Spontaneous decoration of ionic compound at the perovskite interfaces to achieve 23.38% efficiency with 85% fill factor in NiOX-based perovskite solar cells

Geping Qu[1], Deng Wang[2], Xiaoyuan Liu[2], Ying Qiao[2], Yinxin Li[2], Jie Zeng[2], Pengfei Xie[1], Yintai Xu[2], Peide Zhu[2], Limin Huang[2], Yanggang Wang[2], Danish Khan[2], Baomin Xu[2], and Zong-Xiang Xu[2]

[1]Harbin Institute of Technology
[2]Southern University of Science and Technology

March 10, 2023

Abstract

Inorganic hole transporting materials (HTMs), particularly NiOX, have shown significant promise in boosting the efficiency and stability of perovskite solar cells. However, a major challenge facing NiOX-based p-i-n perovskite solar cells (PSCs) is their direct contact with the absorber layer, which can lead to photovoltage and filling factor losses. Additionally, under-coordinated Ni cations can react with the perovskite and cause damage. In this work, we address these issues by using an ionic compound (QAPyBF4) as a perovskite additive to passivate the entire perovskite layer and interact with under-coordinated Ni cations. Our results show that the introduction of QAPyBF4 significantly enhances the performance and stability of NiOX-based PSCs. Specifically, the decorated cells achieved a power conversion efficiency (PCE) of 23.38% and a fill factor (FF) of 85.46%, with no need for complicated surface treatment or NiOX doping. The QAPyBF4 compound passivates the buried NiOX/perovskite interface, effectively reducing photovoltage and filling factor losses. Moreover, the [BF4]- component of the compound interacts with under-coordinated Ni cations to prevent their negative impact on the perovskite layer. Overall, our study proposes a simple and effective approach to optimize the performance and stability of NiOX-based PSCs through the use of ionic compound additives. Our findings suggest that addressing buried NiOX/perovskite interface issues and under-coordinated Ni cation considerations are critical in achieving high-performance and stable NiOX-based PSCs.

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