

## Photodegradation in polymer solar cells

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To achieve commercially viable solution-processed solar modules, materials with a good thermal and photochemical stability are required. For conjugated molecules, the simultaneous exposure to light and in-diffusing oxygen or humidity is particularly challenging. Understanding the photodegradation processes of the molecular semiconducting materials and their effect on electrical performance is therefore a critical question.

We investigated the impact of photo-oxidation of a polymer:fullerene active layer, comprising of a blend of poly[2,3-bis-(3-octyloxyphenyl)quinoxaline-5,8-diyl-alt-thiophene-2,5-diyl] (TQ1) and [6,6]-phenyl-C<sub>71</sub>-butyric acid methyl ester (PC<sub>70</sub>BM), on the solar cell performance. TQ1 was chosen because its electronic structure has shown to be a particular stable compared to other donor polymers.<sup>(1)</sup> The TQ1:PC<sub>70</sub>BM blend was intentionally exposed to simulated sunlight (AM1.5) in air for different lengths of time, before deposition of the cathode. The blend films were investigated by UV-Vis absorption spectroscopy and Fourier-Transform Infrared (FT-IR) spectroscopy. After subsequent cathode deposition, the electrical performance of the ITO/MoO<sub>3</sub>/TQ1:PC<sub>70</sub>BM/LiF/Al solar cells was characterized by I-V measurements and photocurrent spectroscopy (EQE). We find a gradual decrease of all solar cell parameters. In the first 15 minutes of exposure the fill factor (FF) drops very fast, while the short-circuit current (J<sub>sc</sub>) and open-circuit voltage (V<sub>oc</sub>) remain relatively stable. The open circuit voltage decreases to 70% of its original value, while the current drops drastically to 30% of its original value after 10 hours of light exposure in air, a decrease that extends over the whole spectral range.

UV-Vis absorption spectra of the active layer demonstrate that, while the photo-bleaching of pristine TQ1 is rapid, the absorption spectrum of the blend is significantly more stable, indicating that PC<sub>70</sub>BM suppresses the photo-bleaching of TQ1 in the blend, as was earlier demonstrated for PC<sub>60</sub>BM.<sup>(1)</sup> By comparing EQE and absorption spectra, we can conclude that photo-bleaching of the active layer alone does not account for the losses in solar cell performance, further implying that the drastic loss in electrical performance is dominated by changes in the charge transport.

Fullerene derivatives, which are the most commonly electron acceptor materials, are known to photo-oxidize in the presence of oxygen. We have recently shown that PC<sub>60</sub>BM photooxidizes

faster than its larger analogue PC<sub>70</sub>BM.(2) FTIR spectra show that new features gradually grow in the carbonyl region when PC<sub>70</sub>BM and TQ1:PC<sub>70</sub>BM are exposed to light in air. These can be assigned to photo-oxidation of the fullerene cage. As demonstrated by NEXAFS spectroscopy, the LUMO of the fullerene acceptor is drastically affected by this photo-oxidation, which in its turn compromises the transport of electrons.

These results indicate that fullerene acceptors are the main cause of photoactive layer degradation in polymer solar cells. Therefore, new non-fullerene acceptors with a good photochemical stability are needed to achieve photostable polymer solar cells.

## References

- (1) Hansson, R., et al. *Phys.Chem.Chem.Phys.*, 2016, 18, 11132
- (2) Blazinic, V., et al. *Synthetic Metals*, 2017, accepted.