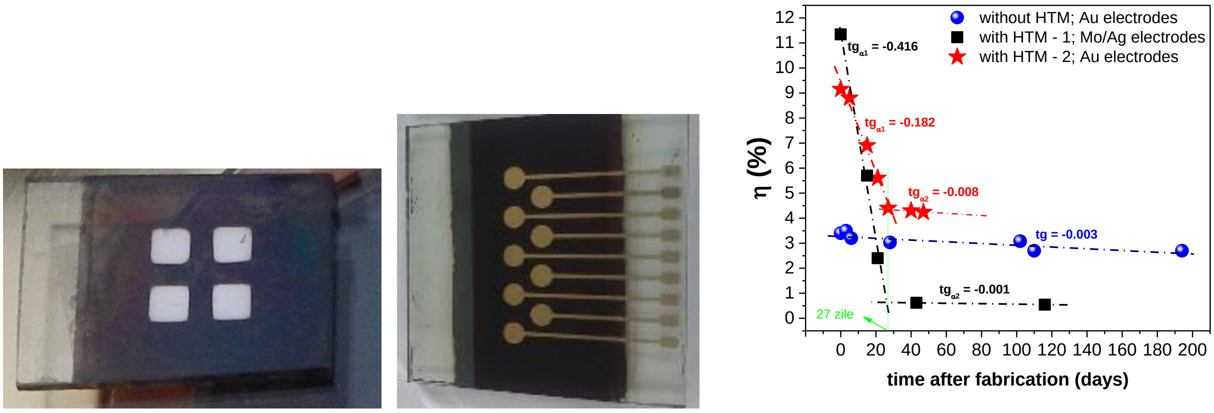
Summary of Phase 2 of the SEE 8 Project

During this phase of the project we have continued the studies on solar cells based on FTO / electron transporter material (ETM) / halide perovskite absorber / hole transporter material (HTM) heterostructure. The perovskite material is obtained by two steps synthesis. As HTM was used only spiro-OMeTAD. To obtain higher efficiency several optimizations of the deposition process were performed for each of the layers. Also, the composition of the halid-perovskite was modified in the sense that a partial substitution of iodine with chlorine has been performed in $CH_3NH_3PbI_3$, forming a mixt perovskite, $CH_3NH_3PbI_{3-x}Cl_x$, for which has been reported enhanced efficiencies and large diffusion lengths for the free carriers. Thus, to obtain $CH_3NH_3PbI_{3-x}Cl_x$ layers with suitable thickness and microstructure, several fabrication and processing parameters have been tested. Due to some problems concerning the reproducibility, the geometry of the metal electrode was redesigned being developed two new configurations. These are shown in Figures 1a and 1b. Stability studies on these structures have shown that the solar cells with spiro-OMeTAD as HTM are not stable in time, their efficiency declining sharply in the first 20 days of the production of the cells (Fig. 1c).



a) b) c)

Fig.1. Perovskitic solar cells: a) on 15x25 mm substrates with contacts having an active area of 0,07065 cm^2 that can be directly connected; b) on 50x50 mm substrates with contacts pulled on the glass substrates having each an active area of 0,12cm^2; c) The power conversion efficiency (PCE=η) on cells „without HTM" (blue circle), „with HTM - 1" (black square) and „with HTM - 2" (red star) over time.

The highest PCE values obtained during this phase of the project were of 12.5% on small cells (Fig.1a) and of 5.1% on the large solar cells (Fig.1b), both having as ETM the titanium dioxide (TiO_2). Studies regarding the replacement of the FTO electrodes with AZO layers have been continued during this phase of the project including the project approach of depositing AZO on metallic nanowebs. These layers have low resistivity ($\sim 2 \cdot 10^{-3}$ Ωcm) and are transparent in visible as can be seen in Fig.2.

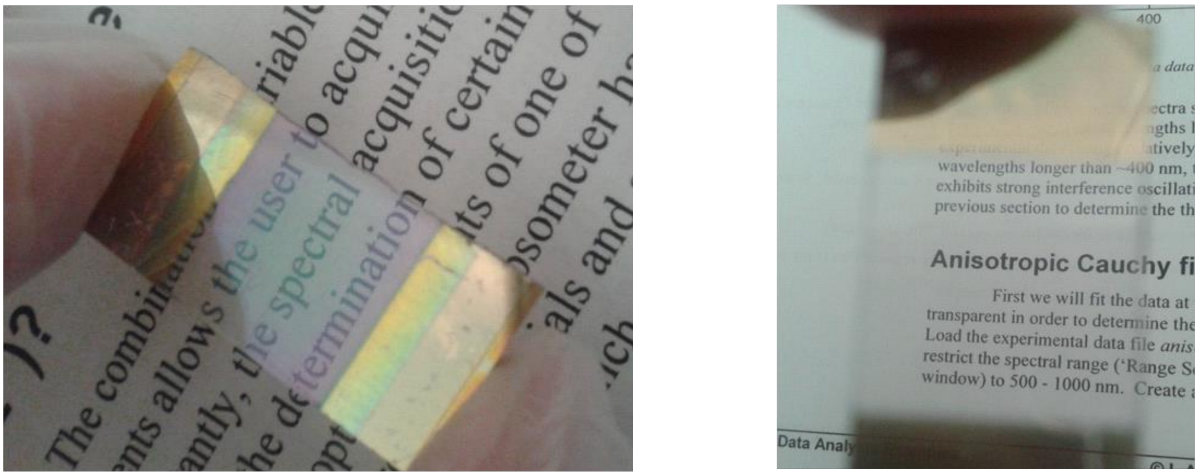


Fig. 2 (a) AZO/metallic nanoweb/glass (b) AZO/glass

Atomistic simulations were performed considering hybrid configurations halide-perovskite-$CH_3NH_3PbI_{3-x}Cl_x$ placed on the surface of rutile TiO_2. It was analyzed the effect of the iodine substitution with chlorine atoms with different concentrations x at the interface with the oxide, the energy bands and the distribution of the electric charge. These simulations have shown that the introduction of chlorine increases the leap of the conduction bands bases in such a way that the transfer of electrons from perovskite into TiO_2 is favored. Another study was dedicated to the combination of halide perovskite structure with columnar ZnO as the alternative material to TiO_2. The advantage of using ZnO is a high electron mobility and reduce the temperature of the sample preparation. ZnO interfaces were considered, as well as aluminum-doped ZnO (AZO). Calculations of transport in cells using methods such as the drift-diffusion and molecular dynamics have been performed. These theoretical modeling show that the charge transfer is faster for mesoporous interfaces than for zigzag surfaces and that it is possible to calculate the I-V characteristics of photoelectric cells using the material parameters of the cell.

There have been developed activities specific to design and manufacturing of the printing equipment's components, based on tests of layers deposition carried out in the laboratories of consortium partners. It has been defined the Concept of "PERPHECT" equipment used for printing layers of perovskite solar cells of 0.5 μm height, by 3 different printing techniques (Screen Printing, Doctor Blade, Wire Bar). Also, there have been designed and modeled the equipment's components together with its command and control system. Based on all of these, manufacturing and assembly processes of "PERPHECT" printing equipment started.