A new Self-Assembled Monolayer as Electron Transport Layer for more stable Organic Solar Cells

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One of the major drawbacks of organic solar cells is the limited lifetime of devices resulting from many intrinsic and extrinsic degradation processes [1] [2]. One of them originates from the electron transport layer material used in inverted (n-i-p) architecture, especially with the commonly used zinc oxide (ZnO) layer. Indeed, ZnO requires UV light activation and presents photocatalytic activity resulting on altered interface with the organic active layer, affecting the power conversion efficiency upon ageing.

As a mean to address these degradation processes, several strategies can be implemented and among them, the use of self-assembled monolayers (SAM) is investigated. The idea consists of either functionalizing the ZnO layer with small molecules, or totally replacing ZnO with a SAM with at least comparable charge extraction capabilities. The first approach has been successfully developed with IC-SAM -a small molecule able to self-assemble at the metal oxide surface- which has proved an ability to passivate ZnO while also improving electron extraction [3]. However, for the second strategy, no use of SAMs has yet been reported to replace the electron transport layer, specifically in the case of inverted architecture. To that end, we show in this work that newly designed SAMs, tailored to optimized molecular dipole, work function, and surface energy, can play the role of an electron transport layer in inverted solar cells by fully replacing the ZnO layer.

In collaboration with Institut Charles Gerhardt Montpellier, a SAM called 2PAPhtal-SAM was designed using a phosphonic acid as an anchoring group on one end, and an electron deficient imide group on the other end, in order to form a negative dipole pointing toward ITO.

Different characterizations among which AFM, Kelvin probe, KPFM, XPS, UV visible absorption, and contact angle have been conducted to understand and optimize the SAM layer formation directly onto the ITO. A favourable shift of work function from -5.16 eV for pristine cleaned ITO to -4.35eV was obtained after SAM deposition, which contribute to a better energy level alignment between the cathode and the LUMO level of the acceptor molecule. Organic photovoltaic devices with PTQ10:Y6 as active layer were fabricated with 2PAPhtal-SAM as ETL and compared to a reference device with ZnO. Devices with SAM as electron transport layer reached up to 9,5% power conversion efficiency (PCE) with V_{oc} around 0.78V, close to the reference devices made with ZnO which presented 11% PCE with a V_{oc} of 0.81V. In comparison, devices without ETL (ITO without 2PAPhtal-SAM) show only poor performances, around 5% PCE and 0.5 V as Voc.

To go further, stabilities studies under continuous light illumination (ISOS-L-2) [4] were performed to determine whether the SAM can prevent the degradation mechanism occurring at the interface. As shown in *Fig.1* the devices with SAM as ETL present a higher stability under UV light than devices with ZnO as ETL. Indeed, the latter undergo a photocatalytic degradation which is absent for SAM-based devices. The additional degradation mechanism, accounting for 50% loss of PCE is due to intrinsic degradation happening within the bulk heterojunction.

From these first results, we can conclude that 2PAPhtal-SAM is a promising candidate for electron transport layer material as a substitute for ZnO, allowing many opportunities for optimisation.

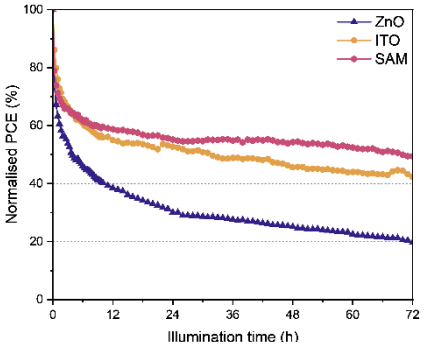

Figure 1 : Comparison of normalised PCE versus illumination time of cells with ZnO, ITO and SAM as ETL under full solar spectrum.

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[3] H. Liu *et al.*, *Adv. Energy Mater.*, vol. 9, no. 34, p. 1900887, Sep. 2019.
[4] M. O. Reese *et al.*, *Sol. Energy Mater. Sol. Cells*, vol. 95, no. 5, pp. 1253–1267, May 2011.