

Improved fullerene materials for plastic photovoltaics

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The power conversion efficiency of plastic photovoltaic cells, based on bulk-heterojunction active layers, is steadily increasing over the last 8 years. Especially the blend of MDMO-PPV and methanofullerene PCBM has been thoroughly investigated and optimized to yield devices with 2.5% efficiency and possibly somewhat higher.¹ This is probably the maximum that can be achieved with this combination of materials. In order to further develop this type of cells, it is of the essence to shift to materials that have a better overlap with the solar spectrum. Many research groups are investigating new donor materials with bandgaps that match the solar spectrum better than the ones presently used in order to raise the current output of the cells. Higher efficiencies were obtained by changing the donor polymer to regioregular P3HT, and by performing a subsequent blend morphology-improving annealing step.²

While others are pursuing efficiency enhancement by improving the polymer constituent (i.e. making low-bandgap polymers), we have investigated the possibility of obtaining a better match in the fullerene part.³ For this, we have first made an intrinsically better absorbing methanofullerene, derived from C₇₀, instead of C₆₀. C₇₀ shows a much stronger absorption in the visible region than C₆₀. In order to mimic the successful methanofullerene PCBM, we have chosen to make the corresponding [70]PCBM derivative. The synthesis of [70]PCBM was performed in an analogous procedure to that described earlier for [60]PCBM. In contrast to the situation with C₆₀, 1,3-dipolar addition to C₇₀ leads to a mixture of regioisomers. From spectroscopic data, we can conclude that a mixture of 85% one isomer and 15% (mainly) two isomers is formed (Figure 1). For the major isomer, the exact structure was elucidated. Until now, we have been unable to separate these isomers, and therefore the mixture was used in all experiments.

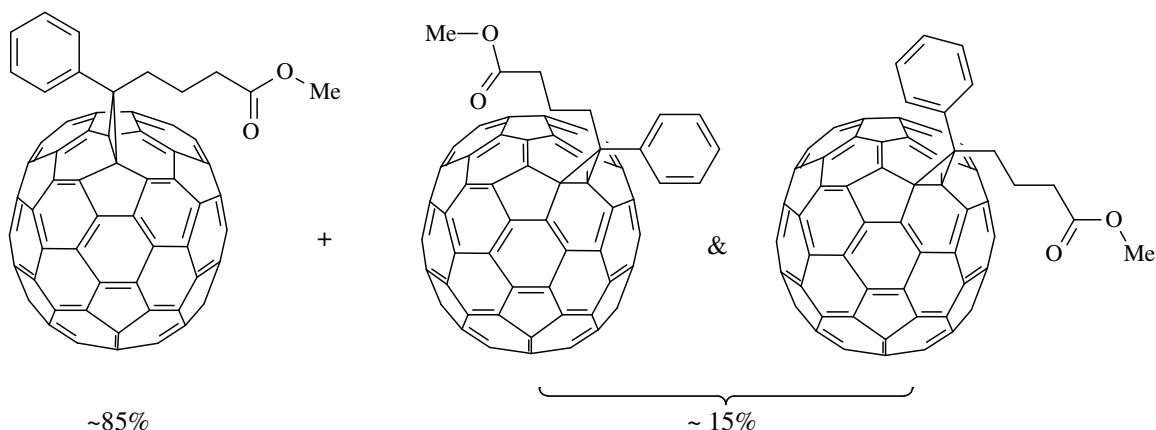


Figure 1: [70]PCBM mixture of isomers

The UV/Vis absorption of the [70]PCBM mixture is shown in Figure 2, together with that of [60]PCBM. The significantly higher absorption coefficient in the visible region is most relevant for the application in photodiodes, photodetectors, and photovoltaics. The [70]PCBM mixture is readily soluble in common solvents.

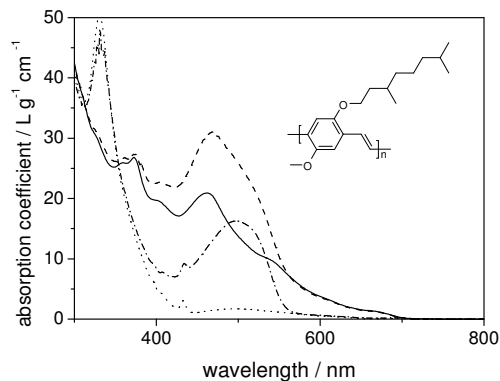


Figure 2 UV/Vis spectra of [70]PCBM (solid line) and [60]PCBM (dotted line), both in toluene. To illustrate the contribution of MDMO-PPV to the absorption, the (normalized) spectra of [70]PCBM:MDMO-PPV (4:1, w/w) (dashed line) and [60]PCBM:MDMO-PPV (4:1, w/w) (dotted dashed line), measured in toluene solution, are also represented. The inset shows the structure of MDMO-PPV.

A crucial step in the evaluation of [70]PCBM was the observation that the standard solvent for making the MDMO-PPV:PCBM blend (chlorobenzene) was *not* the optimal solvent for the corresponding [70]PCBM case. The surface morphology of the blends, made from three different solvents, is shown in Figure 3.

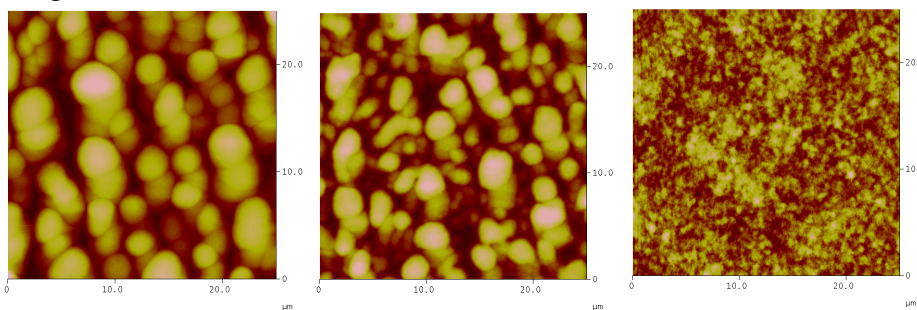


Figure 3. AFM tapping mode height images of [70]PCBM:MDMO-PPV (4:1 w/w) blends on glass, spin coated from chlorobenzene (left, z-range = 86 nm, rms roughness = 12 nm), o-xylene (center, z-range = 37 nm, rms roughness = 7 nm), and ODCB (right, z-range = 8.2 nm, rms roughness = 1.0 nm).

The final result of this work is a PV device with a power conversion efficiency of 3.0%, i.e., a 50% increase in I_{sc} , while the V_{oc} (0.77 V) and the fill factor FF (0.51) were slightly lower than those of the corresponding [60]PCBM cell. We also report on the potential and on our first results concerning the use of derivatives of still higher fullerenes (i.e. C₈₄) in this kind of cells.

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