Effects of structural variation in the fullerene-acceptor part on I_{sc} and V_{oc} of conjugated polymer/fullerene bulk heterojunction PV cells

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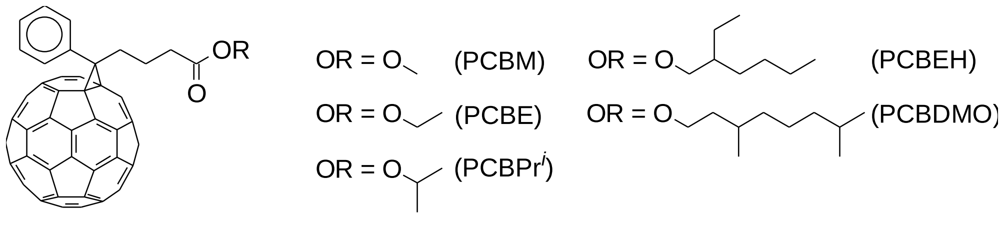
Introduction

Photovoltaic elements based on thin polymer films of solid state composites from conjugated polymer/fullerene (donor/acceptor) compounds have recently proven to be promising candidates for solar energy conversion. An important research topic is to gain insight on the effect of structural changes on the bulk heterojunction and in turn on fundamental photovoltaic parameters. For this reason we have performed two different studies in which the fullerene-acceptor part was varied at both constant, and increasing acceptor strength.

Structural variation in acceptor part at constant acceptor strength

In an initial study we compared the methanofullerene [6,6]-Phenyl C_{61}-Butyric acid Methyl ester (**1**) (PCBM) as acceptor material with structural analogs PCBX in which only the ester moiety was changed (figure 1.).

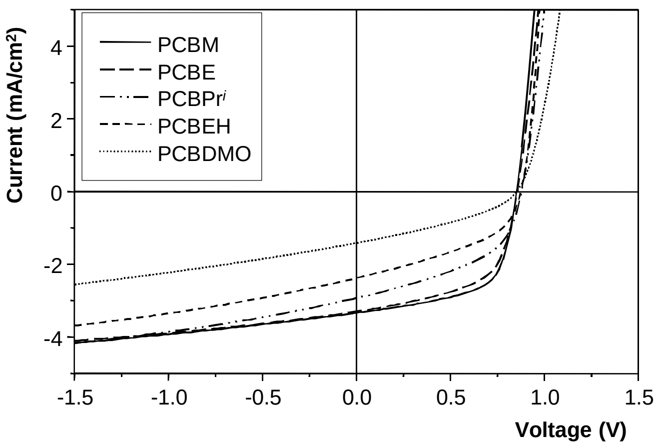
Figure 1.



PCBX

Electrochemical data (CV) verified that the acceptor strength is not altered in going from PCBM to PCBDMO and a typical first reduction potential at ~-760 mV (V vs Ag wire, GCE as working electrode) was found for all compounds. Next, we investigated these materials in bulk heterojunction photovoltaic cells. Thin film photovoltaic devices were produced by spincasting the active layer (MDMO-PPV/PCBX 1:4 (w)) from chlorobenzene solutions on top of a PEDOT/ITO/glass substrate. Subsequent evaporation of a thin layer of lithium fluoride onto the active layer was followed by evaporation of the top aluminum electrode. *I*/*V* curves were recorded under illumination with a solar simulator at 1000 W/m^2 and are depicted in figure 2.

Figure 2.

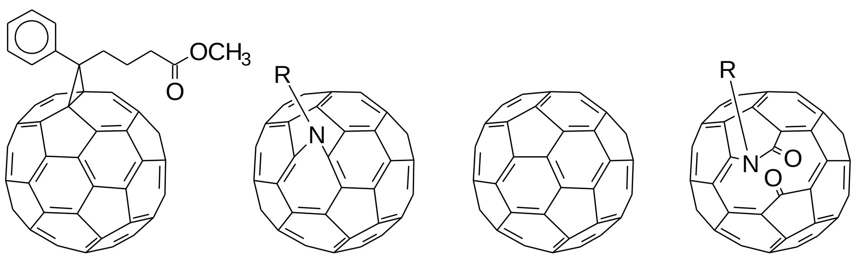


From the I/V characteristics a nearly identical open-circuit voltage (V_{OC}) was observed for all devices at ~850 mV. Surprisingly, a remarkable decrease of short-circuit current (I_{SC}) was observed in going from PCBM (I_{SC} = 3.33 mA/cm^2) to PCBDMO (I_{SC} = 1.41 mA/cm^2). This observation stresses that the performances of the present bulk heterojunction devices are extremely sensitive for small changes in the structure of the fullerene-acceptor. In this specific case, increasing the size of the alkyl chain in PCBX derivatives probably causes a reduced mobility in the fullerene domains due to a higher degree of "insulating greasy chains". In case of PCBDMO there might be an additional effect of minimal phase separation, which could lead to an increase in charge recombination.

Variation in acceptor strength

Different fullerene-acceptor molecules were selected for a study on the relation between acceptor strength and device performance (figure 3).

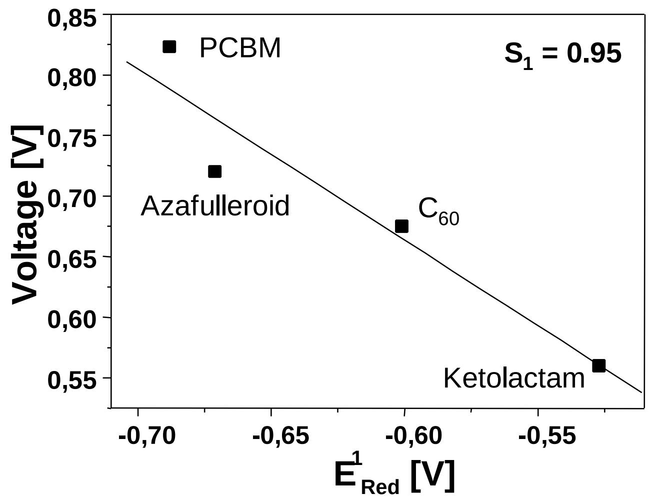
Figure 3.



(E^1=-0.69V) **(E^1=-0.67V)** **(E^1=-0.60V)** **(E^1=-0.53V)**

Among the selected acceptors, C_{60} represents an intermediate acceptor strength (-0.60V) as compared to PCBM (-0.69V) and ketolactam quasifullerene (-0.53V). The acceptors were independently tested in bulk heterojunction photovoltaic devices using MDMO-PPV as the conjugated polymer. The combined results from device measurements (figure 4) show a direct correlation between the first reduction potential of the acceptor and the observed V_{OC}.

Figure 4.



This indicates that V_{OC} is predominantly determined by the energy difference E_{LUMO}(acceptor)-E_{HOMO}(donor).

Acknowledgement

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