Molecular Bulk Heterojunctions: An Emerging Approach to Organic Solar Cells

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Résumé en anglais	The predicted exhaustion of fossil energy resources and the pressure of environmental constraints are stimulating an intensification of research on renewable energy sources, in particular, on the photovoltaic conversion of solar energy. In this context, organic solar cells are attracting increasing interest that is motivated by the possibility of fabricating large-area, lightweight, and flexible devices using simple techniques with low environmental impact. Organic solar cells are based on a heterojunction resulting from the contact of a donor (D) and an acceptor (A) material. Absorption of solar photons creates excitons, Coulombically bound electron?hole pairs, which diffuse to the D/A interface, where they are dissociated into free holes and electrons by the electric field. D/A heterojunctions can be created with two types of architectures, namely, bilayer heterojunction and bulk heterojunction (BHJ) solar cells. BHJ cells combine the advantages of easier fabrication and higher conversion efficiency due to the considerably extended D/A interface. Until now, the development of BHJ solar cells has been essentially based on the use of soluble π-conjugated polymers as donor material. Intensive interdisciplinary research carried out in the past 10 years has led to an increase in the conversion efficiency of BHJ cells from 0.10 to more than 5.0%. These investigations have progressively established regioregular poly(3-hexylthiophene) (P3HT) as the standard donor material for BHJ solar cells, owing to a useful combination of optical and charge-transport properties. However, besides the limit imposed to the maximum conversion efficiency by its intrinsic electronic properties, P3HT and more generally polymers pose several problems related to the control of their structure, molecular weight, polydispersity, and purification. In this context, recent years have seen the emergence of an alternative approach based on the replacement of polydisperse polymers by soluble, conjugated single molecules as donor materials in BHJ cells. In fact, molecular donors present specific advantages in terms of structural definition, synthesis, and purification. In this Account, we present a brief survey of recent work in this nascent field of new single-molecule donors in organic solar cells. Various series of three-dimensional donors built by the attachment of different kinds of conjugated branches on a central node, including silicon, twisted bithiophene, triphenylamine, and borondipyrromethene (BODIPY), are discussed in relation to the performances of the resulting solar cells. Furthermore, it is shown that the concept of a molecular donor with internal charge transfer leads at the same time to improved light-harvesting properties, red-shifted photoresponse, and a higher open-circuit voltage, resulting in a considerable increase of conversion efficiency, up to values now approaching 3%. These results show that soluble molecular donors can lead to BHJ cells that combine high conversion efficiency with the distinct advantages of working with single molecules, including structural definition, synthesis, purification, and reproducibility.
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