

# Ion-Migration Inhibition by the Cation– $\pi$ Interaction in Perovskite Materials for Efficient and Stable Perovskite Solar Cells

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Migration of ions can lead to photoinduced phase separation, degradation, and current–voltage hysteresis in perovskite solar cells (PSCs), and has become a serious drawback for the organic–inorganic hybrid perovskite materials (OIPs). Here, the inhibition of ion migration is realized by the supramolecular cation– $\pi$  interaction between aromatic rubrene and organic cations in OIPs. The energy of the cation– $\pi$  interaction between rubrene and perovskite is found to be as strong as 1.5 eV, which is enough to immobilize the organic cations in OIPs; this will thus lead to the obvious reduction of defects in perovskite films and outstanding stability in devices. By employing the cation-immobilized OIPs to fabricate perovskite solar cells (PSCs), a champion efficiency of 20.86% and certified efficiency of 20.80% with negligible hysteresis are acquired. In addition, the long-term stability of cation-immobilized PSCs is improved definitely (98% of the initial efficiency after 720 h operation), which is assigned to the inhibition of ionic diffusions in cation-immobilized OIPs. This cation– $\pi$  interaction between cations and the supramolecular  $\pi$  system enhances the stability and the performance of PSCs efficiently and would be a potential universal approach to get the more stable perovskite devices.


3.8 to 22.1% within the past few years.<sup>[1–6]</sup> The rocketed improvement of the PSCs is attributed to the easy-crystallized organic–inorganic hybrid perovskite materials (OIPs), which have been demonstrated to be excellent photovoltaic materials, possessing large absorption coefficient, high carrier mobility, long carrier lifetime, and direct bandgap.<sup>[7–9]</sup> However, the outstanding perovskite materials also have much intrinsic flaws, such as the migration and loss of organic cations and halide ions during thermal-annealing process and under illumination conditions.<sup>[10–12]</sup> The ionic migration problem has been considered as the main reason for the degradation in perovskite films and devices, which cannot be avoided by substituting components of perovskite materials or sealing the devices.<sup>[13–16]</sup> In addition, the embarrassing hysteresis in PSCs has been proved to be associated with the ionic migration in perovskite films, which profoundly impacts the practical application of the devices.<sup>[17–20]</sup>

Organic–inorganic hybrid perovskite solar cells (PSCs) possess the advantages of low-cost and high performance, especially the impressive strides of power conversion efficiency (PCE) from

In the past few years, ionic migration has attracted wide attention in OIPs including the investigations through both experimental and theoretical methods.<sup>[21–24]</sup> It has been

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