Popular description of the project achievements

Project NCN SONATA BIS 2015/18/E/ST4/00196 (2016-2021)

"Studies of the interaction of silyl-anchor dyes with metal oxide nanoparticles"

The project aimed at the studies of organic dyes with silyl-anchor units (as alternative to the most popular carboxylic units) interacting with metal oxide nanoparticles (mainly TiO_2) for dye-sensitized solar cells (DSSC). The second part of the project was related to dye-sensitized photoelectrochemical cells for hydrogen production via water splitting using ruthenium dye with another alternative group (phosphate one) anchoring the molecule to TiO_2 (Figure B). Due to the potential better stability of such dyes on TiO_2, a number of different passivation (isolation) methods were tested, like molecular capping, atomic layer deposition or encapsulation in cucurbituril. All of them were expected to prevent from unwanted electron recombination and some of the examples are illustrated in Figure A and C. Moreover, many compositions of electrolyte (e.g. iodide-, cobalt- and copper- based in organic and water-based solutions) and TiO_2 morphologies were also checked. One of the main focuses was on the time constants and quantum yields of charge transfer processes (like electron injection from the dye to TiO_2, dye regeneration by redox couple in electrolyte or molecular catalyst, or electron recombination) measured using different time-resolved spectroscopic methods on the time scales from femtoseconds to seconds.

Certain improvements were observed upon the introduced modifications, and the optimized electrolyte compositions were often revealed. However, the dyes with alternative anchoring groups frequently suffered from more pronounced electron recombination than their standard counterparts with carboxylic groups, therefore the overall better performance of the devices were complex to be achieved. One of the most important results was also the universal observation of the direct correlations between the relative photocurrent of the cells with the efficiency of the fast charge separation processes observed within a first few nanoseconds, confirmed for many different dyes.

In summary, the project resulted in 15 papers in high quality scientific journals (11 of them with Impact Factor higher than 4), two PhD thesis, and 25 presentation during international scientific conferences (14 oral presentation and 11 posters). The findings of the project enabled better understanding of the interaction between organic dyes and inorganic nanostructures. The knowledge should help in better optimization of DSSCs and cells for water splitting in the near future, paving the way to more efficient devices.

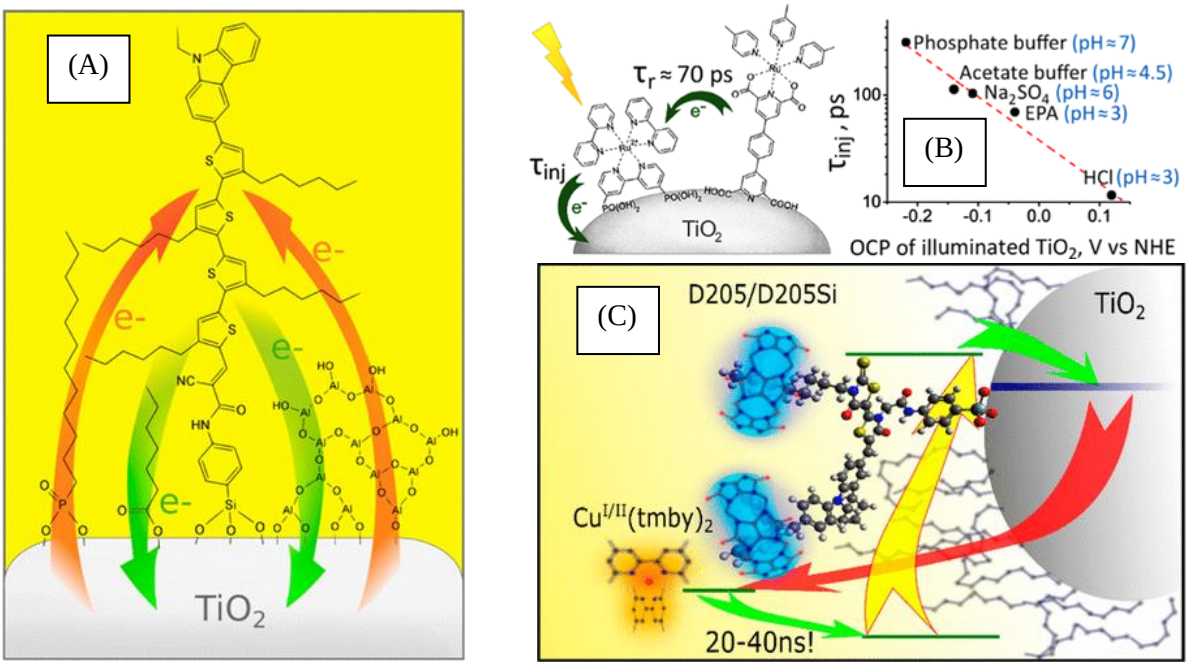

Figure: (A) Carbazole dye with silyl-anchor unit and different passivation of TiO_2 surfaces affecting electron injection (green) and electron recombination (red) processes in DSSC. (B) Ruthenium dye with a phosphate anchoring unit for water splitting, injecting electrons to TiO_2 at rates depending on the electrolyte, and regenerated ultrafast by the molecular water oxidation catalyst. (C) Indoline dye with silyl-anchor unit upon TiO_2 surface passivation or encapsulation with cucurbituril, regenerated very fast by new copper redox pair for DSSC. TOC figures from Open Access papers: (A) https://doi.org/10.1021/acsami.7b03288, (B) https://doi.org/10.1021/acs.jpcc.0c05262, (C) https://doi.org/10.1021/acs.jpcc.9b11778.