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Additive Engineering and Surface Passivation for High Efficiency and Long-term Stability of α-$FAPbI_3$ Perovskite Solar Cells

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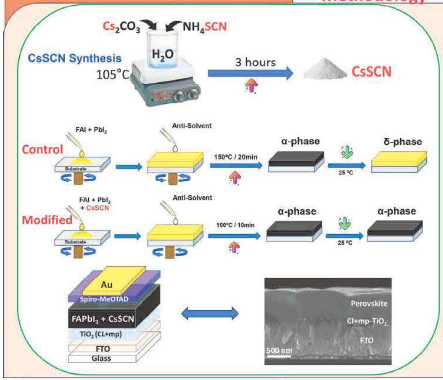
Introduction

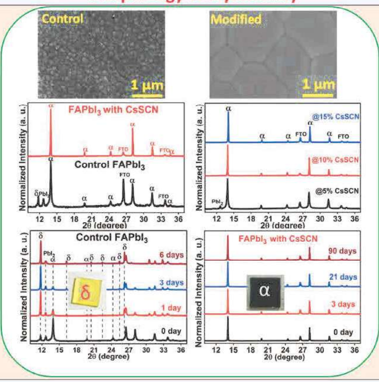
Formamidinium lead triiodide (**$FAPbI_3$**) is a promising semiconductor material for achieving efficient and thermally stable perovskite solar cells (PSCs). However, challenges such as phase instability and defect-related degradation hinder its performance and longevity. To address these issues, we introduce two synergistic approaches: **CsSCN** additive and dual-side surface passivation using **2D-COFs**. CsSCN, incorporated into the perovskite precursor solution, stabilizes the photoactive α-phase of $FAPbI_3$, as confirmed by XRD and MD simulations. This modification improves phase purity, increases grain size, enhances film uniformity, and reduces defects, resulting in a peak PCE of **22.91**% and operational stability exceeding 1000 hours under continuous illumination. Simultaneously, dual-side passivation with (**TFPG-BT-COFs-Cu(CF_3-SO_3)$_2$**) addresses defect traps at the electron and hole interfaces. At the electron-transport layer, the ionic COFs interact with A-site cations (Cs, FA), compensating for defects and reducing nonradiative recombination. At the hole-transport layer, they alleviate lattice stresses and potential barriers, further enhancing stability and efficiency. This comprehensive strategy increased the output performance up to **23.99%** PCE. The combination of CsSCN additive and COF-based dual-side passivation presents a robust pathway to improve efficiency, stability, and durability of PSCs, paving the way for their widespread adoption in photovoltaic applications.

Additive Engineering

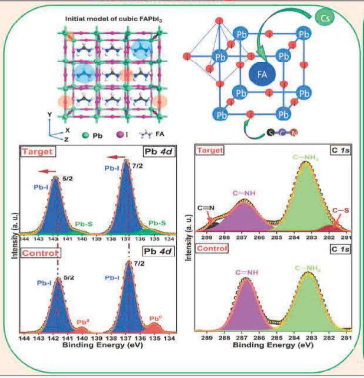
Methodology



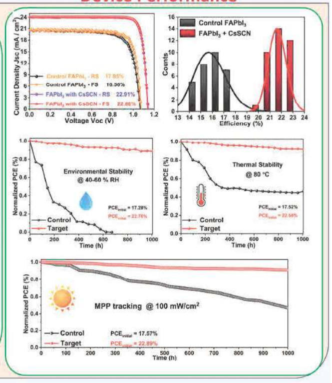
Morphology & Crystallinity



Chemical Bonding

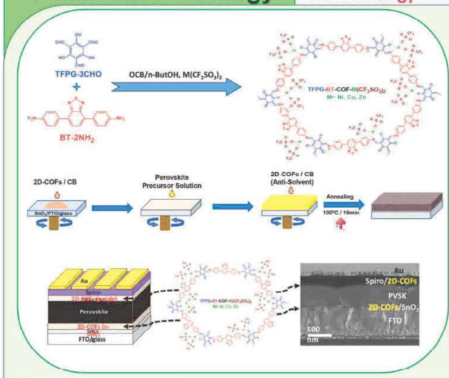


Device Performance

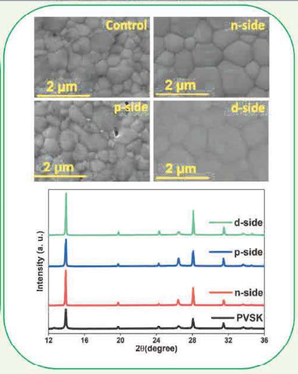


Passivation Strategy

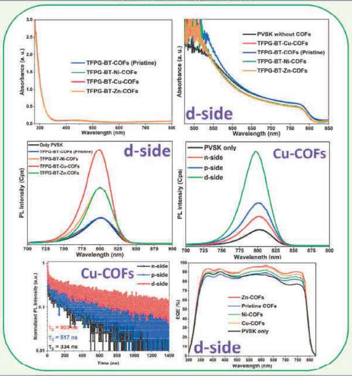
Methodology



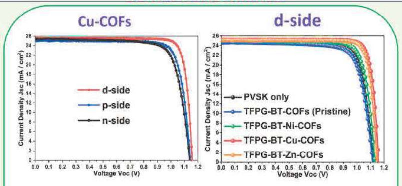
Morphology & Crystallinity



Optical Properties



Device Performance



	Jsc (mA/cm²)	Voc (V)	FF	PCE (%)
Control Perovskite	24.81	1.134	0.779	21.917
TFPG-BT-COFs	24.63	1.126	0.768	21.299
TFPG-BT-Ni-COFs	25.01	1.139	0.795	22.647
TFPG-BT-Cu-COFs	25.19	1.158	0.823	23.988
TFPG-BT-Zn-COFs	25.09	1.143	0.806	23.114

Conclusion

In this work, a dual strategy to improve the efficiency and stability of $FAPbI_3$-based PSCs. By incorporating CsSCN into the precursor solution, α- $FAPbI_3$ is stabilized, enhancing grain size, film uniformity, and phase purity, leading to a PCE of 22.91% and over 1000 hours of operational stability. Additionally, dual-side passivation using 2D-COFs, (TFPG-BT-COFs-Cu(CF_3-SO_3)$_2$), reduces defect traps and lattice stresses, increasing PCE to 23.99%. Together, these innovations significantly enhance PSC performance and durability, offering a robust pathway for their widespread photovoltaic applications.

Acknowledgement

NSTC 國家科學及技術委員會

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