

New materials for organic solar cells

Organic photovoltaics are considered a promising alternative to traditional silicon-based films, benefitting from environmental friendliness and low price. However, the energy conversion rate of conventional fullerene organic solar cells is usually only about 10% to 12%, thus far lower than that of silicon cells (up to 25%) [1]. It was found that the widely used fullerene derivative acceptor [6,6]-phenyl-C-butyric acid methyl ester (PCBM) possess a weak absorption capacity in the visible and near infrared (NIR) regions and limited bandgap variation. In addition, it easily crystallizes and aggregates. All these restrictions hinder the improvement of the power conversion efficiency. To enhance the device efficiency of organic photovoltaics, many solutions have been proposed. Among those, the development of new acceptor or donor materials proved to be highly effective. Compared with fullerene acceptors, non-fullerene acceptors possess significant advantages such as stronger light capturing ability, tunability of bandgaps and energy levels, and absence of strong aggregation. The planarity and crystallinity of different kinds of donors are shown in Figure 1a. According to previous reports, combining of well-matched novel donor materials increases the efficiency of single-junction non-fullerene organic solar cells to above 18%. However, the internal morphology of the active layer build-up from the classic materials (such as P3HT/PCBM combination) and novel donor materials are very different and a study of the internal morphology of the active layers is still challenging. Therefore, it is necessary to observe and study the internal structure of active layer to gain a deeper understanding of how morphology impacts the device performance of organic solar cells.

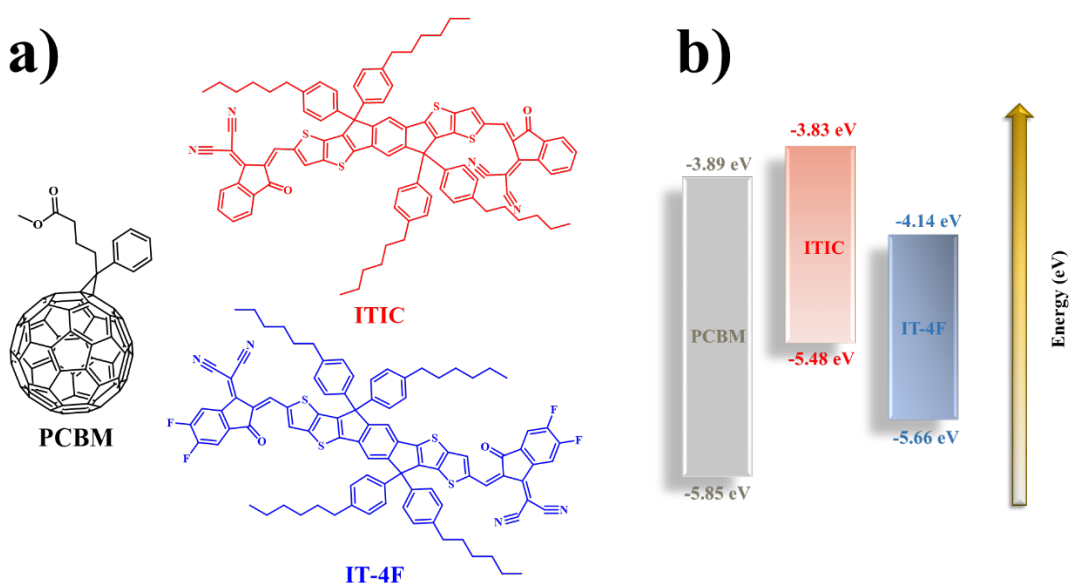


Figure 1: (a) Chemical structure of classic fullerene acceptor PCBM and novel non-fullerene small molecule acceptor ITIC, IT-4F, respectively. (b) Energy levels of the corresponding acceptors.

Based on the above considerations, we use solvent additives 1,8-diiodooctane (DIO) or third components like the conjugated polymer PBDTTPD-COOH to optimize the morphology and crystallites of the organic solar cell active layer [3,4]. The influence of the

additives or third components on the active layers was probed with the advanced scattering methods such as grazing incidence small/wide angle X-ray scattering (GISAXS/GIWAXS). As shown in Figure 2, we fabricated PBDB-T-SF:IT-4F active layers through the slot die printing technique and compared the morphology change before and after DIO addition. It can be clearly seen that the intensity of the peak became boarder along the q_y direction after 0.25 vol% DIO addition. In order to analyze the 2D GISAXS data, horizontal line cuts (red dashed line) are performed at the critical angle (Yoneda region) of PBDB-T-SF. The GISAXS data of printed active layers without or with DIO addition are modeled with three substructures of cylindrical shape, which is a well-established approach to describe the polymer thin film morphology over a large range of length scales. After data modeling, we find that the polymer domains sizes get smaller in the sample doping with DIO, which is favorable for the solar cell performance as the charge transfer from the polymer to the small acceptor molecule is facilitated by gaining interface area. Moreover, a conjugated polymer PBDTTPD-COOH is doped in the bulk heterojunction film to compensate the light absorption of the active layer and to tailor the morphology compatibility of donor and acceptor materials. The results show that adding PBDTTPD-COOH improves the polymer crystallinity and the ratio of the face-on oriented crystallites, which leads to high J_{sc} value in the device performance.

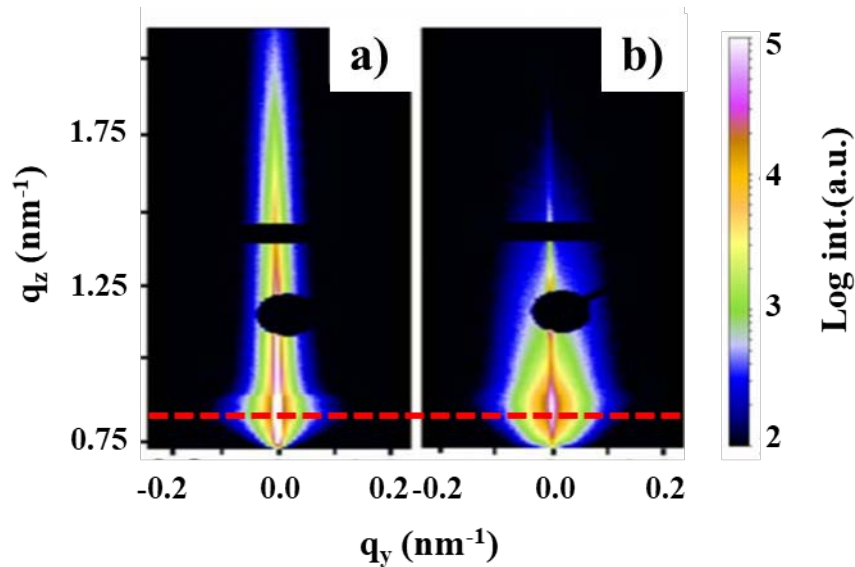


Figure 2: 2D GISAXS data of printed PBDB-T-SF:IT-4F films (a) without or (b) with 0.25 vol% DIO, respectively.

Featured publications:

(1) Song, L.; Wang, W.; Barabino, E.; Yang, D.; Körstgens, V.; Zhang, P.; Roth, S. V.; Müller-Buschbaum, P.: Composition-Morphology Correlation in PTB7-Th/PC71BM Blend Films for Organic Solar Cells. *ACS Applied Materials & Interfaces* **2019**, *11*, 3125–3135.

(2) Yang, D.; Löhrer, F. C.; Körstgens, V.; Schreiber, A.; Bernstorff, S.; Buriak, J. M.; Müller-Buschbaum, P. In-Operando Study of the Effects of Solvent Additives on the Stability of Organic Solar Cells Based on PTB7-Th:PC 71 BM. *ACS Energy Lett.* **2019**, *4*, 464–470.

(3) Wienhold, K. S.; Körstgens, V.; Grott, S.; Jiang, X.; Schwartzkopf, M.; Roth, S. V.; Müller-Buschbaum, P. Effect of Solvent Additives on the Morphology and Device Performance of Printed Nonfullerene Acceptor Based Organic Solar Cells. *ACS Applied Materials & Interfaces* **2019**, *11*, 42313–42321.