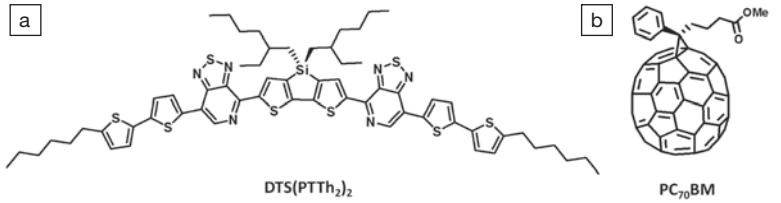
Energy Focus

Solution-processed, small-molecule solar cells show efficiencies of 6.7%

Bulk heterojunction (BHJ) solar cells composed of conjugated polymer-fullerene blends currently display power conversion efficiencies (PCEs) in the range of 6–8%. However, PCE and processing depend on batch variations in solubility, molecular weight, polydispersity, and purity. These problems are absent with solution-processed, small-molecule (SM) BHJ solar cells where the higher degree of molecular precision circumvents the statistical variability of polymers. To date, reported PCEs of SM BHJ solar cells have ranged from 2% to 5%. Recently, however, G.C. Bazan, A.J. Heeger, and co-researchers from the University of California–Santa Barbara, used rational molecular design and an unconventional processing method to fabricate SM BHJ solar cells with a PCE of 6.7%.

Bazan, Heeger, and co-researchers report their synthesis of a new small-molecule donor, DTS($PTTh_2$)$_2$ (see Figure) in the November 6, 2011 online edition of *Nature Materials* (DOI: 10.1038/NMAT3160). Based on a core acceptor/donor/acceptor framework with donor end-capping units, DTS($PTTh_2$)$_2$ displays excellent solubility in organic solvents, strong optical absorption from 600 nm to 800 nm, and a field-effect hole mobility of ~0.1 $cm^2V^{-1}s^{-1}$.

The planarity of DTS($PTTh_2$)$_2$ was designed to increase charge-carrier mobilities by promoting intramolecular π-delocalization and intermolecular π-π-stacking, and the substituted bithiophene end caps serve both to extend π-conjugation and improve film formation. In fact, the absorption peak for the cast thin film is red-shifted with respect to DTS($PTTh_2$)$_2$ in solution, which is consistent with an ordered structure and an optical bandgap of ~1.5 eV.



The molecular structure for (a) the small-molecule donor: 5,5′-*bis*{(4-(7-hexylthiophen-2-yl)thiophen-2-yl)-[1,2,5]thiadiazolo[3,4-c]pyridine}-3,3′-di-2-ethylhexylsilylene2,2′-bithiophene, abbreviated DTS($PTTh_2$)$_2$; and (b) the [6,6]-phenyl C_{70}-butyric acid methyl ester, abbreviated $PC_{70}BM$. Reproduced with permission from *Nature Mater*. (2011), DOI: 10.1038/NMAT3160. © 2011 Macmillan Publishers Ltd.

The researchers investigated photovoltaic characteristics using a conventional layered architecture, ITO/MoO_x/DTS($PTTh_2$)$_2$:$PC_{70}BM$, where ITO is indium tin oxide, MoO_x is a molybdenum oxide anode, and $PC_{70}BM$ is [6,6]-phenyl C_{70}-butyric acid methyl ester (see Figure). The DTS($PTTh_2$)$_2$:$PC_{70}BM$ ratio of 70:30 displayed the highest PCE (4.5%). Solar cells with the most successful compositions displayed a maximum incident photon conversion efficiency of 68% at about 600 nm.

The researchers also found that 1,8-diiodooctane (DIO), which is commonly added to the solutions from which polymer BHJ layers are cast, actually decreases device performance at a concentration typically used for polymer films but increases performance at lower concentrations. DIO also alters the nanomorphology of the BHJ blend. The BHJ films cast with 0.25% v/v DIO have 15–20 nm domains, while films cast without DIO have 20–30 nm domains, with lattice planes covering a significant fraction of both films. The researchers inferred crystal overlap from the presence of overlapping planes, and postulated that smaller domains result in more efficient charge-carrier generation due to larger donor–acceptor interface areas.

The researchers said that their results "provide important progress for solution-processed organic solar cells, and demonstrate that such solar cells fabricated from small donor molecules can be competitive with their polymeric counterparts."

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