Science Bulletin 65 (2020) 1231–1233

Contents lists available at ScienceDirect

Science Bulletin

journal homepage: www.elsevier.com/locate/scib

Research Highlight

The new era for organic solar cells: non-fullerene small molecular acceptors

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Organic solar cells (OSCs) is a promising renewable energy technology as their prospect in producing large-area photovoltaic modules via low-cost roll-to-roll processing and their widespread application including photovoltaic farms, building integration, and portable electronics, etc. [1]. The key component of an OSC is its photoactive layer, which is a bulk-heterojunction blend of an electron donor and an electron acceptor [2]. The electron donors are p-type semi-conducting conjugated polymers or small molecules, and the electron acceptors were predominated by fullerene derivatives in OSC history. The power conversion efficiencies (PCEs) of fullerene-based OSCs have been promoted to ≈11% via ~20 years of effort by researchers all over the world [3]. After that, the fullerene-based OSCs have encountered bottlenecks in both device performance and stability due to the intrinsic drawbacks of fullerene acceptors including poor light-harvesting ability, difficulty in energy level control, and photon-induced dimerization, etc.

Therefore, researchers in the OSCs field have shifted their interests into alternative electron acceptors with an aim at overcoming the drawbacks associated with fullerene acceptors. A pioneering work was done by Lin et al. [4], who reported the fused-ring A–DD'D–A type molecular design for developing non-fullerene small molecular acceptors (SMAs). A benchmark molecule is ITIC, which consists of an indacenodithieno[3,2-*b*]thiophene core with four 4-hexylphenyl groups on it and two 2-(3-oxo-2,3-dihydroinden-1-ylidene)malononitrile end groups. After that, numerous SMAs with various core units, side chains, and end groups were developed based on this A–DD'D–A type molecular design. Combined with the progresses in high-performance polymer donors, delicate morphology control, organic/electrode contact optimization, and device engineering, OSCs based on A–DD'D–A type SMAs can afford PCEs approaching 15% in fully optimized single-junction cells [5] and over 17% in tandem cells [6].

More recently, a more promising A–DA'D–A type molecular design for SMAs proposed by Yuan et al. [7] has brought OSCs into a new era. The milestone molecule based on this design is Y6 (Fig. 1), which offered a prominent PCE of 15.7% in single-junction OSCs along with external quantum efficiency exceeding 80% at a voltage loss (V_{loss}) of only 0.50 V in its first report. This success has inspired widespread research activities in OSC field rapidly. Shortly afterwards, a few new SMAs (Fig. 1) based on the same design rationale have been developed via appropriate backbone modification, end group modification, and side chain control, which all produced decent device performance in OSCs (Table 1) [8–13]. Meanwhile, the device performance of OSCs has been improved to higher level upon the use of matched polymer donors and optimized device fabrication conditions. Up to date, the highest PCE of 18.2% in single-junction OSCs has been achieved based on Y6 [14]. Moreover, a recent study by Liu et al. [8] reported an unprecedently low voltage loss of 0.17 V due to non-radiative recombination loss in single-junction OSCs based on an analogue of Y6 (Y11, Fig. 1).

Y6 employs a ladder-type central fused ring (dithienothiophen [3,2-b]-pyrrolobenzothiadiazole) based on an electron-deficient benzothiadiazole core and two 2-(5,6-difluoro-3-oxo-2,3-dihydroinden-1-ylidene)malononitrile end groups. The electron-deficient benzothiazole unit with quinoidal character significantly extended the optical absorption of the molecule to near-infrared region with an absorption onset at 930 nm. The molecule consists of two conjugated planes with a small twist due to the steric hindrance in the center, and the bulky side chains on the central nitrogen atoms are orthogonal to the conjugated planes, which can prevent over-aggregation in solid state. With these unique characteristics in structure, the molecule offers good solubility in common solvents and efficient intramolecular charge transfer effect [7]. The single-crystal structure of a similar molecule (BTIC-CF_3-γ, Fig. 1) was revealed by Lai et al. [11] very recently, which can help to understand the marvelous photovoltaic performance of this kind of SMAs. In the single-crystal of BTIC-CF_3-γ, the central fused rings form H-aggregation in the perpendicular direction and the end groups form J-aggregation in the horizontal direction, which collectively result in a three-dimensional interpenetrating network for intermolecular charge transport.

Overall, the recent achievements based on Y6 and its analogues demonstrate that PCEs of 20% in single-junction cells and 25% in tandem cells are conceivable for OSCs in the near future via

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https://doi.org/10.1016/j.scib.2020.04.030

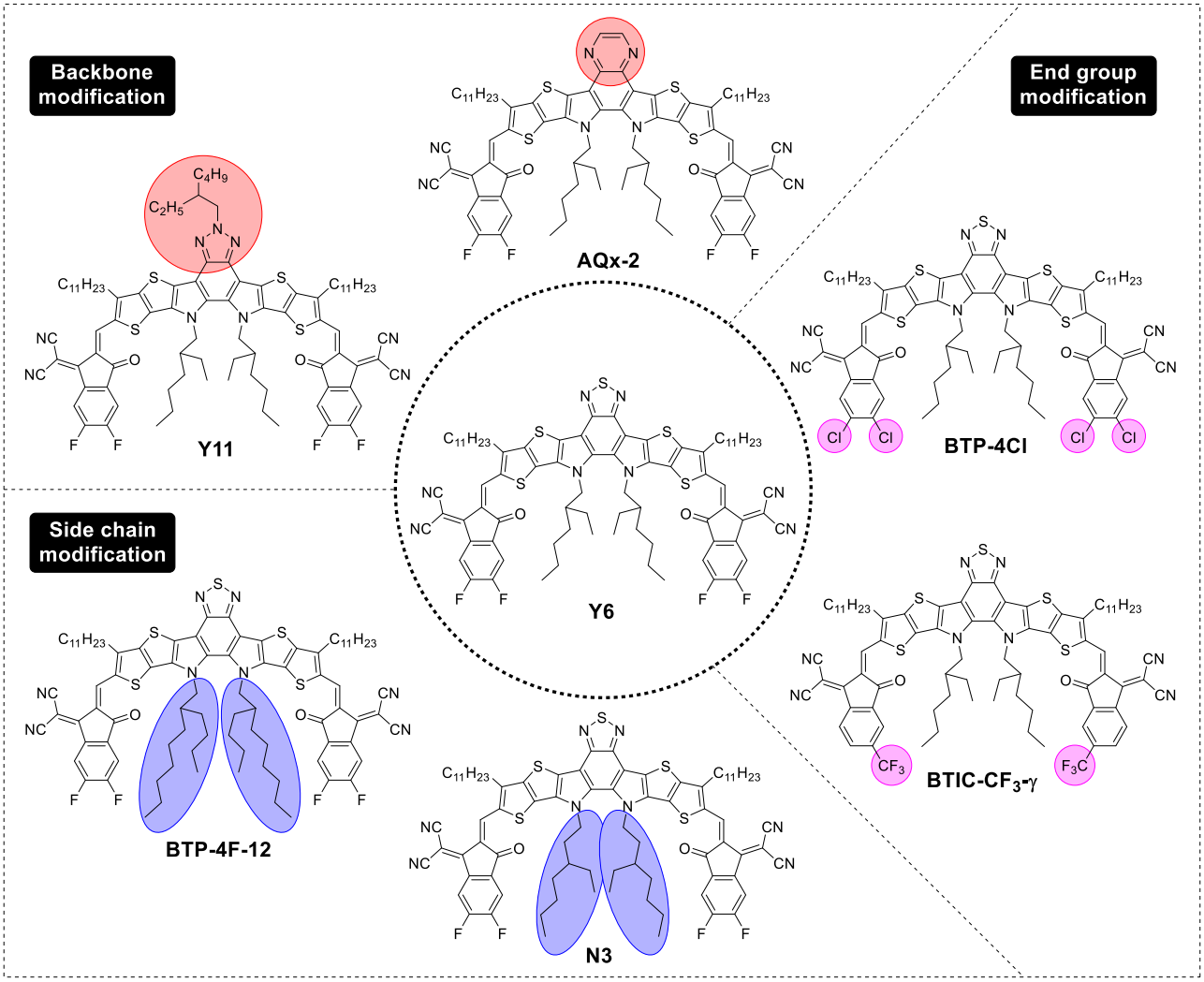

Fig. 1. (Color online) The chemical structures of representative small molecular acceptors with an A–DA'D–A framework.

Table 1
Device performance of binary OSCs based on the representative A–DA'D–A type small molecular acceptors.

Acceptor	V_{oc} (V) [a]	J_{sc} (mA cm^{-2}) [b]	FF [c]	PCE (%)	V_{loss} (V) [d]	Ref.
Y6	0.83	25.3	0.75	15.7	0.50	[7]
Y11	0.83	26.7	0.74	16.5	0.50	[8]
AQx-2	0.86	25.4	0.76	16.6	0.47	[9]
BTP-4Cl	0.87	25.4	0.75	16.5	0.46	[10]
BTIC-CF_3-γ	0.85	25.2	0.73	15.6	0.48	[11]
N3	0.84	25.8	0.74	16.0	0.49	[12]
BTP-4F-12	0.86	25.3	0.76	16.4	0.47	[13]

[a] Open-circuit voltage;
[b] Short-circuit current density;
[c] Fill factor;
[d] Voltage loss, which is given by $V_{loss} = E_g/q - V_{oc}$, where E_g is the bandgap acquired from the EQE onset, and q is the elementary charge.

synergetic efforts from synthetic chemists and device scientists. Further understanding on the working mechanism of these acceptors will help to boost the efficiency.

Conflict of interest

The authors declare that they have no conflict of interest.

Acknowledgments

This work was supported by the National Key Research and Development Program of China (2017YFA0206600, 2019YFA0705900) and the National Natural Science Foundation of China (21875072, 51773045, 21772030, 51922032, and 21961160720).

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