Soutenance de thèse

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Investigation of Interfaces in Perovskite-based Optoelectronic Devices

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Abstract

Perovskite (PSK) solar cells (PSCs) have recently gained attention due to a rapid increase in best-cell power conversion efficiency (PCE), allowing them to compete with the established silicon solar cell technology. Nevertheless, the novelty of hybrid PSK materials and the employment of reactive or unstable selective carrier extraction layers (SCTLs) has hindered fast marketization. In this regard, much of the improvements in PCE and stability have come from a deeper understanding of the optoelectronic properties of the materials inside PSCs.

In this context, this PhD thesis focused on coupling advanced characterization techniques, such as Kelvin probe (KP), Kelvin probe force microscopy (KPFM), X-ray photoemission spectroscopy (XPS), and transient surface photovoltage (TrSPV), with 2D drift-diffusion based (DD) simulations, employed to interpret the outcome of the experiments and gain information on the optoelectronic properties of the materials in the solar cell stack.

Two lateral heterojunction (LHJ) devices have been produced and studied. These samples are essentially PSCs with a full-back-contact design, leaving the PSK surface available for characterization. We studied the LHJs using XPS, interpreting the results with the help of the DD model. The analysis allowed us to evaluate a maximum effective doping density in the PSK layer of about 10^{11} cm^{-3}. This value is low enough to consider the thin PSK layer employed in PSCs as intrinsic and of high electronic quality.

We also studied structures where the PSK has been deposited onto a selective electron transport layer (ETL), namely TiO_x. KP and KPFM have been employed to study the response of PSK/TiO_x structures to continuous illumination and the relaxation after switch-off. The acquired response in the [1 s, 1 hr] range shows a large positive surface photovoltage (SPV) amplitude of about 300 mV and a long SPV decay time ($\tau_{PSK/TiOx}$ = 700 s). The interpretation with our DD-based simulations led us to postulate the presence of deep donor traps in the ETL as the only possible electronic cause of the observed response.

Finally, we used TrSPV measurements in the [1 ns, 0.5 s] range to study the response of PSK/TiO_x structures to ns laser pulses. A parametric DD model, including the deep TiO_x donor defects suggested by the previous KP/KPFM study, has been built to reproduce the experiment. By fitting the experimental data, we obtained various material parameters, not only related to TiO_x, but also to the PSK layer, which showed, in particular, the existence of a large concentration of shallow electron acceptor traps.