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

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Organic photovoltaics (OPV), a third generation of photovoltaics technology, is noteworthy by the use of organic semiconductors allowing to both tune precisely the bandgap of interest and create flexible, semi-transparent, light weight and overall low energy pay-back time modules. However, devices still present limited lifetime of devices due to many intrinsic and extrinsic degradation processes[1]. Which among the direct interaction between the electron transport layer material used in inverted (n-i-p) architecture, zinc oxide (ZnO), and the organic active material layer[2]. Indeed, ZnO requires UV light activation and presents photocatalytic activity resulting on altered interface with the organic active layer ultimately affecting the performances. As a mean to address these issues, several strategies can be implemented such as the use of self-assembled monolayers (SAM). 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[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 a newly designed SAM, 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.

A molecule called 2PAP-SAM was designed and synthesised in order to get a favourable molecular dipole. 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 suitable 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 2PAP-SAM as ETL and compared to a reference device with ZnO. Devices with SAM as electron transport layer reached up to 10% power conversion efficiency (PCE) with Voc around 0.78V, close to the reference devices made with ZnO which presented 11% PCE with a Voc of 0.81V. In comparison, devices without any ETL show only poor performances.

To go further, stabilities studies in dark and protected environment (ISOS-D-1) or under continuous light illumination (ISOS-L-2)[4] were performed and showed that devices with SAM as ETL present a higher overall stability during storage in the dark and under light spectrum than devices with ZnO. From these first results, we can conclude that 2PAP-SAM is a promising candidate for electron transport layer material as a substitute for ZnO, allowing many opportunities for optimisation.

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