RESEARCH HIGHLIGHTS

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The origin and evolution of Y6 structure

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During last several years, electron acceptors for organic solar cells (OSCs) have experienced three major innovations. The first invention was a fused-ring electron acceptor (FREA), ITIC, reported by Zhan *et al.* in 2015, which consists of an indacenodithienothiophene (IDTT) donor core and two 3-dicyanomethylene-1-indanone (IC) as the end-groups[1]. ITIC cells exhibited comparable performance to $PC_{61}BM$ cells, and inspired the development of hundreds nonfullerene acceptors (NFAs). The second breakthrough is the 14.08% power conversion efficiency (PCE) delivered by a low-bandgap nonfullerene acceptor CO_i8DFIC with strong NIR absorption, invented by Ding *et al.*[2, 3]. The third star acceptor is Y6, developed by Zou *et al.* in 2019[4]. Y6 and its derivatives (Y-series NFAs) are very promising[5, 6]. Ding *et al.* developed polymer donor D18 and its outstanding derivatives[7–10], and the D18:Y6 cells gave a PCE of 18.22%[7], which was the first time for OSCs to deliver PCEs over 18%.

The core of Y6, dithienothiophen[3,2-*b*]pyrrolobenzothiadiazole, was derived from unit DTPBT (Fig. 1), which was reported by Cheng *et al.* in 2011[11, 12]. This ladder-type unit fuses central electron-deficient benzothiadiazole (BT) and two electron-rich thiophenes by two pyrroles, and it endows its copolymers with strong intermolecular π–π interaction, enhanced light absorption, and decent photovoltaic performance[12]. Zou *et al.* developed ladder-type unit dithieno[3,2-*b*]pyrrolobenzotriazole (BZTP) and used it as the core of acceptor BZIC[13]. BZIC presented broad absorption with a low optical bandgap of 1.45 eV, high lowest unoccupied molecular orbital (LUMO) energy level, and strong π–π interactions, and HFQx-T:BZIC cells gave a PCE of 6.30%. Then, acceptor Y1 was synthesized by replacing two thiophenes of BZIC's core with thieno[3,2-*b*]thiophenes[14]. With octacyclic dithienothiophen [3,2-*b*]pyrrolobenzotriazole as the D-A-D core, Y1 exhibited a red-shifted absorption, a low voltage loss of 0.57 V and a short-circuit current density (J_{sc}) of 22.44 mA/cm^2, yielding a PCE of 13.42%. Zou *et al.* changed benzotriazole unit of Y1 to benzothiadiazole for higher charge transport, and grafted alkyl chains at the terminals of the D-A-D core, producing Y5[15]. PBDB-T:Y5 cells offered a PCE of 14.1%. Derivated from Y5, Y6 was obtained by modifying the alkyl chains on thieno[3,2-*b*]thiophenes, and fluorinating the terminals[4, 16]. Y6 employs an A-DA′D-A molecular configuration with ladder-type core, fusing an electron-deficient BT in the middle. Y6 possesses enhanced intermolecular and intramolecular interactions for good electron mobility. As a strong electron-donating unit, N-alkyl pyrroles not only upshifted the highest occupied molecular orbital (HOMO) energy level to reduce the bandgap[17], but also suppressed over-aggregation and enhanced solubility[18]. The alkyl chains on both sides of DA′D core can help to lock conformation to enhance the order of molecular stacking[19]. Y6 cells exhibited high photocurrent, less non-radiative recombination and reduced voltage losses, giving a PCE of 15.7%[4, 20]. More Y6 derivatives were developed in a short time, pushing the PCE to 19%[6].

Y-series NFAs present universal compatibility and excellent photovoltaic performance. First, they always exhibit pretty high PCEs when combining with many polymer donors, even some of them were designed to match fullerene acceptors or ITIC derivatives[5]. Second, they have been used in almost all high-performance OSCs, ternary or all-small-molecule devices (SM-OSCs)[21, 22]. Some efficient polymer acceptors were developed by polymerizing Y-series NFAs, and over 17% PCEs from these all-polymer solar cells (all-PSCs) were delivered[23–25].

In summary, to enhance PCE further, the electron mobilities for Y-series NFAs need to be improved, and the energy loss needs to be minimized. We should understand well the relationship between molecular structures and non-radiative recombination[26]. To pave the road to commercialization, more efforts should be put into molecular design to invent more high-performance acceptors and donors.

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References

[1] Lin Y, Wang J, Zhang Z G, et al. An electron acceptor challenging fullerenes for efficient polymer solar cells. Adv Mater, 2015, 27, 1170

[2] Xiao Z, Jia X, Li D, et al. 26 mA cm^{-2} J_{sc} from organic solar cells with a low-bandgap nonfullerene acceptor. Sci Bull, 2017, 62,

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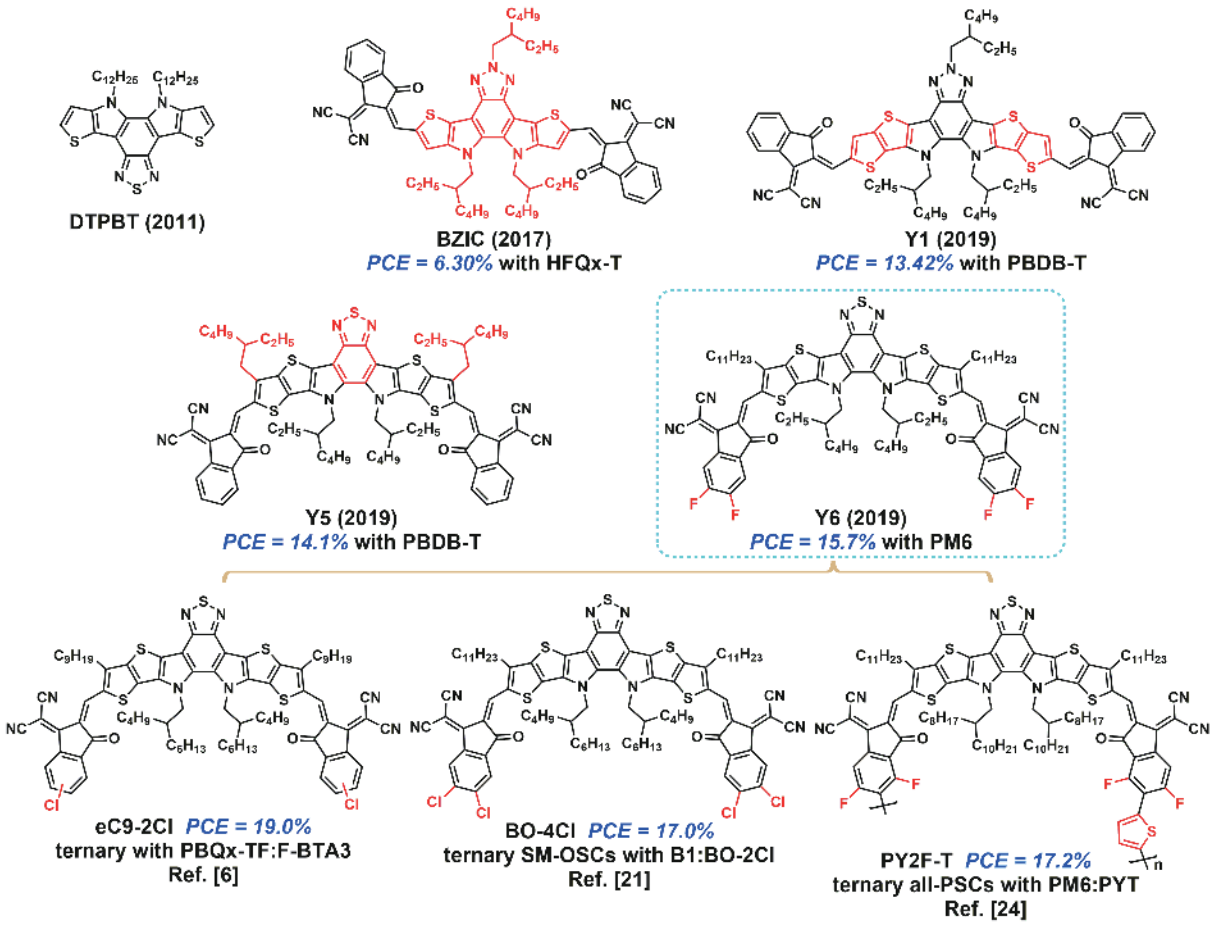

Fig. 1. The origin and evolution of Y6 structure.

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[3] Xiao Z, Jia X, Ding L, et al. Ternary organic solar cells offer 14% power conversion efficiency. Sci Bull, 2017, 62, 1562

[4] Yuan J, Zhang Y, Zhou L, et al. Single-junction organic solar cell with over 15% efficiency using fused-ring acceptor with electron-deficient core. Joule, 2019, 3, 1140

[5] Li S, Li C Z, Shi M, et al. New phase for organic solar cell research: emergence of Y-series electron acceptors and their perspectives. ACS Energy Lett, 2020, 5, 1554

[6] Cui Y, Xu Y, Yao H, et al. Single-junction organic photovoltaic cell with 19% efficiency. Adv Mater, 2021, 33, 2102420

[7] Liu Q, Jiang Y, Jin K, et al. 18% Efficiency organic solar cells. Sci Bull, 2020, 65, 272

[8] Qin J, Zhang L, Zuo C, et al. A chlorinated copolymer donor demonstrates a 18.13% power conversion efficiency. J Semicond, 2021, 42, 010501

[9] Jin K, Xiao Z, Ding L. 18.69% PCE from organic solar cells. J Semicond, 2021, 42, 060502

[10] Meng X, Jin K, Xiao Z, et al. Side chain engineering on D18 polymers yields 18.74% power conversion efficiency. J Semicond, 2021, 42, 100501

[11] Cheng Y J, Chen C H, Ho Y J, et al. Thieno[3, 2-*b*]pyrrolo donor fused with benzothiadiazolo, benzoselenadiazolo and quinoxalino acceptors: synthesis, characterization, and molecular properties. Org Lett, 2011, 13, 5484

[12] Cheng Y J, Ho Y J, Chen C H, et al. Synthesis, photophysical and photovoltaic properties of conjugated polymers containing fused donor-acceptor dithienopyrrolobenzothiadiazole and dithienopyrroloquinoxaline arenes. Macromolecules, 2012, 45, 2690

[13] Feng L, Yuan J, Zhang Z, et al. Thieno[3, 2-*b*]pyrrolo-fused pentacyclic benzotriazole-based acceptor for efficient organic photovoltaics. ACS Appl Mater Interfaces, 2017, 9, 31985

[14] Yuan J, Huang T, Cheng P, et al. Enabling low voltage losses and high photocurrent in fullerene-free organic photovoltaics. Nat Commun, 2019, 10, 570

[15] Yuan J, Zhang Y, Zhou L, et al. Fused benzothiadiazole: a building block for n-type organic acceptor to achieve high-performance organic solar cells. Adv Mater, 2019, 31, 1807577

[16] Wei Q, Liu W, Leclerc M, et al. A-DA′D-A non-fullerene acceptors for high-performance organic solar cells. Sci China Chem, 2020, 63, 1352

[17] Xie L, Zhang Y, Zhuang W, et al. Low-bandgap nonfullerene acceptor based on thieno[3, 2-*b*]indole core for highly efficient binary and ternary organic solar cells. Chem Eng J, 2022, 427, 131674

[18] Duan C, Ding L. The new era for organic solar cells: non-fullerene small molecular acceptors. Sci Bull, 2020, 65, 1231

[19] Yuan J, Zhang C, Chen H, et al. Understanding energetic disorder in electron-deficient-core-based non-fullerene solar cells. Sci China Chem, 2020, 63, 1159

[20] Liu S, Yuan J, Deng W, et al. High-efficiency organic solar cells with low non-radiative recombination loss and low energetic disorder. Nat Photonics, 2020, 14, 300

[21] Qin J, Chen Z, Bi P, et al. 17% efficiency all-small-molecule organic solar cells enabled by nanoscale phase separation with a hierarchical branched structure. Energy Environ Sci, 2021, 14, 5903

[22] Jin K, Xiao Z, Ding L. D18, an eximious solar polymer. J Semicond, 2021, 42, 010502

[23] Ji X, Xiao Z, Sun H, et al. Polymer acceptors for all-polymer solar cells. J Semicond, 2021, 42, 080202

[24] Sun R, Wang W, Yu H, et al. Achieving over 17% efficiency of tern-

ary all-polymer solar cells with two well-compatible polymer acceptors. Joule, 2021, 5, 1548

[25] Fan Q, Xiao Z, Wang E, et al. Polymer acceptors based on Y6 derivatives for all-polymer solar cells. Sci Bull, 2021, 66, 1950

[26] Yuan J, Zhang H, Zhang R, et al. Reducing voltage losses in the A-DA′D-A acceptor-based organic solar cells. Chem, 2020, 6, 2147

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