Publishable Summary

INNOVASOL project aimed at developing radically new nanostructured materials for photovoltaic (PV) excitonic solar cells (XSCs) really competitive with traditional energy sources. The target was to leapfrog current limitations of third-generation PV devices through a drastic improvement of the materials used for assembling XSCs (with particular attention to light absorbers, hole transport materials and electron transport solids). Taking into account that the state of the art DSC device was 11% efficiency, INNOVASOL XSC device target was to reach 11-15% efficiency.

As a first activity, benchmarking analysis to evaluate the effect of commercially available organic dyes, titanium dioxide, conductive SnO_2:F (FTO) coated glasses and electrolytes on the efficiency of laboratory "spot-cells" (being typically between 0.16 and 0.64 cm^2 in size) was carried out: this activity was fundamental to measure the performances of new INNOVASOL materials in a reproducible and comparable fashion. A detailed analysis of literature data and their comparison with preliminary results of INNOVASOL project was carried out especially during the first year of the project, in order to select the most promising candidates for the core materials of the new XSC devices. In particular, the screening involved four classes of XSC materials: i) quantum dot light absorbers (QD), ii) molecular relays, iii) hole transport materials, iv) mesoscopic electron transport materials. In this respect, development of innovative preparation routes allowing the optimization of new core materials needed to increase the actual performances of XSC devices.

The physico-chemical performances of these solids were studied by using a multidisciplinary experimental approach augmented by computational studies. Novel computation procedure to define the properties of solids for XSC devices were developed. In the frame of INNOVASOL project different quantum dot absorbers were synthesised. Obtained results indicated that the most promising materials to achieve the objectives of the INNOVASOL project are nanocrystals (NCs) based on the IV-VI semiconductors class, especially those of PbS and PbSe. They are also the most promising with respect to multi-exciton generation. Tailoring of the synthetic protocols for CdSe, CdSe/ZnS core/shell and CdSe/CdS/ZnS core/shell/shell nanocrystals, the materials with high reaction yields for preparation of composites with specially designed NIR absorbing squaraine (also developed in the frame of the project) dyes, was also made. As far as the development of novel dyes is concerned, the INNOVASOL project allowed the optimization of more than 30 new squaraines and relatives intermediates (with absorption bands in the 600-850 nm range), reaching reaction yields higher than 75%. The synthesis procedures were scaled up from milligrams to tens of grams. Specific experiments demonstrated that energy transfer processes may occur between selected light absorbing QDs and molecular relays through FRET mechanism, and suggested that long chains dye trap QDs and act as linkers between TCO layers and sensitizer (QD). Novel hole transporting materials were developed in the frame of the project, and different classes of solids were tested as additives for the stabilisation of liquid electrolytes and for the preparation of stable electrolyte in the gel form (more suitable for screen printing processes). A wide number of porous solids and layered materials were explored for these purposes. At the end of the project, the most suitable materials for the preparation of quasi-solid electrolytes were identified. Finally, novel TCO architectures were developed for efficient interface energy transfer and electron diffusion. The integration of novel nanostructured materials in XSC devices to assess the impact of core materials developed in the frame of INNOVASOL project was realised, as well as prototypes specifications, design and validation protocol for product development applications were carried out. The optimization of core materials was done aiming at the enhancement of PV device lifetime and at decreasing cost production of materials (*i.e.* by upscaling material preparation). Concerning the target proposed in the INNOVASOL project, the Consortium succeeded in the preparation of XSC on glass and thin glass substrates, with a power density of 13 mW/cm^2 (proposed target 10-15 mW/cm^2). Spot cells (0.1 cm^2) with 13% efficiency have been prepared by using the most promising project materials. Furthermore, XSC modules of 65 cm^2 with efficiency of 6.4% were fabricated. Degradation of overall cell efficiency less than 2% was reached.