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Synergetic effect of tetraoctylammonium chloride in suppressing photoinduced phase segregation in mixed halide perovskite solar cells

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ABSTRACT

Phase segregation, caused by halide ion migration under illumination, is a critical challenge limiting the commercialization of mixed-halide perovskites. In this study, a facile and effective strategy is introduced to mitigate photoinduced phase segregation in the $FA_{0.83}Cs_{0.17}Pb(I_{0.6}Br_{0.4})_3$ mixed halide perovskite film by employing tetraoctylammonium chloride (TOAC) as both an additive and surface passivation for the first time. The results demonstrate that TOAC effectively reduces halide ion migration, stabilizes the perovskite phase, and suppresses phase segregation, particularly in the combined additive-passivation configuration. Mixed-halide perovskite solar cells fabricated with this dual TOAC approach achieve the highest efficiency of 15.8 %, with enhanced stability under continuous illumination and reduced hysteresis. The study highlights the critical role of TOAC in suppressing phase segregation, and improving the stability and performance of mixed-halide perovskite solar cells by addressing both surface and bulk defects, facilitating the development of more stable and efficient mixed-halide perovskite solar cells.

1. Introduction

Perovskite solar cells (PSCs) have rapidly gained prominence in the field of photovoltaic material research due to their remarkable efficiency improvements. Over the past decade of development, single-junction PSCs have achieved power conversion efficiencies (PCEs) exceeding 26 % [1–3]. This rapid advancement is attributed to their cost-effective fabrication methods [4] and excellent optoelectronic properties such as high absorption coefficients [5], long carrier diffusion lengths [6], and tunable bandgaps [7]. The bandgap tunability is thanks to variable composition of mixed halide perovskites ABX_3 where A is typically $MA^+ = CH_3NH_3^+$ / $FA = CH(NH_2)_2^+$ / Cs^+, B is Pb^{2+}/Sn^{2+}, and X is $I^-/Br^-/Cl^-$. By varying their chemical composition, the bandgap can be tuned across a wide range, approximately 1.2–2.3 eV [8–11]. This bandgap tunability is particularly advantageous for tandem solar cell applications, where combining materials with different bandgaps can overcome Shockley-Queisser limit for single junction solar cell. Tandem configurations, such as perovskite-perovskite and perovskite-silicon solar cells, have shown great progress in recent years, achieving efficiencies that exceed those of traditional silicon solar cells [2,3,12,13].

Despite their promising characteristics, the instability of perovskite materials poses a major challenge to the commercialization of perovskite-based devices [14,15], particularly under prolonged exposure to oxygen [16], humidity [17,18], or light [19]. In mixed-halide perovskites, a notable phenomenon known as halide segregation has emerged as a significant factor contributing to instability [19]. Photoinduced halide segregation is a process where, under illumination above the material's bandgap or upon charge carrier injection, the halide ions (I^- and Br^- in typical mixed-halide perovskites) spatially separate, forming iodide-rich and bromide-rich domains [20]. This phase separation results in regions with lower and higher bandgap perovskites, respectively, compared to the average composition of the film. The precise mechanism of halide segregation is complex, but it is generally accepted that photoexcitation plays a crucial role. Upon illumination, electrons and holes are generated within the perovskite lattice. These charge carriers can interact with the ionic lattice, providing the energy to overcome activation barriers for halide ion migration. Halide vacancies, which are inherent defects in the perovskite structure, facilitate

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