Decoupling engineering of formamidinium–cesium perovskites for efficient photovoltaics

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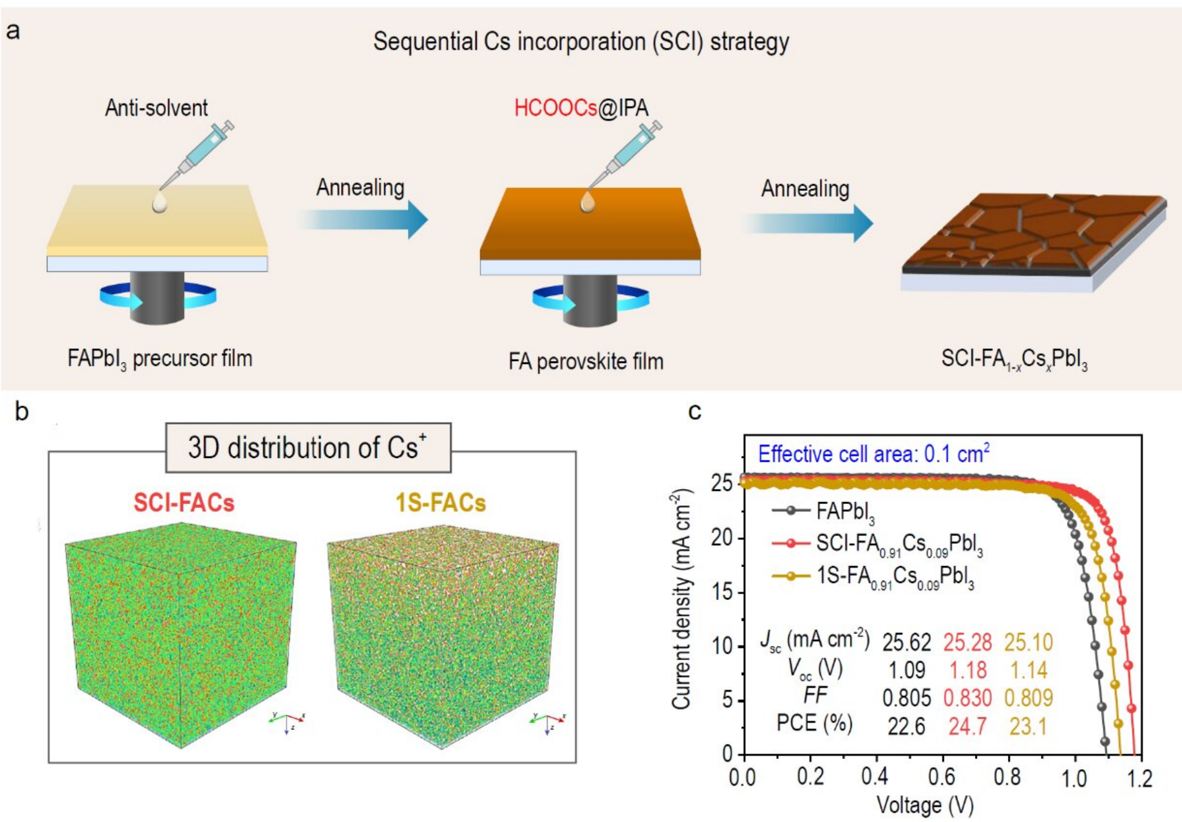

(a) Schematic diagram of the SCI-FA1-xCsxPbI$_3$ perovskite films fabricated by decoupling the crystallization process of formamidinium and cesium. (b) 3D distribution of Cs^+ in the SCI-$FA_{0.91}Cs_{0.09}PbI_3$ and 1S-$FA_{0.91}Cs_{0.09}PbI_3$ film by ToF-SIMS analysis. (c) The J-V curves of the champion solar cell devices based on $FAPbI_3$, SCI-$FA_{0.91}Cs_{0.09}PbI_3$ and 1S-$FA_{0.91}Cs_{0.09}PbI_3$ perovskites. Credit: Science China Press

Metal halide perovskites (ABX_3) have emerged as promising candidates for various optoelectronic applications due to their excellent optoelectronic properties and low-cost fabrication. At present, the light-absorbing layer of the highest-efficiency single-junction perovskite solar cells (PSCs) is almost all based on $FAPbI_3$ perovskite, achieving power conversion efficiency (PCE) that is comparable to commercial crystalline silicon cells.

However, the photoactive black-phase $FAPbI_3$ readily transforms to a photo-inactive yellow phase under humid conditions. Composition engineering such as A/X-site alloying has been developed to stabilize the black-phase $FAPbI_3$.

Notably, alloying FA^+ with Cs^+ to formpure-iodide FA-Cs perovskite ($FA_{1-x}Cs_xPbI_3$) is an ideal approach to obtain PSCs with high efficiency and stability. However, due to the complex crystallization kinetics between $FAPbI_3$ and $CsPbI_3$, $FA_{1-x}Cs_xPbI_3$ perovskite prepared by typical one-step (1S) crystallization exhibits poor compositional homogeneity and high trap density, which limits the device performance and long-term stability.

To tackle this challenge, Professor Yixin Zhao from Shanghai Jiao Tong University and co-workers recently developed a strategy of sequential cesium incorporation (SCI) to decouple the crystallization of FA-Cs triiodide perovskite with highly efficient and stable PSCs achieved.

In this work, cesium formate (HCOOCs) as a cesium source is sequentially introduced into high-quality FA precursor film. By cooperating with Professor Feng Gao from Linköping University, a new stabilization mechanism for Cs doping to stabilize $FAPbI_3$ is also revealed. This research article is published in *National Science Review*.

In their work, high-quality $FA_{1-x}Cs_xPbI_3$ (x=0.05-0.16) perovskites are obtained by the SCI method. The ratio of FA to Cs in these SCI-$FA_{1-x}Cs_xPbI_3$ perovskites can be facilely tuned by adjusting the content of the cesium source.

Compared with the conventional one-step-prepared 1S-$FA_{1-x}Cs_xPbI_3$ perovskites, SCI-$FA_{1-x}Cs_xPbI_3$ perovskites have demonstrated a much more uniform Cs distribution. "The uniform composition distribution of Cs is the key to the enhancement of device performance," Zhao says, while the PSCs based on SCI-$FA_{0.91}Cs_{0.09}PbI_3$ films achieved a PCE of 24.7% (certified 23.8%), which is the highest value among the FA-Cs triiodide PSCs reported so far.

Moreover, the collaboration with Gao's group further revealed a new stabilization mechanism for this Cs doping. The incorporation of Cs into $FAPbI_3$ significantly reduces the electron-phonon coupling strength and lattice fluctuation, thereby suppressing ionic migration and the formation of iodide-rich clusters. As a result, the stability of FA-Cs based devices has been greatly improved.

Overall, this work opens up new possibilities to strategically develop high-quality mixed-cation perovskites with good control over the crystallization kinetics, presenting a milestone towards the rational construction of highly efficient and stable perovskite-based optoelectronic applications, including but not limited to solar cells, light-emitting diodes, and lasers.

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