MONOLAYER AS A HOLE-SELECTIVE CONTACT FOR EFFICIENT PEROVSKITE SOLAR CELLS

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Currently, the fastest growing technology in the field of solar energy harvesting is perovskite solar cells (PSCs). With the efficiencies already surpassing 23% and coming closer to the Si-based solar cells, it is very important to ensure competitive price and stability of the perovskite-based devices. Stability of the final devices is not only dependent on the perovskite absorber material, but also on the selective layers, as well as all the interfaces.

In most of the best-performing PSCs organic materials, deposited by spin-coating, are used for the hole-selective layer formation. To ensure good charge transport they are usually used in a doped, partially oxidized state. However, the presence of the cation-radicals could lead to a reduces stability of the devices. In addition, morphological instability of the films, formed from the small-molecule hole transporting materials (HTMs) introduces additional issues for the devices under operational conditions [1].

To avoid problems associated with the doping, we are proposing an alternative approach for the formation of the hole-selective layer. In particular, by using a one-molecule-thick layer, transport is not anymore limited by the bulk of the organic semiconductor. In addition, use of such films would reduce the required amount of material to the minimum, thus contributing to the lower price of the final device. To achieve this goal, new carbazole-based HTM, functionalized with anchoring phosphonic acid group (**V1036**) was synthesized (Fig. 1). Organic phosphonic acids are known to bind to the surface of indium tin oxide (ITO), while substituted carbazole fragment is known to be used in a several efficient organic HTMs. Using **V1036** as a model compound, deposition method for the formation of the hole-selective monolayer on ITO was developed.

PSCs with **V1036** demonstrated the power conversion efficiency of 17.8% [2], which was close to that of the standard devices with PTAA (19.2%). Initial stability assessment showed good shelf life-time of the monolayer HTM-based devices, with the drop in performance of less than 3% after more than 4000 h. After the initial success, the concept was further developed by means of molecular engineering. A new generation of the monolayer HTMs (**V1193**, **V1194**) ensured high open-circuit voltage values of up to 1.19 V, which in a combination with over 80% fill factors resulted in a highest power conversion efficiency of 21.2%. This value surpassed the one obtained with PTAA, and is on par with the state-of-the-art inverted PSCs (21.5%) [3], without any interlayers and/or perovskite post-treatments.

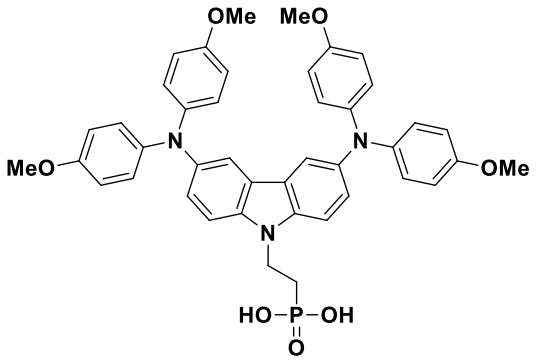

Fig. 1. Structure of the first-generation material **V1036**, used for the monolayer formation

In conclusion, we were able to show the great promise of the monolayers as a hole-selective contact in PSCs. Our work lays a foundation for the further exploration of the possible molecular structures, in particular by using molecules with additional functionalities. One more possible advantage is a conformal monolayer formation on a textured surface, which is important for the tandem solar cell application. More detailed study of the influence of the monolayer contact layer on the degradation of the device is currently undergoing.

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