Light-activated interlayer contraction leads to high-efficiency in 2D perovskite solar cells

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Despite their improved stability and versatility, 2D layered perovskites' solar cell efficiencies lag behind those of their 3D counterparts, which currently exceed 25%[1]. Through a proper selection of the organic spacer, 2D perovskites can be synthetized in different configurations adopting various phases such as the Ruddlesden-Popper (RP), the Alternating Cation Interlayer (ACI) or the Dion-Jacobson ones[2]. Tailoring the organic spacer type has been shown to enhance the electronic coupling along the layered perovskite stacking axis and thereby enhance carrier transport resulting in improved efficiencies[3]. In prior works related to 3D perovskites, steady light soaking of the solar cells affected their device performance[4] and resulted in improved efficiencies[5]. Here[6], we show that continuous illumination of the DJ and the ACI 2D hybrid halide perovskites results in a lattice contraction that presents more than 1% decrease in the lattice parameter in the out-of-plane direction and 0.4% decrease in the in-plane direction. X-ray photoemission spectroscopy measurements reveal that the terminal iodine atoms become electron poor (positively charged) upon light illumination. This triggers an enhancement of I--I interactions across the organic barrier leading to an out-of-plane contraction. Noteworthy, the onset of the out-of-plane contraction in the in-situ device coincides with an abrupt 3-fold step like increase in the carrier mobility. Theoretical calculations reveal that the localization of holes on the iodine atoms result in larger electronic dispersion along the stacking axis consistent with the experimental observation of enhanced charge transport. The improved charge transport leads to an increase in the efficiency of a DJ-based solar cell from 15.6% to 18.3% mainly reflected in an increase in the fill factor and the open-circuit voltage (Fig. 1a-d).

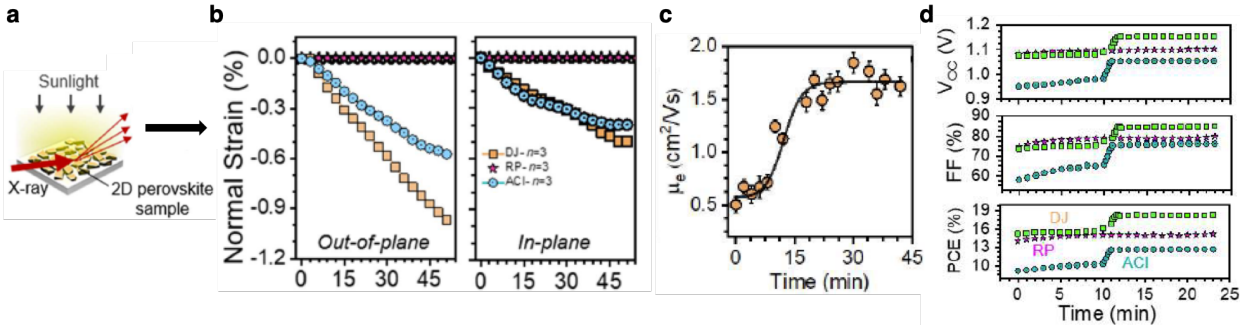

Figure 1. a) 2D sample under light illumination. b) lattice parameters variation, c) electron mobility and c) solar cell characteristics under light illumination.

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