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Photoinduced Charge and Energy Transfer Dynamics in novel Diketopyrrolopyrrole Transparent Dye-Sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) are one of the most promising, emerging candidates for solar energy conversion applications. Our target is to utilize novel NIR organic dyes [1,2], advantageous for applications such as the production of quasi-fully transparent devices and in parallel to enhance the efficiency approaching the theoretical limit (ca.20 %) [3]. We have already demonstrated that when associated with an anatase TiO_2 photoanode, the selective NIR-DSSC based on cyanine derivatives can display a record 3.1 % power conversion efficiency, with up to 76 % Average Visible Transmittance [4]. We report here combined Femtosecond Transient Absorption and Fluorescence Up-Conversion studies of a novel NIR absorbing dye in solution phase as well as, incorporated in complete prototype devices of operating TiO_2 and of non-productive high bandgap semiconductor (SC) Al_2O_3, as reference. The system under investigation, the DPP derivative **TB207** exhibits in EtOH a strong absorption band peaking at 760 nm (ε=138'000 $M^{-1}cm^{-1}$) and covering 650-850 nm when attached on SC nanoparticles. After thorough optimization, the best efficiencies reach 3.9 %. Anticipating that the main efficiency limitation of these systems is aggregate formation, inducing self-quenching processes, and monomer-to-aggregate energy transfer (ET), which antagonise the electron injection to TiO_2, we used the co-adsorbent CDCA (50:1 to dye molar concentration ratio) to reduce the dye-aggregation in the DSSCs. By comparing with the reference Al_2O_3 DSSC, we identify e-injection to occur in the range 1-30 ps with injection efficiency reaching 40 %. This means that 60 % of the excited molecules are non-productive since they are quenched by energy transfer to aggregates. Finally, the next experiments are focusing on new promising dyes designed to overcome aggregation issues and tuning the absorption spectrum with high ε values and taking into consideration the human's eye phototropic response for an increased the average visible transmittance of the DSSC devices.

[1] T. Geiger, Int. J. Photoenergy, 2014, 258984, 10 pages
[2] S. Kuster, Dyes & Pigments, 2010, 87, 30
[3] Snaith, H. J. Advanced Functional Materials, 2010, 20, 13–19
[4] W. Naim, JACS Au, 2021, in press

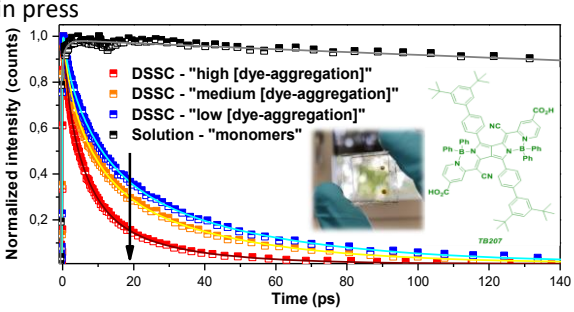

Figure 1 : Fluorescence kinetic traces of **TB207**, obtained with a Broadband-Fluorescence Up-Conversion Set-Up, detected over several wavelengths of the fluorescence spectrum for TiO_2 DSSC of Dye-CDCA concentration ("high") [1:0], ("medium") [1:50], ("low") [1:100] and for solution ("monomers").