The challenges of fullerenes for organic solar cell stability

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To achieve commercially viable solution-processed solar modules, materials with a good thermal and photochemical stability are required. Understanding the degradation processes is therefore a critical issue to enhance the stability of organic solar cells, which are continuously exposed to external factors such as light, heat, in-diffusing oxygen and humidity. Fullerene derivatives, which are among the most used electron-acceptor materials, have a tendency to photooxidize in the presence of oxygen. Finding non-fullerene acceptors with a good photochemical stability is one of the new challenges for the field.

We studied the photodegradation in air of fullerenes and fullerene:polymer blends used as active layer materials in polymer solar cells. In particular, we have studied changes in composition and electronic structure of the fullerene derivatives $PC_{60}BM$, $PC_{70}BM$, and blends of those with conjugated polymers, using near-edge X-ray absorption fine structure (NEXAFS), X-ray Photoelectron Spectroscopy (XPS) and FT-IR spectroscopy. On the contrary, exposure of $PC_{60}BM$ films in air to light strongly affects its occupied as well as its unoccupied molecular orbitals. This change could be assigned to a transition of sp^2 to sp^3 hybridized carbons in the C_{60} cage, as a consequence of photo-oxidation. Changes in the carbonyl region of the IR spectra suggest possible photo-oxidation products. Moreover, when these changes to the electronic structure of pristine TQ1 and PCBM films are compared to those in TQ1:$PC_{60}BM$ (1:3) blend films, we found that the photo-degradation of the $PC_{60}BM$ is accelerated by the presence of TQ1, while the photobleaching of the TQ1 is slowed down by the fullerene.