Highly Efficent and Stable Non-Fullerene Organic Solar Cells

Improved efficiency and thermal stability of organic solar cells enabled by an additive material using supramolecular fluorinated interactions

In recent years, organic-based non-fullerene acceptors (NFA) with a multifused-ring central core end-capped with two acceptors are revolutionary n-type materials for organic solar cells (OSCs) because of their enhanced light-harvesting ability, better matched energy levels, and better molecular packing properties. In 2019, a new nitrogen-bridged NFA, known as Y6, was developed. When it was paired with a p-type polymer donor PM6, the device achieved an unprecedented power conversion efficiency (PCE) of 15.7% (**Fig. 1**).[1] Since then, tremendous efforts have been devoted to methods of molecular modification on the basis of the Y6 structure, including aliphatic side-chain, conjugated main-chain, and end-group engineering. To date, a series of Y6-based NFA molecules have increased the PCE to over 18%. Approaching the ultimate goal of a PCE over 20% is foreseeable in the near future. Despite the great success of Y6 in molecular architectures, maintaining the thermal stability of the Y6-based device performance remains a challenge.

In 2017, Yen-Ju Cheng (National Yang Ming Chiao Tung University) developed a nonvolatile additive material bis(perfluorophenyl)pimelate, denoted as BF7, with two perfluorophenyl (C_6F_5) groups linked to a linear aliphatic chain through an ester linkage (**Fig. 1**).[2] They found that the C_6F_5 moieties of BF7 retained in the film after

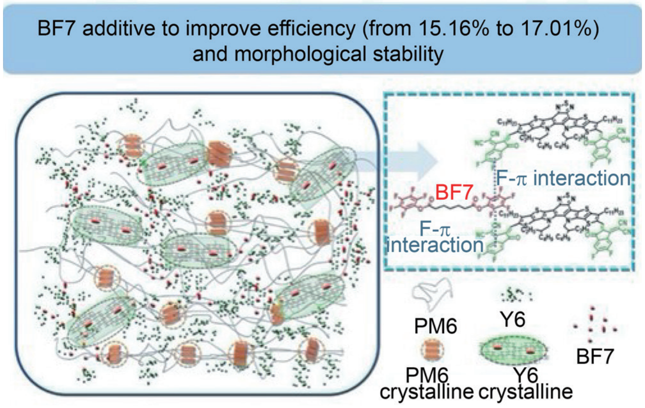

Fig. 1: Schematic of PM6:Y6 morphology in the presence of BF7 to induce F-π interaction with Y6. [Reproduced from Ref. 3]

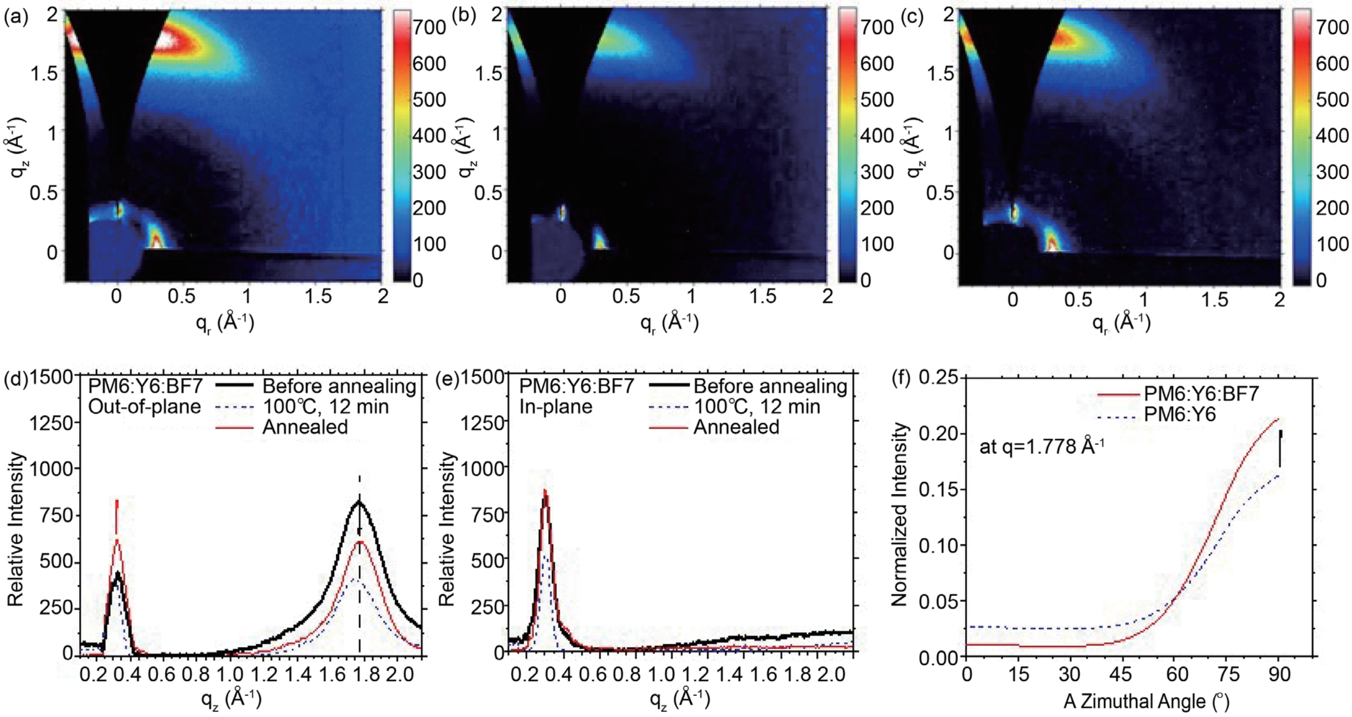

Fig. 2: (a–c) Time-resolved GIWAXS patterns of the PM6:Y6:BF7-0.5% thin films measured before, during, and after 100 °C annealing for 12 min. (d) Out-of-plane and (e) in-plane profiles extracted from the corresponding 2D GIWAXS patterns. (f) Azimuthal-angle dependent GIWAXS profiles at 1.778 Å^{-1} each taken from the 2D GIWAXS patterns of the two films after annealing. [Reproduced from Ref. 3]

processing could form supramolecular physical attractions with the fullerene derivatives, thereby suppressing fullerene aggregation. Consequently, the BF7-incorporated PCBM-based solar cells exhibited improved efficiency and greatly improved thermal stability.[2] If BF7 is introduced as a nonvolatile additive to the representative NFA-based OSC of a PM6:Y6 active layer, the perfluorophenyl C_6F_5 moieties in BF7 would induce F-F, F-H, and F-π interactions with the difluorophenyl-based FIC-end-groups of Y6, thereby modulating the phase segregation and crystallization of Y6 and PM6 for improved PCE and thermal stability. With 0.5-wt% BF7 in the active layer, the efficiency of the PM6:Y6-based device was enhanced dramatically to 17.01% from 15.16% of that without BF7. Moreover, 97% of the best efficiency could be maintained after isothermal heating at 100 °C for 72 h.[3]

The evolution of PM6:Y6 thin-film morphology with and without BF7 additive was highly correlated with device performance, and the stability was thoroughly investigated by U-Ser Jeng (NSRRC) and his coworkers including Chun-Jen Su at **TLS 23A1**; these researchers used grazing-incidence time-resolved wide-angle X-ray scattering (GIWAXS) measurements with *in situ* annealing and grazing-incidence small-angle X-ray scattering measurements (GISAXS), as shown in **Fig. 2**.[3] The experimental results demonstrated that the underlying mechanism of the double-effects of BF7 was associated with delicately controlled phase segregation and crystallization of the acceptor Y6 from the weakly ordered networks of the polymer donor PM6 through the selective supramolecular interactions of BF7 with Y6 to form a Y6-BF7 ordered complex of higher thermal stability than that of neat Y6 crystallites. The theoretical calculations consistently revealed preferred F-π noncovalent supramolecular interactions between the perfluorophenyl moieties of the nonvolatile additive BF7 and the difluorophenyl-based FIC end groups of Y6. In addition, they found that BF7 could have similar bifunctional effects of improving PCE and thermal stability on another well-known OSC system of PM6:IT-4F with the small-molecule acceptor IT-4F of similarly featured FIC end-groups.

In summary, the improvement of OSCs is primarily dependent on the rapid development of superior NFA n-type materials. The control and optimization of the morphology of the NFA:polymer blends by the incorporation of an additive material through supramolecular interactions can further improve the efficiency and impart morphological stability against thermal heating. The study of morphological evolution plays a crucial role in understanding the mechanism of molecular packing under the influence of an additive. The GIWAXS and GISAXS techniques at **TLS 23A1** used by Jeng and his coworkers offer insightful information on the nanostructures of the organic thin films. (Reported by Yen-Ju Cheng, National Yang Ming Chiao Tung University)

This report features the work of Yen-Ju Cheng and U-Ser Jeng published in Adv. Energy Mater. ***12****, 2270047 (2022).*

TLS 23A1 Small/Wide Angle X-ray Scattering

- GIWAXS, GISAXS
- Materials Science, Thin-film Chemistry.

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Orientational Control of Artificial Water Channels by Water-Induced Self-Assembly

Water-induced self-assembly (WISA) is a smart approach to control the dual-axis alignment of soft water channels.

Transport of water in cell membrane systems is well known to occur along Aquaporin channels. Thus, channels with a diameter of ~0.25 nm only allow the transport of water while simultaneously preventing the passage of other solutes. This selectivity mechanism is based on size exclusion, electrostatic repulsion, and water-molecule dipole reorientation. Currently, most studies on biomimetic membrane technology are based on this concept. Artificial water channels are typically composed of a water-permeable central pore surrounded by an external hydrophobic shell.