Ultrafast spectroscopy of transparent solar cells designed for the near-IR

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New approaches to make solar cells alternative to roof-top Silicon panels include Dye-Sensitized Solar Cells (DSSCs) [1]. They use organic dyes, which under the action of light liberate electrons and inject them into the semiconductor anode, on which they are grafted (fig. 1). The electron transfer process is ultrafast, i.e. it occurs within a picosecond or less (10^{-12} s). The dyes are regenerated to their neutral form on a slower micro-second time scale through an electrolyte, and the whole solar cells is then a source for electric current.

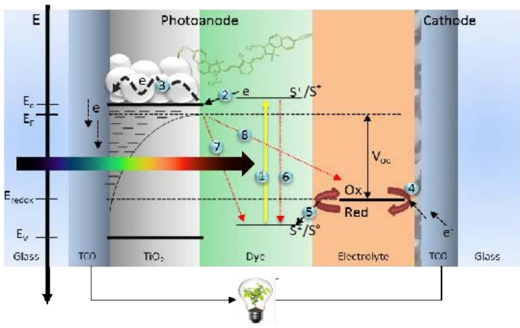

FIGURE 1: SCHEMATIC OF A DSSC, INCLUDING THE ENERGY LEVELS OF TIO_2, DYE AND ELECTROLYTE. FEMTOSECOND SPECTROSCOPY MEASURES THE PRIMARY STEP « 2 », THE INJECTION OF ELECTRONS INTO THE TIO_2 SEMICONDUCTOR. FROM PHD THESIS V. NOVELLI.

The whole power conversion efficiency (PCE) of the device is a result of many detailed molecular steps, but in many instances the first limiting step is the primary electron transfer [2] from the dye into the TiO_2. In our lab, we can measure the speed and the efficiency of the reaction via femtosecond transient absorption spectroscopy (fs-TAS), and compare for instance different molecules, thereby identifying the most efficient systems.

Our team is involved in the French national project "VISION-NIR", which develops DSSCs specifically for the near-IR portion of sun light. These devices are almost fully transparent, and could be used on large window surfaces for "building-integrated" photo-voltaics. The project partners, including the contributions from an ongoing PhD project in our team, have recently obtained a world-record near-IR solar cell, however with a moderate PCE of 3.1% [3]. New dyes, which have recently reached higher PCE values (unpublished), call for further fs-TAS and ultrafast fluorescence (FLUPS) in order to identify the most promising chemical design routes for further improvement. This project therefore will be extended within the present PhD project.

In this context, we search for a PhD candidate with a strong motivation in this applicative area of molecular spectroscopy. The student will be trained in femtosecond spectroscopy by the supervisor and in making of DSSCs by the project partners at LRCI Amiens (Dr. F. Sauvage). Organic dyes, electrolytes and the semiconductors will be provided by the project partners in Amiens and Nantes. We will address the central questions such as "is the carrier injection process the limiting step for high PCE ?" and "to which extent are molecular aggregates impairing the injection efficiency ?". A direct comparison of the injection efficiency measured by fs-TAS and of the PCE measured on the same devices will be carried out (coll. T Heiser, ICube Strasbourg). Another new aspect is to investigate the effect of the excitation wavelength on the carrier injection efficiency, which can be addressed by two-dimensional femtosecond spectroscopy, a powerful technique currently under development in our team.

[1] B. O'Regan and M. Grätzel Nature, **353**, pp. 737-740 (1991).
[2] Novelli V., Barbero N., Barolo C., Viscardi G., Sliwa M., Sauvage F., *Phys. Chem. Chem. Phys.* **19**, 27670-27681 (2017)
[3] A. Waad, V. Novelli, I. Nikolinakos, et al., JACS Au, in press (2021).