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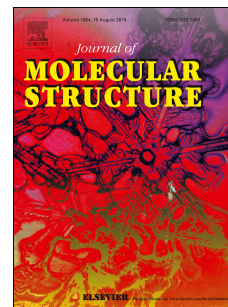
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Targeting ideal acceptor-donor materials based on hexabenzocoronene

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A series of new hybrid donor-acceptor materials based on hexabenzocoronenes (HBC) functionalized with electron donors is investigated by combining a variety of quantum mechanical and molecular dynamic methodologies for use in organic photovoltaic (OPV) devices. Segments of a low band gap alternating copolymer constructed of benzo[1,2-*b*;3,4-*b'*]dithiophene and thieno[3,4-*c*]pyrrole-4,6-dione were attached to the conjugated HBC core. The copolymer was chosen for its known high performance in OPVs, and both moieties were singled out due to their exceptional resistance to photo-oxidation, an important requirement for such applications. The macromolecular topology of these systems are expected to induce supra-molecular columns, such as those common to discotic liquid crystals, conducive to the effective percolation of electrons in OPV devices. A challenge with these systems, that of the mixing of the electronic structures of the donor and acceptor moieties that result in excitonic losses and charge recombination, was diminished by trialling a range of linking units. It was found possible to propose ideal donor-acceptor structures with enhanced charge dissociations and transfers in the π -stacking direction for use in OPV and other organic electronic devices.

Keywords: hexabenzocoronene, discotic liquid crystals, charge dissociation, organic photovoltaics.

1. Introduction

Over the last fifteen years or so, polymer-based organic photovoltaic (OPV) devices have relied on the blend of poly(3-hexylthiophene):[6,6]-phenyl C₆₁ butyric acid methyl ester (P3HT:PC₆₁BM) as a benchmark for the transformation of visible light into electricity. P3HT was one of the first polymers to show acceptable yields in this type of device[1, 2, 3], whereas fullerene C₆₀ derivatives have been used as *n*-type materials since the discovery of ultrafast electron transfer at the beginning of the 90s[4].

Fullerene based materials, such as PC₆₁BM, are still by far the most commonly used *n*-type materials in OPVs[5, 6, 7], regardless of the *p*-type material. Their success is based on their unrivalled electron acceptor properties which arise from: (i) their high electron mobility; (ii) the delocalisation of the LUMO over the whole surface of the molecule permitting 3D electron transfer and transport; (iii) their reversible electrochemical reduction profile; (iv) the formation of domains appropriate to charge percolation when blended with a *p*-type polymer.

It has been shown, however, that the latter property is not easily controlled, and with exposure to radiation or thermal stress, PC₆₁BM excessively aggregates forming large μm scale crystals that damage devices[8, 9, 10, 11]. Furthermore, this leaching of PC₆₁BM reduces contact areas and increases the average diffusion lengths of excitons to the phase boundaries.

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