Crystallization and Morphology Tailoring via Functionalized Ligands for Efficient and Stable Perovskite Solar Cells

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Perovskite solar cells have been regarded as one of the most promising alternatives to conventional polycrystalline silicon solar cells due to their excellent photovoltaic properties, flexibility, and relatively low cost. However, there is still a big gap in transitioning laboratory scale devices to industrial large area solar cell modules. The enlarged device area makes the decomposition initiated by pinholes and defects more significant, largely affecting the performance of the solar devices. Enormous efforts have been made to optimize the slot-die coating system. Most researchers limit their attention to regulating the crystallization process of perovskite film during the slot-die process. Thus, it is necessary to find a strategy to not only modify the crystallization but also suppress detrimental defects through defect passivation. It is hypothesized that a long-chain ligand with fluorine groups can effectively tune the crystallization route and stabilize the surface of perovskite film. During crystallization, the fluoride group on the ligand which can coordinate with lead and the amine group will interact with the inorganic part of perovskite, thus modifying the crystallization process. The fluoride on the grain boundaries can significantly stabilize the surface and inhibit the formation of cation vacancies. The results show that incorporating 2-(5'''-fluoro-3''',4'-dimethyl-[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl) ethan-1-ammonium (F4Tm) iodide can regulate the crystallization process and increase the grain sizes. As a result, the solar cell device performance and stability increases with the assistance of additive F4Tm. The results from the small-area devices show great potential of applying F4Tm ligand in slot-die printed perovskite solar cells.