THE IMPACT OF MATERIALS PHOTO-DEGRADATION ON THE PROPERTIES OF POLYMER-BASED SOLAR CELLS

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PCBM ([6,6]-phenyl-C_{61}-butyric acid methyl ester) is a commonly used electron acceptor in polymer solar cells. We have studied the photo-stability in air of spin-coated films of PCBM using C K-edge near-edge X-ray absorption fine structure (NEXAFS), and X-ray Photoelectron Spectroscopy (XPS) of the core levels and valence band (VB). The significant changes observed in the shape of the VB and NEXAFS spectra imply that the occupied as well as the unoccupied molecular orbitals of PCBM are strongly affected by exposure in air to simulated solar light (AM1.5). In particular, we observe a photodegradation of the conjugated structure of the PCBM molecules at the surface of the thin films, which gets more severe with longer exposure times. Assigning the NEXAFS resonances to molecular moieties is possible through comparison of the experimental spectra of PCBM with DFT-calculated sum spectra of individual carbons for an isolated molecule. Comparison with results of analogous experiments on vacuum-deposited C_{60} films, we can conclude that exposure of PCBM to white light causes extensive degradation of the carbon cage of PCBM molecules.

Poly[2,3-bis-(3-octyloxyphenyl)quinoxaline-5,8-diyl-alt-thiophene-2,5-diyl] (TQ1) is a polymer that has demonstrated a high solar cell efficiency in blends with PCBM and a substantially improved stability compared to P3HT. We have studied the photo-degradation in air of the blend film and how the photo-degradation affects the solar cell performance. Changes to the electronic structure of TQ1 and PCBM caused by illumination in ambient air were investigated and compared between the pristine materials and the blend. The NEXAFS spectra show that the photo-degradation of PCBM is accelerated by blending it with TQ1. While the NEXAFS spectrum of TQ1 remains unchanged upon illumination in air, its valence band spectrum shows that the occupied molecular orbitals are weakly affected. Yet, UV-Vis absorption spectra demonstrate photo-bleaching of TQ1, which is attenuated in the presence of PCBM in blend films.

This shows that the photobleaching, as well as the changes in the electronic structure of the molecules, are affected by their molecular environment. The effect on device performance is studied through analysis of the current-voltage characteristics under illumination of solar cells with photodegraded active layers. Illumination of the active layer of TQ1:PCBM solar cells prior to cathode deposition causes severe losses in electrical performance. The decrease in photocurrent, open circuit voltage and fill factor can be assigned partly to the decreased absorption of the active layer, but also to the less efficient charge transport due to the loss of conjugated character of the fullerene acceptor. Further studies include the FT-IR spectroscopy of photodegraded PCBM films to identify the degradation products, as well as depth profiling by dynamic secondary ion mass spectrometry to determine how deep into the film the material is affected.