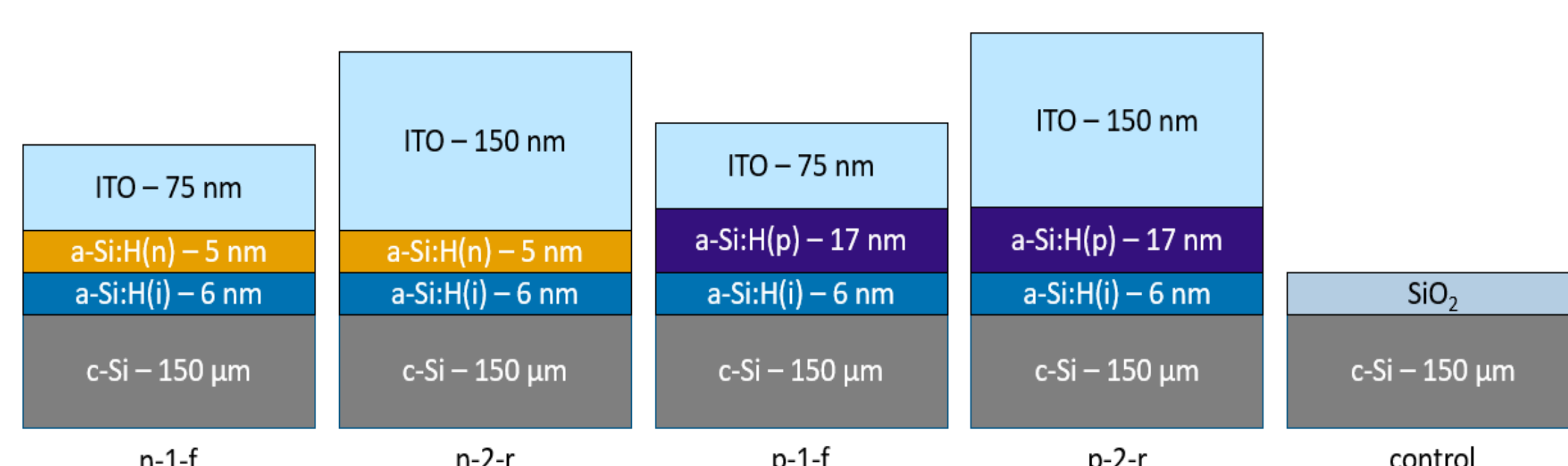
Silicon heterojunction PV among most efficient industrial-scale PV.

Goals:

- Decouple effects of encapsulation degradation from stack deterioration
- Rapid screening process for unencapsulated cells to probe fabrication variables

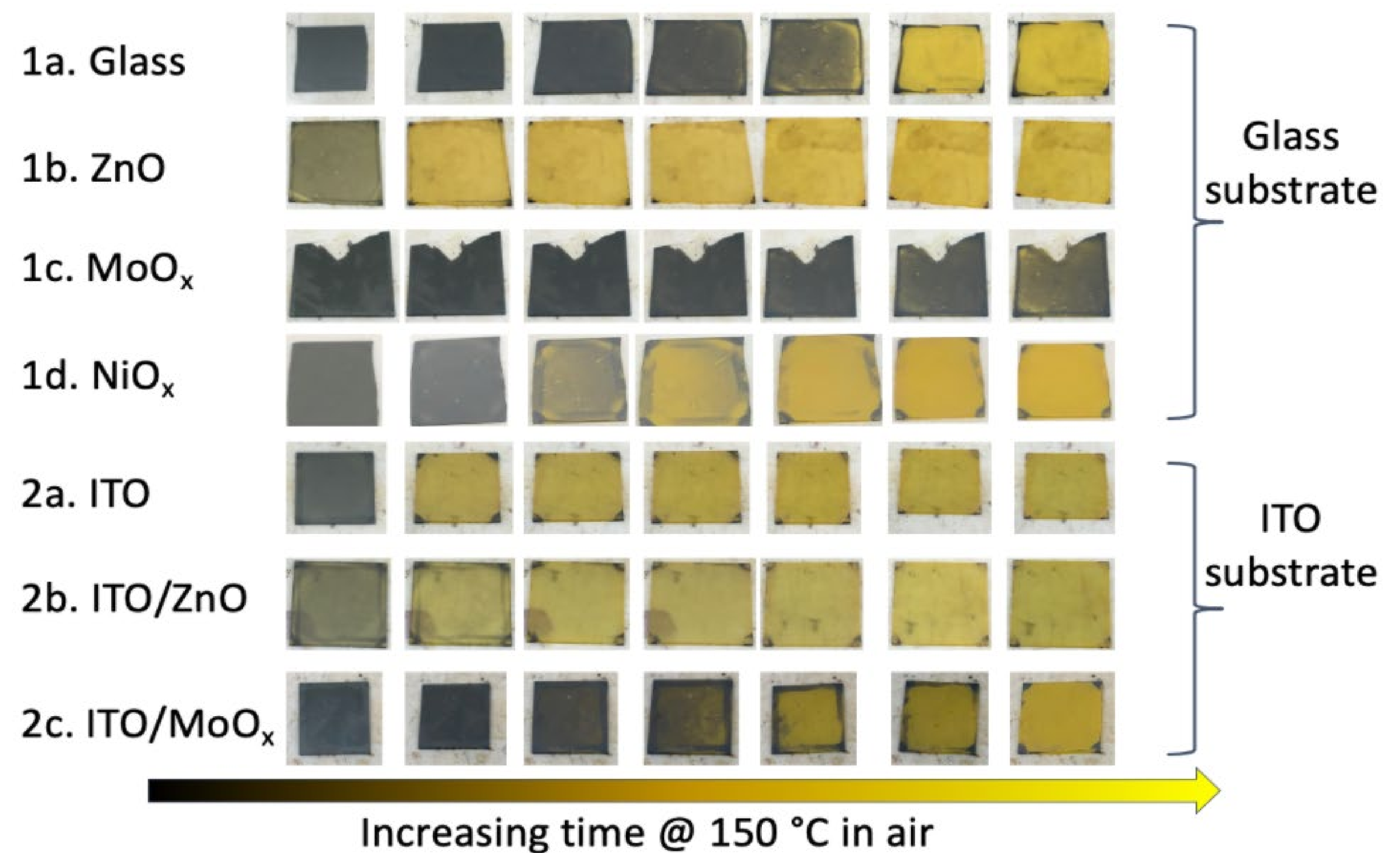
Focus on UV-induced degradation of film stacks:

- Step-wise aging study
- ToF-SIMS, XPS, spectroscopic ellipsometry
- Tracking hydrogen transport



Pb-Based Perovskite Films

- Emerging PV absorber – record devices over 20% efficient [1]
- Moisture and temperature sensitive
- Complex effects of aging on multilayer systems



Results

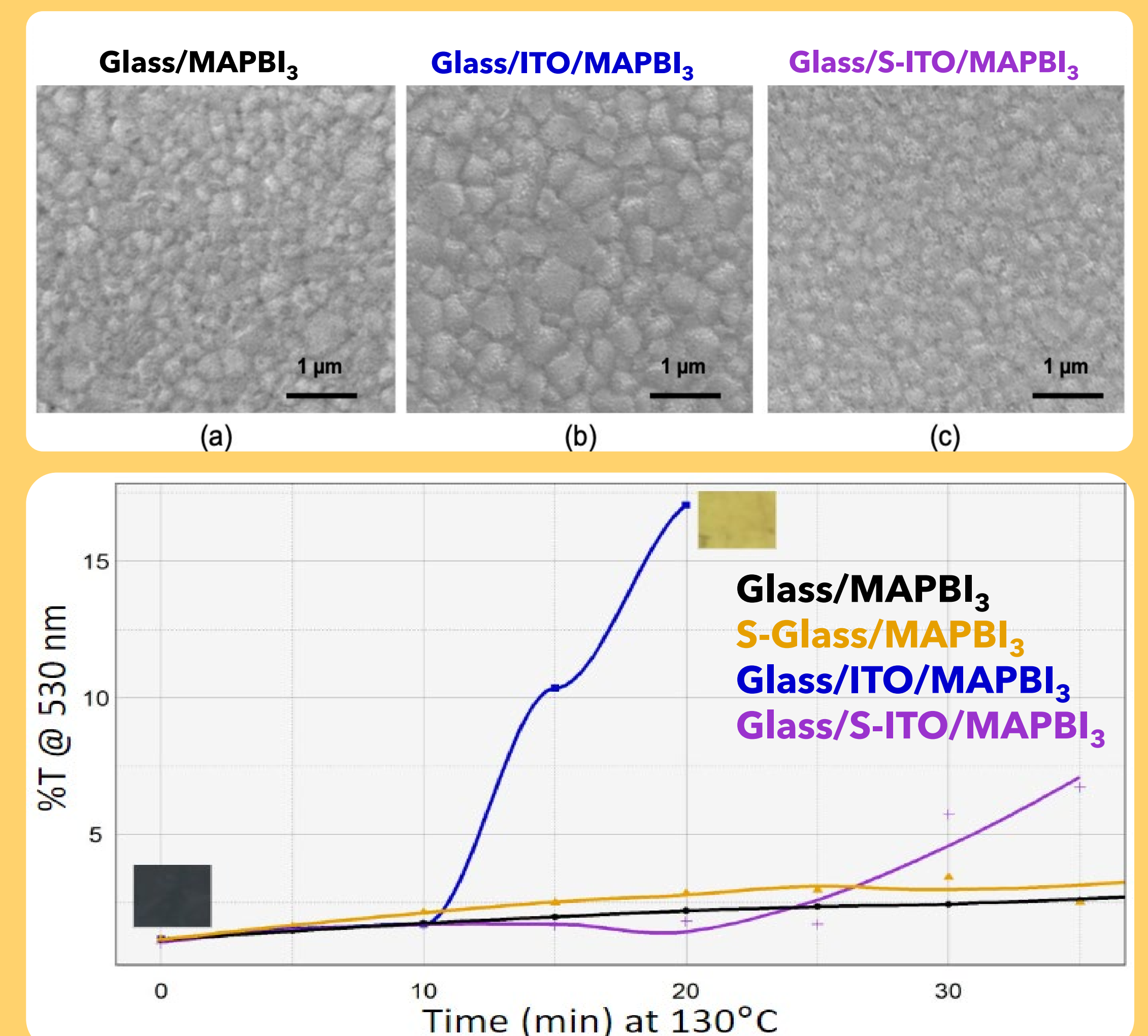
BPTMS passivates perovskite/TCO interface, affecting morphology and degradation profile.

MAPbI₃ Grain Growth:

- BPTMS modification leads to smaller grains on ITO
- Grains on S-ITO comparable to those grown on glass

MAPbI₃ Degradation:

- BPTMS mitigates degradation on ITO compared to control
- Decouples effects of grain size from interfacial chemistry



Conclusions and Next Steps

Results highlight importance of film studies under device-relevant conditions.

- Organofunctional silanes can be used as molecular modifiers to passivate a TCO/perovskite interface
- Interfaces/interfacial modifiers have multifaceted effects on film morphology and lifetime

Future work:

- ToF-SIMS to track differences in atomic composition profiles through samples with and without silane layers

Contact

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References

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- [2] *ChemSusChem*, 10 (2017), 3794-3803. DOI: 10.1002/cssc.201701262.
- [3] *Journal of Materials Chemistry A*, vol. 5, no. 4, pp. 1658-1666, 2017.
- [4] *ACS Appl. Energy Mater.*, vol. 6, no. 2, pp. 667, 2023.

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