Engineering fibrillar morphology for highly efficient organic solar cells

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The power conversion efficiency (PCE) for single-junction organic solar cells (OSCs), wherein the photoactive layer is a typical bulk-heterojunction containing donor and acceptor materials, has surpassed 19%^[1-4]. The advance is ascribed to the development of Y-series non-fullerene acceptors (NFAs)^[5, 6] and polymer donors^[7–13], and the refined control of the blend film morphology. The design of donor or acceptor structures is to achieve optimal energy level alignment or to broaden the absorption range, thereby improving charge generation and maximizing photon capture. The organic semiconductors exhibit low dielectric constants and strong electron localization, leading to the generation of Frenkel excitons. Additionally, the organic semiconducting materials (OSMs) display a relatively low charge carrier mobility associated with the formation of polarons and charge carrier trap centers, which harm the transport and extraction of charge carriers. The photovoltaic performance of OSCs depends on the electronic structure of the active materials, molecular stacking, phase separation, and miscibility regulation. Therefore, how to control the nanoscale phase separation to realize optimal morphologies in photoactive layers is quite critical for OSCs.

Benefiting from previously developed star polymer donors and Y-series NFAs, including D18, PM6 and L8-BO (Fig. 1), the optimal bicontinuous network morphology has been achieved by manipulating domains and crystallinity of the blend films. Such morphological structures are advantageous for minimizing energy losses and enhancing charge carrier generation, thus enhancing the power output of OSCs. Liu *et al.* constructed a bicontinuous network with nanofibril aggregates in PM6:Y6 and D18:Y6 films by using solvent vapor annealing, achieving PCEs of 16.53% and 17.98% in single-junction OSCs, respectively^[14]. This achievement can be attributed to the formation of bundled nanofibril structures in the blend films after solvent annealing, which can facilitate charge transport and reduce charge recombination.

Liu *et al.* devised ternary OSCs based on PM6:D18:L8-BO, giving a PCE of 19.6%. The incorporation of polymer crystallization and NFA fibril assembly yielded a dual-fibril network^[15]. Wang *et al.* further used a solid additive to make fine fibril-like morphology, leading to a PCE of 19% for D18:L8-BO

binary system^[16]. Similarly, Hou *et al.* introduced a second polymer donor or highly volatile additives to regulate the aggregation behavior in the blend films with PBQx-TCl or PBQx-TF, yielding a PCE over 19%^[17, 18].

All-polymer solar cells (all-PSCs) with high performance also face the difficulty of constructing bicontinuous fibril-like network in the active layer. Hou *et al.* introduced PM6 with high molecular weight into the blend of PBQx-TF:PY-IT, realizing a precise adjustment of the bicontinuous network. This adjustment resulted in a short π – π stacking distance, and all-PSCs based on PBQx-TF:PM6:PY-IT offered a PCE of 18.2%^[19]. Liu *et al.* employed a combined strategy with solid additive, thermal annealing and solvent annealing to control polymer crystallization and film surface structure. This approach yielded a highly crystalline and bicontinuous network, greatly enhancing the exciton dissociation and charge carrier transport. All-PSCs based on PM6:PY-IT achieved a PCE over $19\%^{[20]}$.

The above studies emphasize the significance of morphology optimization in OSCs. With appropriate donor and acceptor materials, trying to attain an optimal fibril-like morphology is one of the foremost strategies for improving OSC performance.

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Fig. 1. (Color online) Chemical structures for the star donors and acceptors.

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