Numerical investigation of the effect of interface conditions in HTM-free and printable WO_x based perovskite solar cells

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One of the remaining issues, impeding the commercialization of the low cost and high efficiency perovskite solar cells (PSCs) is whether the halide perovskite materials have sufficient stability. Two main instabilities are the light-induced degradation[1] and the scan-dependent performance, namely the hysteresis effect[2]. Following the observation and the atomic computation, the interfaces of perovskite/WO_x and perovskite/Au are numerically investigated by reproducing the experimental current-voltage (J-V) and capacitance-voltage (C-V) characteristics[3]. As a result, the build in potential (V_{bi}) variation, open circuit voltage (V_{OC}) loss and hysteresis effects are explained. The effect of mobile ions is additionally taken into account in the drift-diffusion model for the realistic modelling, including the ionic current, the dopant-like behavior and the polarization effect between ions and the other charges. The interaction between interface traps and mobile ions is assumed to lead the anomalous hysteresis. Furthermore, a new approach is proposed to the modelling of Kelvin Probe Force Microscopy (KPFM) of hetero-structures in dark and under illumination, aiming at estimating the surface states on the top of electron transport materials and understanding the carrier operation inside the cells.

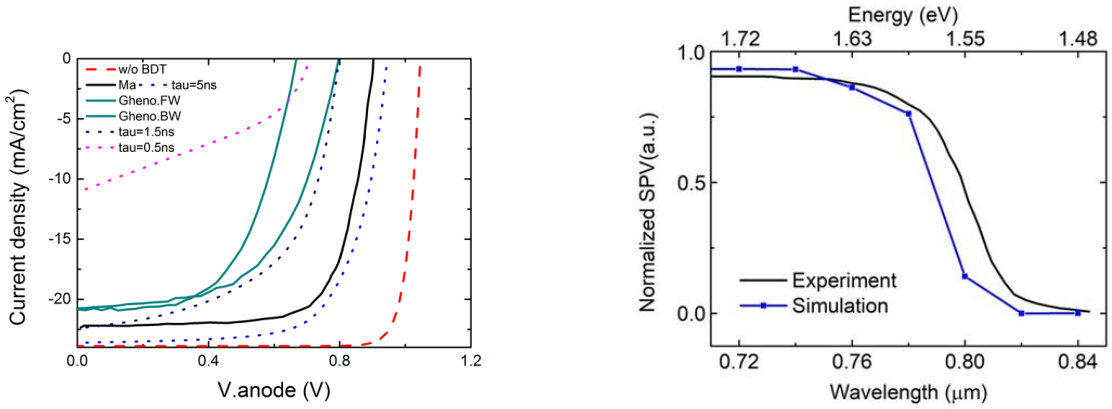

Fig. 1. Left) V_{OC} loss caused by non-radiative recombination. Right) Surface photovoltages spectroscopy of $MAPbI_3$.

1. Nie, W. *et al.* Light-activated photocurrent degradation and self-healing in perovskite solar cells. *Nat. Commun.* **7,** 11574 (2016).
2. Snaith, H. J. *et al.* Anomalous Hysteresis in Perovskite Solar Cells. *J. Phys. Chem. Lett.* **5,** 1511–1515 (2014).
3. Huang, Y. *et al.* Influence of Schottky contact on the C-V and J-V characteristics of HTM-free perovskite solar cells. *EPJ Photovolt.* **8,** 85501 (2017).