Supporting information for

Effect of SrI₂ substitution on the perovskite film formation and its photovoltaic property via two different deposition methods

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Fig. S1 *J-V* curves of the 10 mol% Sr-substituted PSC obtained with forward and reverse scanning methods.



Fig. S2 UV-visible absorption spectra (a) and Tauc plots (b) of 0~20 mol% Sr-substituted perovskite films. Inset is the corresponding band gaps.

As we can see from the UV-visible absorption spectra (Fig. S2a), each film has an absorption range covering visible light region, and the absorbance of Sr-substituted perovskite films is higher than that of the pristine one. It should be interpreted that the increased grain boundaries caused by Sr substitution (see Fig. 7g~j) can enhance the light scattering in the perovskite film. According to the equation: $(\alpha h\nu)^2 = A(h\nu - E_g)$, where α is the absorption coefficient and $h\nu$ is the photon energy, Tauc plot of each sample is obtained (Fig. S2b). Extrapolating the linear part of Tauc plot to coordinate axis, the optical band gap (E_g) for each sample is achieved. It is observed that the band gap changes little with increasing Sr content.



Fig. S3 (a) XPS survey spectra of the pristine and 10 mol% Sr-substituted films. Inset is the enlarged view at around 280.0 eV. (b) Partial spectra in the Pb 4f region. (c) Partial spectra in the I 3d region.

In Fig S3a, the XPS patterns of the pristine and 10 mol% Sr-substituted films are similar. The peak at binding energy of around 269.0 eV confirms the presence of Sr. The two peaks at binding energy of around 138.5 eV and 143.5 eV (Fig. S3b) are in accordance with the values of Pb interacting with I in the perovskite.¹ For the pristine sample. The shoulder peaks at around 141.5 eV and 136.5 eV which disappear in the 10 mol% Sr-substituted film are the signals of metallic Pb.^{2, 3} It indicates that Sr substitution can effectively suppress the metallic Pb which may act as non-radiative recombination centre in the perovskite film. The two peaks at binding energy of around 618.5 eV and 630.5 eV are attributed to the signals of I 3d. From both Fig. S3b and Fig. S3c, a slight right-shift of Pb 4f and I 3d signals is observed, which may arise from the different interactions between I⁻ and Sr²⁺ or Pb²⁺.⁴ Therefore, we consider that Sr replaced Pb in the perovskite crystal lattice.



Fig. S4 EDX elemental mapping of Sr, Pb and I in the 10 mol% Sr-substituted perovskite film.

References

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