

# Multi-cation thiocyanate-based pseudohalide perovskite solar cells with MASCN additive

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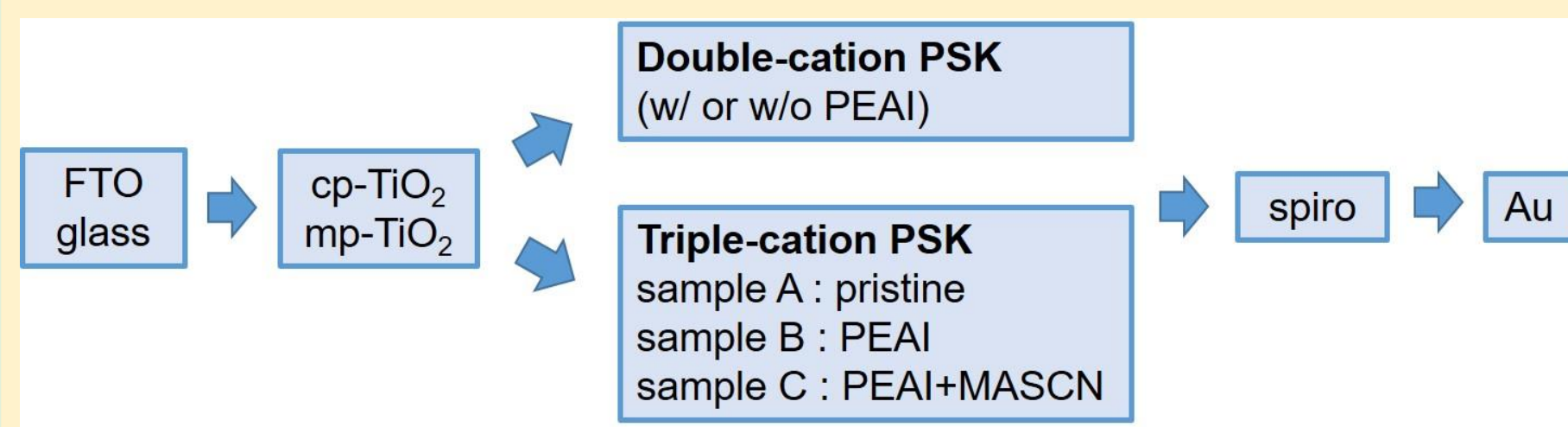
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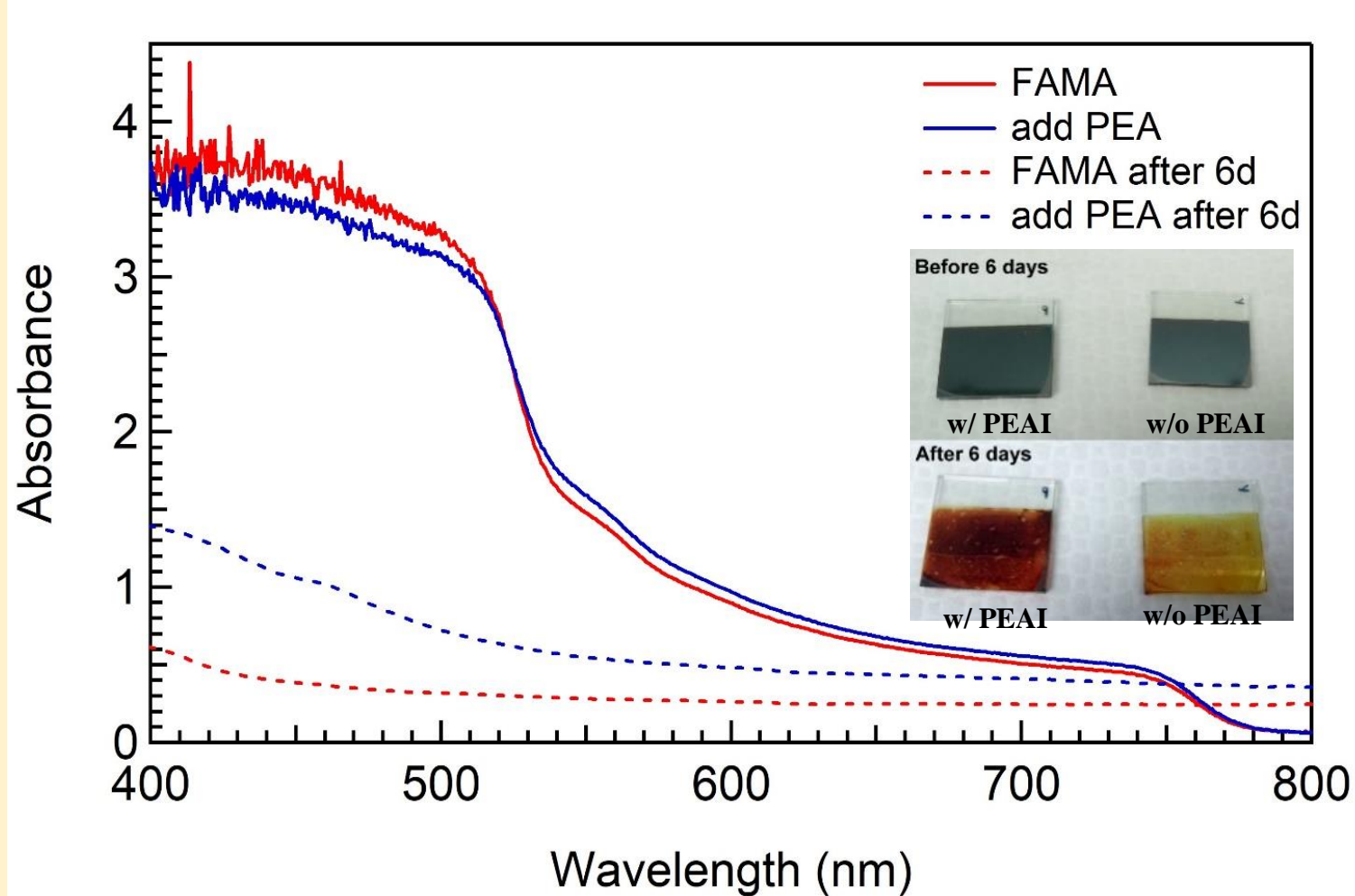
## Abstract

Currently, the organic-inorganic hybrid perovskite solar cells (PSCs) have achieved high efficiency; however, their stability remind a concern under ambient condition for real application. The purpose of this study is to enhance the perovskite stability in virtue of composition engineering by doping large-sized cation and pseudohalide SCN<sup>-</sup> into perovskite. Mixed cations and halides (or pseudohalide) in perovskite have been demonstrated to stabilize the perovskite lattice structure. For example, addition of Pb(SCN)<sub>2</sub> in thermal unstable and moisture sensitive methylammonium lead triiodide (MAPbI<sub>3</sub>) perovskite enhances the MAPbI<sub>3</sub> grain size, reduces defects state and improves the film stability. In addition to the composition engineering, introduction of two-dimensional (2D) perovskite into three-dimensional (3D) perovskite could significantly enhance the stability of perovskite active layer and the perovskite solar cells. Thus, we incorporated a large-sized aromatic cation phenethylammonium (PEA<sup>+</sup>) into double-cation perovskite (FAPbI<sub>3</sub>)<sub>0.85</sub>(MAPbBr<sub>3</sub>)<sub>0.15</sub> and triple-cation perovskite FA<sub>0.85</sub>MA<sub>0.1</sub>Cs<sub>0.05</sub>Pb(Br<sub>0.15</sub>I<sub>0.85</sub>)<sub>3</sub>. We further add MASCN into PEAI-doped triple-cation perovskite to enhance the stability of the perovskite solar cells.

## Process flow diagram

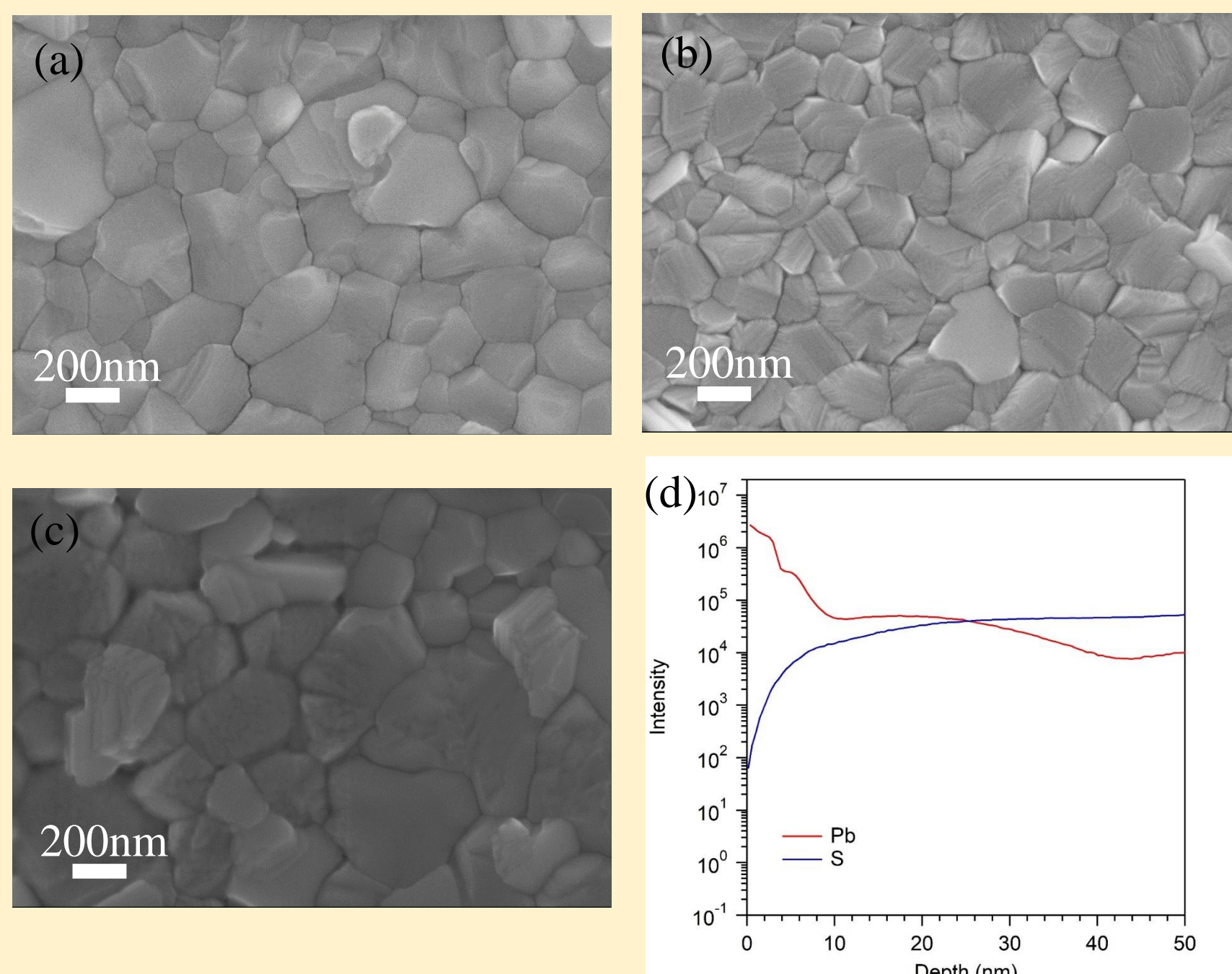


## Stability of double-cation perovskite



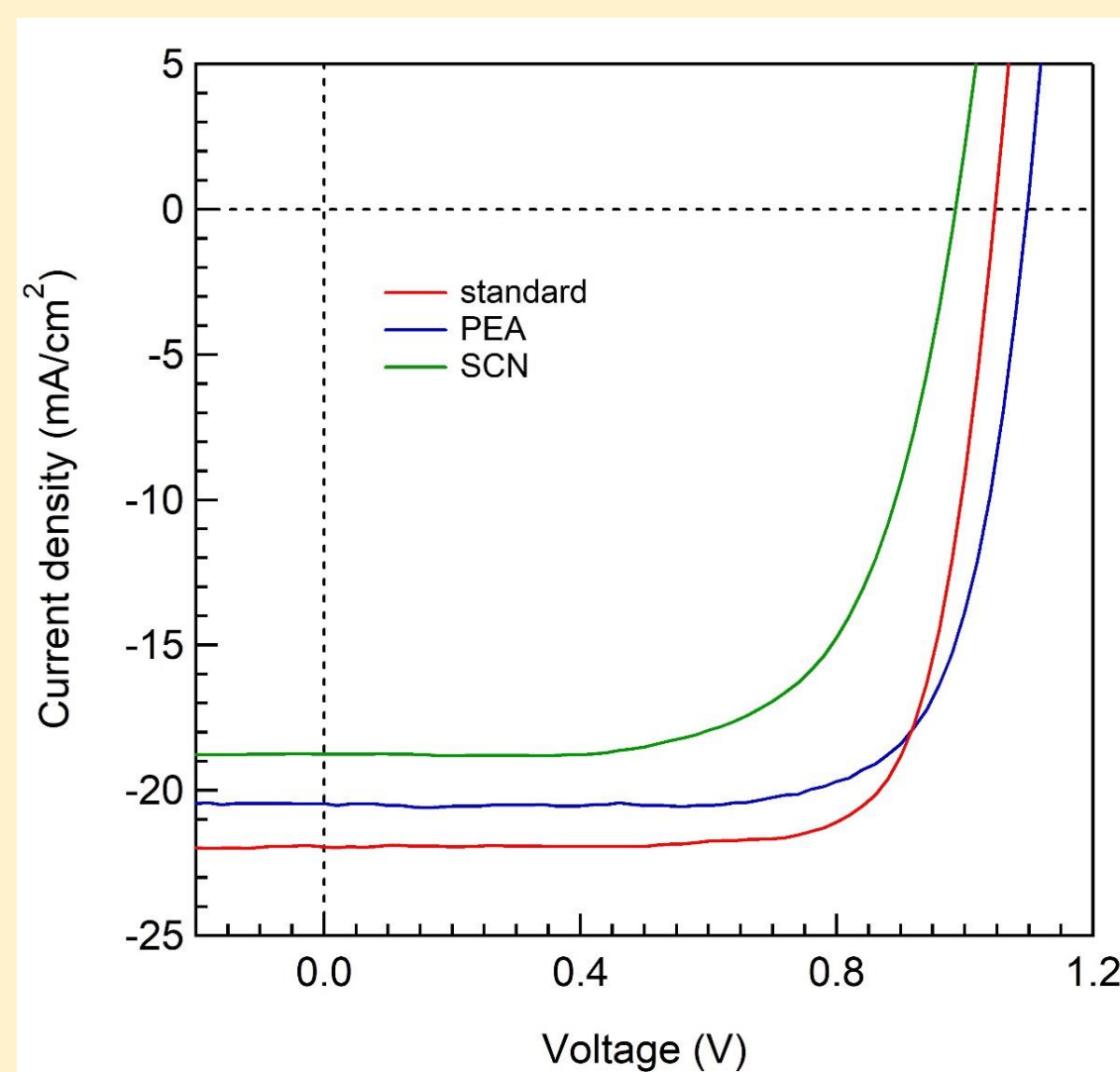
**Fig.1** UV-vis spectra of double-cation perovskite with (red) and without (blue) PEA dopant and that of perovskite film storage with a relative humidity of  $60 \pm 5\%$  after 6 days. Corresponding photographs are shown for comparison.

## Material characteristic



**Fig.2** SEM images of (a) triple-cation perovskite film, (b) PEAI-doped, and (c) PEAI+MASCN doped triple-cation perovskite film. (d) The SIMS depth profile for PEAI+MASCN doped triple-cation perovskite film.

## Photovoltaic performance

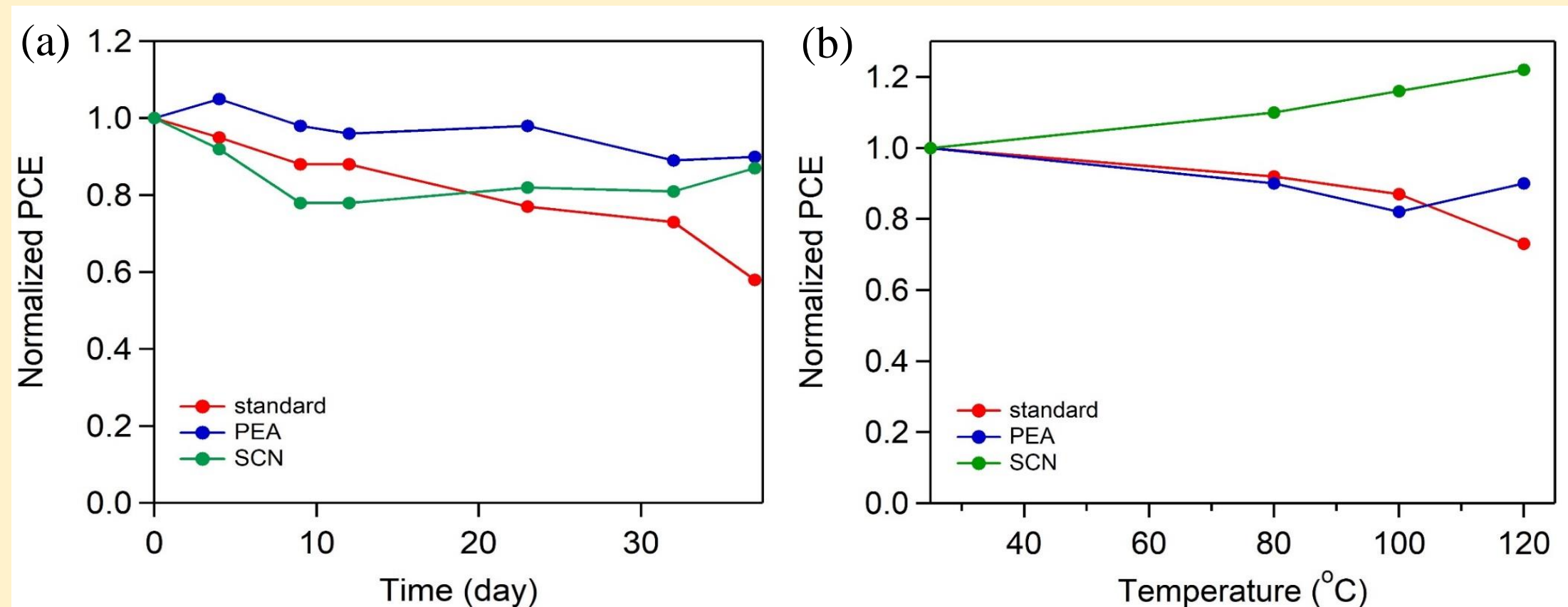


**Table.1** The photovoltaic parameters of as-fabricated perovskite solar cells.

Devices	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
standard	1.04	21.94	75.44	17.33
PEA	1.09	20.45	73.78	16.61
SCN	0.98	18.75	65.22	12.05

**Fig.3** J-V curves of perovskite solar cells based on triple-cation perovskite (standard), PEAI-doped (PEA), and PEAI+MASCN doped (SCN) triple-cation perovskite.

## Stability of triple-cation perovskite solar cells



**Fig.4** (a) Efficiency tracking for devices (without encapsulation) under a relative humidity of 40-50% for a period of 37 days. (b) Thermal stability test for devices placing on the hot plate for 30 min. Relative humidity is controlled within 15-20%.

## Conclusions

- The PEAI-doped perovskite film shows superior water resistance than the pristine triple-cation perovskite which is presumably attributed to the formation of 2D layered perovskite as passivation against moisture. Further doping of MASCN in the PEAI-doped triple-cation perovskite significantly enhances the perovskite grain size.
- The optimized pseudohalide-doped perovskite solar cell achieves a PCE of 12% with good stability when the devices are soaked under high relative humidity and heating.

## ACKNOWLEDGMENTS

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