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*Published in:*

ELECTRONIC PROPERTIES OF NOVEL MATERIALS - PROGRESS IN MOLECULAR NANOSTRUCTURES

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*Document Version*

Publisher's PDF, also known as Version of record

*Publication date:*

1998

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Knol, J., & Hummelen, J. C. (1998). Fullerenes and nanostructured plastic solar cells. In H. Kuzmany, J. Fink, M. Mehring, & S. Roth (Eds.), *ELECTRONIC PROPERTIES OF NOVEL MATERIALS - PROGRESS IN MOLECULAR NANOSTRUCTURES* (pp. 523-526). (AIP CONFERENCE PROCEEDINGS; Vol. 442). MELVILLE: University of Groningen, Stratingh Institute for Chemistry.

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# Fullerenes and nanostructured plastic solar cells

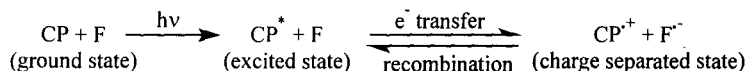
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**Abstract.** We report on the present on the present status of the plastic solar cell and on the design of fullerene derivatives and  $\pi$ -conjugated donor molecules that can function as acceptor-donor pairs and (supra-) molecular building blocks in organized, nanostructured interpenetrating networks, forming a bulk-heterojunction with increased charge carrier mobilities. Finally, we report on the first and basic steps towards the preparation of such molecular building blocks.

## INTRODUCTION

The need to develop inexpensive renewable energy sources continues to stimulate new approaches to the production of efficient, low-cost photovoltaic (PV) devices. The recent discovery of photoinduced electron transfer<sup>1</sup> in composites of conducting polymers (CP's) as donors and suitable fullerene (F) derivatives as acceptors provided a molecular approach to high-efficiency photovoltaic conversion. Because the time scale for photoinduced charge transfer is ultrafast as compared to charge recombination, the charge separated state can be described as being meta-stable (lifetime  $\sim 10^{-4}$ s) with a quantum efficiency close to unity (Scheme 1).

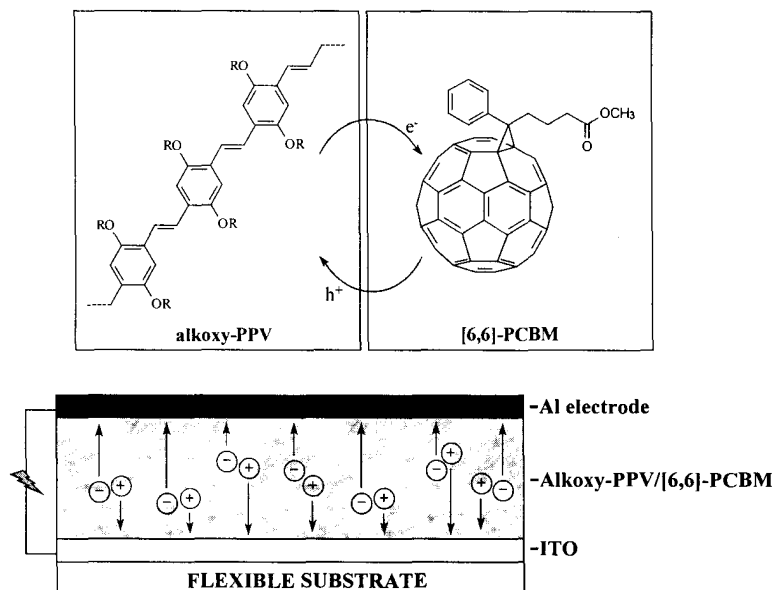


*Scheme 1. Photoinduced electron transfer in composites of conducting polymers and fullerenes.*

In contrast to single junction devices (e.g. *n*-Si/*p*-Si), PV devices consisting of blends of CP and suitable fullerene derivatives (CPC blends) behave like bulk-heterojunction materials with interpenetrating networks of donors and acceptors in which the whole blend is photoactive.

Recently, it has been shown that such "all plastic" (except for the electrodes) PV devices consisting of blends of alkoxy-poly(phenylene vinylene) (alkoxy-PPV) and

the soluble fullerene derivative<sup>2,3</sup> 1-(3-methoxycarbonyl)propyl-1-phenyl [6,6]C<sub>61</sub> (denoted as [6,6]-PCBM) can be made reproducibly with active areas of 4 cm<sup>2</sup> without loss of efficiency<sup>4</sup> (see Figure 1). Device manufacturing includes a single spincoat procedure of the alkoxy-PPV/[6,6]-PCBM blend from solution upon a flexible substrate coated with ITO followed by deposition of the upper aluminum electrode.



*Figure 1.* Schematic representation of PV device.

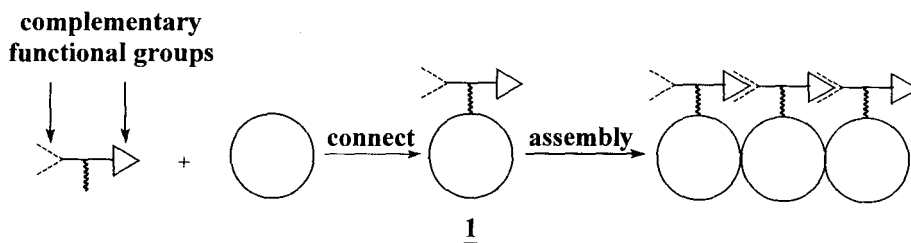
Due to the presence of electrodes with different work functions an internal electric field is generated, along which the separated charges (i.e. hole and electron) move in opposite directions.

There are two major points of interest for further development of this type of PV cell: lifetime (stability) and charge carrier mobility. Since the bulk-heterojunction is a rather disordered assembly on the nanometer scale, it is expected that the overall charge carrier mobility within the PV cell is still low. With respect to the fullerene phase, optimum charge carrier mobility (i.e. electron transport) would be achieved if the independent fullerene units could be assembled in a more or less straight alignment between the two electrodes.

### **Towards assembly of novel functionalized fullerene derivatives**

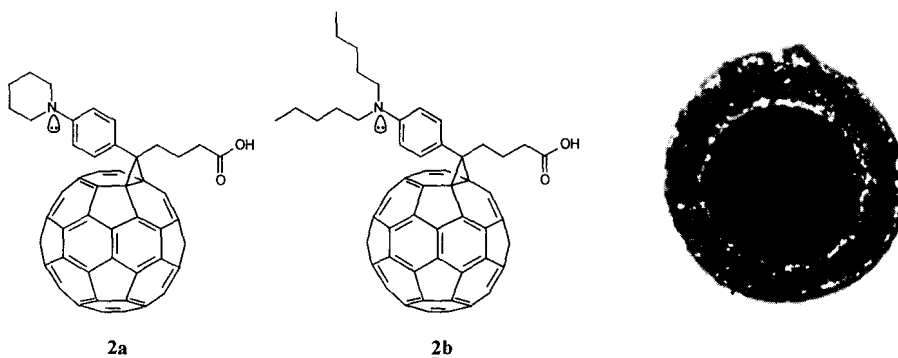
Through the rich chemistry of addition reactions to fullerenes<sup>5</sup>, a variety of functional groups can be introduced that affect macroscopic properties (e.g. solubility).

We have studied the introduction of complementary functional groups (“lock” and “key”) that can induce head-to-tail assembly of fullerene units on the molecular level. The connection of complementary functional groups to the fullerene core yields a fullerene derivative **1** that is expected to give a spontaneous head-to-tail assembly via multiple “lock”-“key” interactions (Scheme 2).



*Scheme 2.* Assembly of fullerenes through complementary functional groups.

For this reason we have prepared methanofullerenes **2a** and **2b** which are structurally related to [6,6]-PCBM (see Figure 2).<sup>6</sup> Both compounds have been characterized by several spectroscopic techniques (IR, UV/VIS, NMR). Especially **2b** shows remarkable solubility in different solvents such as carbon disulfide, toluene, tetrahydrofuran and *o*-dichlorobenzene which is an important factor during the manufacturing of PV devices. Both **2a** and **2b** meet the criterion of bearing complementary functional groups including the carboxylic- (acidic “key”) and the *N,N*-dialkylamino- (basic “lock”) functionalities. We have found that recrystallization of **2b** under carefully controlled conditions leads to the formation of polycrystalline bowl-shaped superstructures of ~0.4 mm (!) outer-diameter as identified by microscopy (see Figure 2).



*Figure 2.* Structures of methanofullerenes **2a** and **2b** and top-view of bowl-shaped polycrystalline superstructures of **2b**.

We speculate that the actual assembly involves a poly hydrogen bonded array of fullerene units. A further study of the assembly features of both **2a** and **2b** in the solid state and in solution is needed to unambiguously answer this question.

## Nanostructured interpenetrating CP/fullerene networks

There are numerous ways in which one could think of modifying the structure of a bulk-heterojunction involving interpenetrating networks of CP's and fullerenes. Three different types of interactions can be distinguished in such networks:

(a) Interactions between CP-units; (b) interactions between fullerene-units (as discussed in the previous paragraph); (c) CP/fullerene interactions within the bulk-heterojunction. Control over CP/fullerene interactions on the nano-level might be achieved by linking the independent CP- and fullerene-units together. This process could involve either linking of CP and fullerene through covalent bonds and/or linking through a spontaneous assembly process of functional groups (i.e. the principle of "lock" and "key"). Currently we are selecting and investigating suitable molecular building blocks materials for this particular purpose. Ultimately, the impact of the linking process on the architecture of the bulk-heterojunction and physical PV device parameters such as exciton transport, electron transfer efficiency, charge recombination, charge carrier mobilities etc. is to be verified.

## Acknowledgments

Prof. N.S. Sariciftci, Dr. C. Brabec and Mr. F. Padinger of the Johannes Kepler University Linz (Austria) are acknowledged for the work on PV devices. Dr. R.A.J. Janssen and Ir. B. de Waal of the Technical University Eindhoven (The Netherlands) are acknowledged for the work on CP's. This work was financially supported by The Netherlands' Agency for Energy and the Environment (Novem).

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