Modulating Defects in Wide Bandgap Tin Perovskite Solar Cells through Molecular Passivation

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Perovskite-based tandem photovoltaic (PV) devices show promise for surpassing single-junction efficiency limits.[1] However, the use of toxic lead in perovskites hampers their application in silicon or perovskite/perovskite tandem structures. Addressing lead toxicity is crucial for the commercial viability and environmental safety of these advanced solar cells. Researchers are developing lead-free alternatives, such as tin-based perovskites, to overcome this challenge.[2]

Tin perovskite could be an alternative to be compiled as subcells in tandem structure. Herein, we present the fabrication of lead-free, wide band gap Sn-based halide perovskite, an optimal candidate for top cell applications. The WB-Sn-HP perovskite solar cells (PSCs) achieved a promising power conversion efficiency (PCE) of over 11% using $ASnI_2Br$ perovskite, enhanced by molecular surface passivation with fluorobenzyl derivative. Enhancing device performance hinges on meticulously engineering both the surface and bulk properties of the WB-Sn-HP film through molecular treatment, which benefits from the stronger electrostatic potential and interactions with molecular functionalities. This surface treatment mitigates defect chemistries by adjusting the surface chemistry and interfacial energy. In this report, we will discuss the film growth properties, materials chemistry, and photo-physics correlating with device performance and device stability.[3,4]

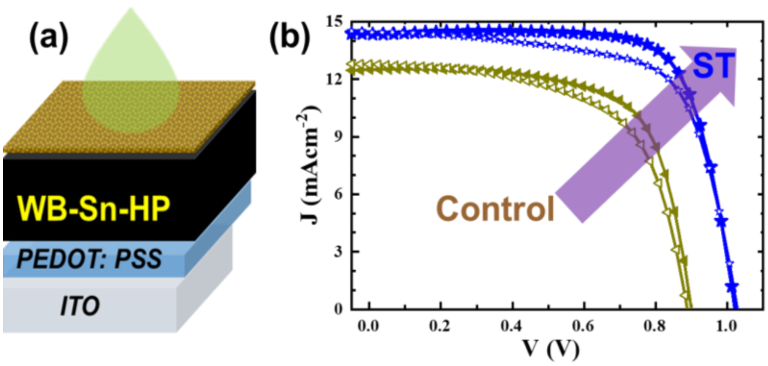

Figure 1: (a) Schematic illustration of device fabrication. (b) J-V characteristics of control and surface treated (ST) WB-Sn-PSCs.

Reference:

1 D. B. Khadka, Y. Shirai, M. Yanagida, T. Tadano and K. Miyano, *Adv Energy Mater*, 2022, **12**, 2202029.
2 D. B. Khadka, Y. Shirai, M. Yanagida, J. W. Ryan, Z. Song, B. G. Barker, T. P. Dhakal and K. Miyano, *Solar RRL*, DOI:10.1002/solr.202300535.
3 D. B. Khadka, Y. Shirai, M. Yanagida, T. Tadano and K. Miyano, *Chemistry of Materials*, 2023, **35**, 4250–4258.
4 D. B. Khadka, Y. Shirai, M. Yanagida and K. Miyano, *ACS Appl Energy Mater*, 2021, **4**, 12819–12826.