ABSTRACT:

Molecular Engineering of a Tailored Additive for Morphology Control and Performance Enhancement in mixed Pb-Sn Perovskite Solar Cells

Perovskite solar cells based on mixed tin-lead compositions are attracting increasing interest because of their narrow bandgap and potential for efficient low-toxicity photovoltaic technologies. However, the development of high-performance Sn-Pb devices is still limited by film inhomogeneity, defect formation, and poor operational robustness. In this contribution, we report the design, synthesis, and application of a new cyano-functionalized benzothieno-benzothiophene derivative, BTBT-CN, as a multifunctional small-molecule additive for mixed Sn-Pb perovskite solar cells. A major focus of this work is placed on the synthetic strategy leading to BTBT-CN, developed to provide a structurally well-defined, conjugated additive combining the rigid BTBT scaffold with a polar cyano functionality. This molecular design was conceived to promote favorable interactions with the perovskite matrix while preserving good chemical stability and process compatibility. After synthesis and full molecular characterization, BTBT-CN was incorporated into mixed Sn-Pb perovskite precursor formulations and evaluated in p-i-n devices. The introduction of BTBT-CN was found to influence the formation of the perovskite layer, leading to improved film quality and a more homogeneous surface morphology. Structural and spectroscopic characterization suggest that the additive contributes to modulating the local film environment and to mitigating non-ideal interfacial features. These effects are reflected in the photovoltaic response of the corresponding devices, which showed improved performance and enhanced stability compared to reference samples prepared without the additive. This work highlights how targeted organic synthesis can provide effective molecular tools for perovskite engineering. BTBT-CN emerges as a promising example of how rationally designed small molecules can bridge synthetic chemistry and device optimization in next-generation tin-lead perovskite photovoltaics.