Engineering of Semiconductor Interfaces in Perovskite Photovoltaics

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Perovskite solar cell (PSC) is called 'young sister' of the dye-sensitized solar cell [1]. The key component of the negative electrode (photoanode) is a compact thin film of oxide semiconductor (TiO_2 or SnO_2). It transport electrons from the photoexcited perovskite (or sensitizing dye) to the collecting terminal (FTO) and prevents recombination of these electrons with a hole-transport medium and/or the photoabsorber. The film should be pinhole-free, allowing fast electron injection and transport, and its conduction band minimum (CBM) must be properly aligned with the CBM of perovskite [2] or LUMO of the dye. Amorphous ALD-made SnO_2 or TiO_2 films block holes for thicknesses down to several nm, but amorphous and crystalline SnO_2 films differ in their CBM positions. They are usually measured by photoelectron spectra (XPS, UPS). An electrochemical alternative is the determination of the flatband potential. Electrochemical studies of single crystal TiO_2 (anatase, rutile, brookite) together with vacuum/near-ambient pressure XPS studies and theoretical (DFT) modelling point at the effect of interface, influencing the CBM positions [3]. This knowledge provides relevant inputs not only for PSC development, but also for solar-driven water splitting [4]. Even 1-2 monolayers of water cause significant CBM shifts. TiO_2 rutile thin films and or rutile/anatase double-layers turned out to be useful for PSC, too, outperforming even the anatase layers. They can be most simply prepared by thermal oxidation of Ti at FTO [5]. The hole-collecting terminal (e.g. Au) is interfaced to hole-transporting medium. A promising hole-conductor to replace *spiro*-OMeTAD is CuSCN, particularly if it is separated from Au by a film of reduced graphene oxide (rGO). The natural p-doping of CuSCN is demonstrated by both Hall-effect and by Mott-Schottky plots [6]. Along with small improvement of the performance metrics (efficieny, fill factor, open-circuit votlage) the long term stability of CuSCN/rGO/Au is the main benefit of this PSC architecture. **Acknowledgement**: This work was supported by the Czech National Science Foundation (contract No. 18-08959S).

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