ON THE EQUILIBRIUM ELECTROSTATIC POTENTIAL AND LIGHT-INDUCED CHARGE REDISTRIBUTION IN HALIDE PEROVSKITE STRUCTURES

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Lead halide perovskites are semiconductor materials which are employed as non-intentionally doped absorbers inserted between two selective carrier transport layers (SCTL), realizing a p-i-n or n-i-p heterojunction. In our study, we have developed and investigated a lateral device, based on methylammonium lead iodide (MAPbI$_3$) in which the p-i-n heterojunction develops in the horizontal direction (see Figure 1a). To study this device, we coupled X-ray photoemission spectroscopy (XPS) data and drift diffusion simulations. Our research suggests that the effective doping level in the MAPbI$_3$ film should be very low, below 10^{12} cm^{-3}. Along the vertical direction, this doping level is not enough to screen the electric field of the buried heterojunction with the SCTL. The perovskite work function and surface potential are therefore affected by the SCTL underneath, as shown in Figure 1b for acceptor trap density values below 10^{15} cm^{-3} (yellow curve). From drift-diffusion simulations we show that intrinsic perovskite-SCTL structures develop mV range surface photovoltages (SPVs) under continuous illumination. However, perovskite-SCTL structures can develop SPVs of hundreds of mV, as confirmed by our Kelvin probe force microscopy measurements. We therefore analyzed the compatibility between low doping and low defect densities in the perovskite layer and such high SPV values using numerical modelling. It is shown that these high SPV values could originate from electronic processes due to large band offsets in the buried perovskite-SCTL heterojunctions, or at the SCTL - transparent conductive oxide (TCO) buried heterojunction. However, such electronic processes can hardly explain the long SPV persistence after switching off the illumination, which could be a sign that light-induced physicochemical processes are at work.
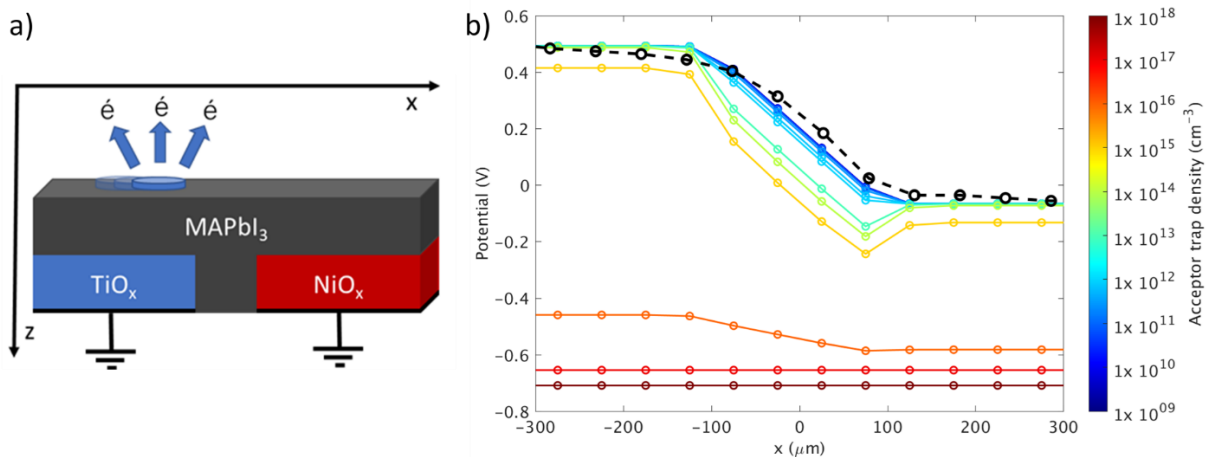
Figure 1: MAPbI$_3$ perovskite lateral heterojunction solar cell layout (a) with TiO$_x$ and NiO$_x$ at the two sides of the channel, acting as electron and hole transport layers respectively. XPS scan represented on the picture. (b) Electrostatic potential across the channel measured by XPS (dashed black line) from the TiO$_x$ to the NiO$_x$ side, compared with the surface potential obtained from drift diffusion simulations for different values of acceptor trap density in the perovskite layer. The surface potential $V(x)$ is referenced here to the intrinsic Fermi level $E_i(x)$: $V(x) = (E_F - E_i(x))/q$, and the origin of the x axis is taken in the middle of the channel.