Anatase, rutile, and brookite TiO_2 electron transport layers for mesoporous carbon-based perovskite solar cells

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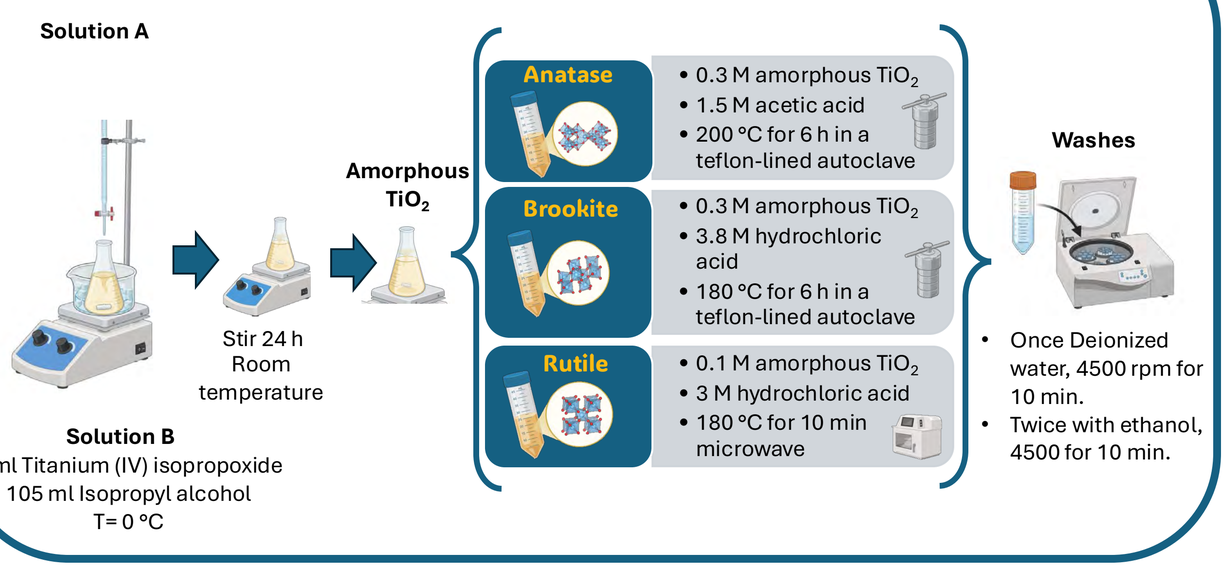
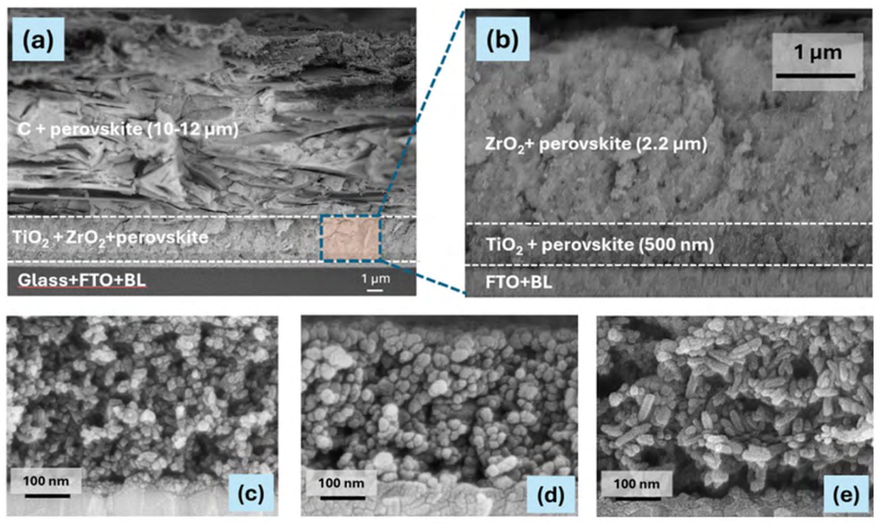
This work investigates the influence of the TiO_2 crystal structure and nanomaterial morphology on the effectiveness of the electron selective contact in triple-stack mesoporous, carbon-based perovskite solar cells (C-PSCs) and evaluates the impact of the relative humidity (45% and 60% RH) during the infiltration on the device characteristics.

Methodology:

Synthesis

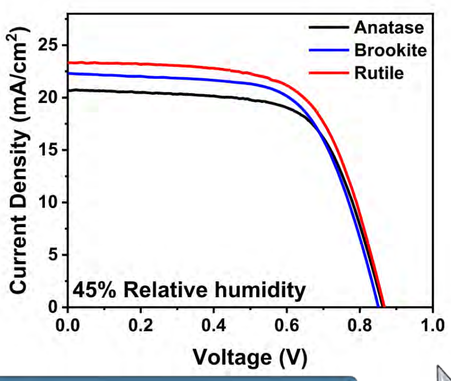


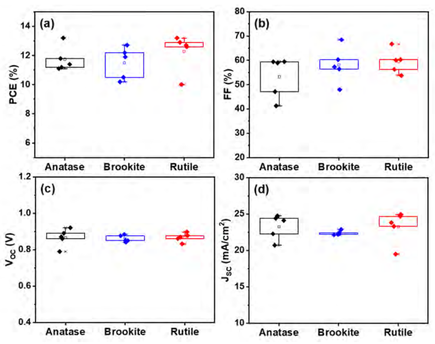
SEM

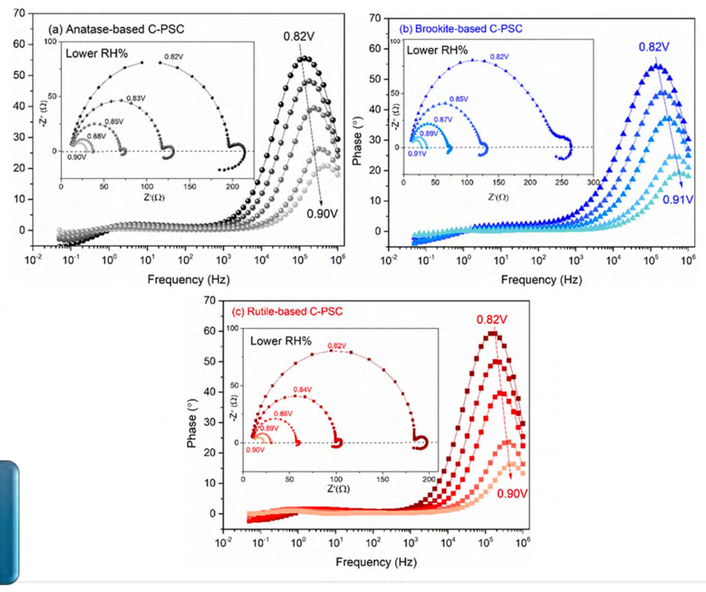


Results:

45% RH







Better conduction band alignment
Fewer interfacial defect states
→ Better electron extraction efficiency
Reduction of the recombination losses

More open pore network
→ Improve perovskite infiltration.
Promote de formation of larger perovskite grains
→ Improving charge transport
Mitigating recombination

The results demonstrate that variations in TiO_2 crystallographic phase have minimal influence on recombination kinetics, interfacial dynamics, and capacitive responses.

High humidity introduces phase-dependent variations in interfacial processes and ion dynamics.

Conclusions:

- Photovoltaic measurements showed robust performance of all C-PSC configurations at 45% RH, with rutile-based devices slightly outperforming anatase- and brookite-based counterparts.
- At higher humidity (60% RH), anatase-based cells demonstrated the highest resilience
- These results emphasize the inherent robustness and scalability potential of triple-stack C-PSCs for manufacturing under realistic and challenging conditions, particularly in humid climates.

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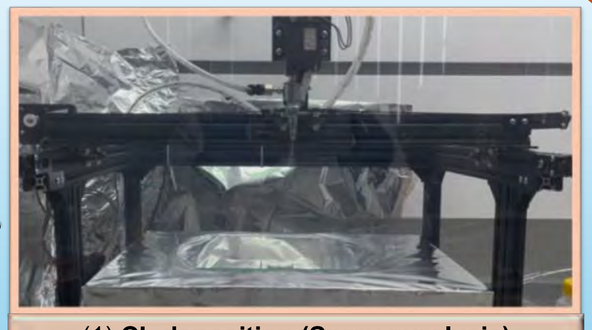
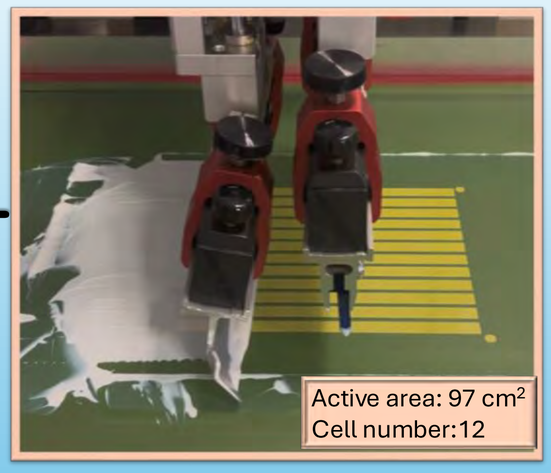
Step 1



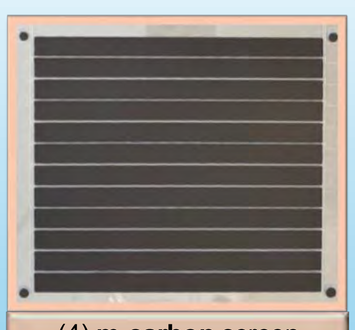
(1) **CL deposition (Spray pyrolysis)** 10% v/v titanium diisopropoxide bi(acetylacetonate) in IPA at 280 ° C. Heat treatment at 400 ° C for 10 min.

Step 2



(2) m-TiO_2 screen printing and heat treatment at 510 ° C for 45 min

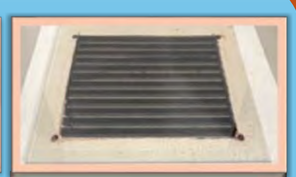
(3) m-ZrO_2 screen printing and heat treatment at 400 ° C for 30 min



(4) **m-carbon** screen printing and heat treatment at 400 ° C for 30 min

Step 3

(5) **Infiltration** 1.1MPbI_2 , 1.1M MAI, 0.33M 5-AVAI, 9:1 (v/v) GBL:anhydrous methanol, 20%RH.

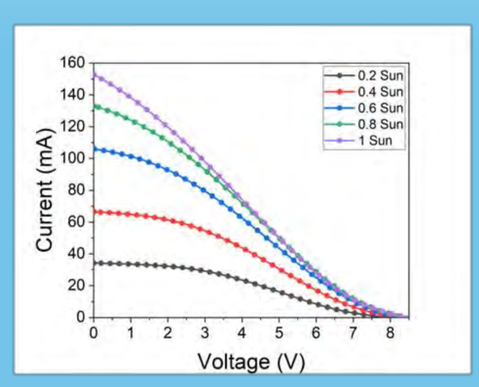


(6) **Perovskite conversion** at 52 ° C

Step 4

(7) **Parylene-C** deposition at room temperature and 3.3 Pa.

(8) **Edge seal** butyl rubber (Quanex) at 90 °C and 800 mbar for 15 min.



Sample	Irradiance	Eff(%)	FF (%)	V_{oc} (V)	I_{sc} (mA)
A1	1 Sun	3.1	24	8.4	153
A1	0.8 Sun	3.7	26	8.4	133
A1	0.6 Sun	4.3	29	8.2	106
A1	0.4 Sun	4.4	32	8.1	66
A1	0.2 Sun	4.7	34	7.8	34

The encapsulation and sealing of the modules was carried out at Newcastle University in collaboration with Susana Iglesisas-Porras and Elizabeth A. Gibson.

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