Polymer Solar Cells with novel fullerene derivatives

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Fullerenes have been used as active components within polymer solar cells for more than one decade by now. Due to their relatively high electron affinity the fullerenes serve within the conjugated polymer matrix as excellent electron acceptors. The process that dissociates the exciton – formed by photoexcitation on the conjugated polymer – is known as photoinduced charge transfer.[1] Furthermore, the fullerenes provide efficient charge transport pathways for the electrons to the corresponding electrode.

To increase the solubility as compared to bare C_{60}, a fullerene derivative C_{61} bearing phenyl-[6,6] butyric acid methyl ester side-group substitutions (PCBM) was synthesized,[2] and has not been overcome in performance by any other fullerene derivative within the last decade.

To start a systematic investigation on potential improvements, a set of novel methanofullerenes was synthesized and characterized by ^{1}H and ^{13}C NMR spectroscopy. The molecular structures of new derivatives resemble closely the structure of the "running horse" PCBM. In spite of some variations in the size and shape of attached organic residues in the synthesized methanofullerenes, their reduction potentials are virtually the same and very close to those of PCBM.

Bulk heterojunction solar cells were produced by blending these novel fullerenes with poly[3-hexyl thiophene] (P3HT) and characterized by standard methods like current-voltage characteristics and spectral photocurrent. A comparison is drawn with identically prepared P3HT:PCBM solar cells.

We find a clear trend between the solubility of the lower soluble fullerene derivatives and the achieved photovoltaic performances. Further, the higher soluble fullerene derivatives show similar high photocurrents and partly higher open circuit voltages than PCBM in the optimized polymer solar cells.

[1] N.S. Sariciftci, L. Smilowitz, A.J. Heeger, and F. Wudl, *Science* **258**, 1474-1476 (1992).

[2] J.C. Hummelen, B.W. Knight, F. LePeq, F. Wudl, J. Yao, and C.L. Wilkins*, Journal of Organic Chemistry* **60**, 532-538 (1995).