Critical role of Interface and perovskite lattice in high-efficiency and photostable solar cells

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Hybrid perovskites have recently seen an unprecedented improvement in the power conversion efficiency in photovoltaics devices, and therefore are very promising materials for developing efficient and low-cost single junction solar cells [1-3]. However, a critical issue is the limited understanding of the correlation between the degree of crystallinity and the emergent perovskite/hole (or electron) transport layer on device performance as well as photo-stability.

Los Alamos National laboratory (LANL) developed an efficient growth procedure for 3D halide perovskites in inverted perovskite cell architecture using PEDOT-PSS as a p-type hole transporting material (HTM) [4]. The initial collaboration between FOTON/ISCR and LANL led to the observation of a reversible self-healing mechanism under light soaking [5] and showed that the aging of the precursor solution plays a role in the nucleation of the perovskite crystallites [6]. In this study, we show that growth of methylammonium lead perovskites ($MAPbI_3$) on nickel oxide (NiO) HTM, results in the formation of ordered and crystalline thin-films with enhanced crystallinity, leading to characteristic XRD Bragg peak width reminiscent of exclusively observed in the tetragonal phase in single-crystals. Photo-physical and interface sensitive measurements reveal a reduced trap density at the $MAPbI_3$ perovskite/NiO interface in comparison with perovskites grown on PEDOT: PSS. Photovoltaic cells exhibit a high open circuit voltage (1.12 V), indicating a near-ideal energy band-alignment. Moreover, we observe photo-stability of photovoltaic devices up to 10-Suns, which is a direct result of the enhanced crystallinity of perovskite thin-films on NiO. These results elucidate the critical role of the quality of the perovskite/HTL interface in rendering high-performance and photo-stable optoelectronic devices [7].

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