Efficient Role of Brominated Metalloporphyrin Additive in Improvement of Performance and Stability of Carbon-Based Planar Perovskite Solar Cells

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Abstract

Despite the great promotion of perovskite solar cells, the polycrystalline nature of the perovskite layer leads to the formation of defect trap states at surfaces and grain boundaries, hampering photovoltaic functionality. Motivated by porphyrin molecules tunable optoelectronic characteristics, we introduce zinc(II)*β*-tetra-bromo-meso-tetra-phenyl-porph yrin as an additive in the perovskite layer to improve the performance and stability of perovskite solar cells. The electronegative bromine atoms alter the distribution of electron density within the metalloporphyrin. Through Fourier transform infrared spectroscopy (FTIR) analysis, it has been observed that there is an interaction between the modified electron density of metalloporphyrin and the charge trap state, particularly the under-coordinated Pb^{2+} deep traps. The potential for passivating defect states has been confirmed through space-charge limited current (SCLC) measurements using electron-only devices and a quantitative assessment of trap density. Moreover, the V_{OC} alteration in response to light intensity suggests a reduced rate of trap-assisted recombination and effective prevention of electron trapping in the vacancy sites of the crystal structure in the modified layer. Additionally, XRD analysis demonstrated a notable increase in the intensity of peaks associated with the perovskite crystal structure within the modified perovskite. On the other hand, besides the positive impact on the quality of perovskite crystallinity, validated by the UV-Vis absorption and photoluminescence spectrum, the energy levels alignment between the perovskite, metalloporphyrin, and hole transport material leads to the development of a graded band structure to assists the efficient transport of electron-holes towards the hole transport layer, as evidenced by the photoluminescence spectra and the SCLC measurements. As a result, the efficiency of the best device is up to 18.5%, a factor of 15% increase to that of the reference cell with a value of 16.1%, which is superior in planar device structure with copper indium disulfide (CIS) as a hole transport material and carbon as back contact. Furthermore, enhanced hydrophobicity and crystalline quality improve the stability of devices, and the modified device maintained 96% of its initial efficiency after 40 days in comparison with the control device, which displayed a 38% drop in its performance.

Keywords

Planar Perovskite Solar Cells, Metalloporphyrin, Additive, Grain Boundary, Passivation, Defect State, Charge Transfer