In an advance that makes more efficient in organic photovoltaics (OPVs), University of Central South researchers, Prof. Yingping Zou have developed non-fullerene acceptor organic photovoltaics (NFA-OPV) devices that can achieve 15.7% efficiency.

The research was published in Joule and has been heated discussion on the OPVs field. Before that research came out, Prof. Yingping Zou cooperated with Prof. Yang Yang from UCLA, and Prof. Feng Gao from Linköping University reported a successful strategy to tune the optoelectronic properties by introducing electron-deficient-core-based fused structure into non-fullerene acceptors. In this work, both devices exhibited a low voltage loss of 0.57 V and high short-circuit current density of 22 $mAcm^{-2}$, resulting in high power conversion efficiencies of 13.4 %. These unconventional electron-deficient-core-based non-fullerene acceptors with near-infrared absorption lead to low non-radiative recombination loss in resulting organic photovoltaics, contributing to a certified high-power conversion efficiency of 12.6%. The research," Enabling low voltage losses and high photocurrent in fullerene-free organic photovoltaics" was published in Nature Communications.

The two design rules for highly efficient OPVs

Organic photovoltaics (OPVs) have several advantages, such as potential low cost, inexpensive manufactured in roll-to-roll capability, and absorption tunability. Despite these advantages, OPVs have lacked the power conversion efficiencies (PCEs) required to compete with inorganic counterparts. One of the most significant factors, which hinders OPVs devices performance, is the relatively large loss in open-circuit voltage (Voc) with respect to the optical gap.

In an ideal OPV, maximum Voc can be achieved only when sources of voltage losses are limited to an unavoidable radiative recombination of absorption species above the optical gap. However, for the state-of-the-art OPVs, there are strong nonradiative recombination present leading to significant voltage losses, evidenced by electroluminescence quantum efficiency (EQEEL) measurement. Recombination of radiative charge-transfer (CT) states can also be present sue to energetic offsets between the donor (D) and the acceptor (A) components.

In the team's work, two design rules are formulated aiming at reducing the voltage loss and increasing the efficiency of OPVs:

(1) Small energy offset between the donor and acceptor materials.

(2) High luminescence yield of the lower-gap single component (and hence the blend).

Among the materials candidates meeting these design rules, A-D-A-structured non-fullerene acceptors (NFAs) are extremely promising since they exhibit strong level tunability, and good molecular crystallinity. These features allow NFAs to become potential candidates for achieving an efficient charge separation and low voltage losses simultaneously as per the design rules.

Maximize spectral absorption and elevate HOMO

For the aspect of molecular design, synthesis of donor and acceptor materials with complementary absorption profiles intended to maximize the coverage of the solar spectrum has been one of the prerequisites for achieving a high photocurrent. Thus, a variety of narrow optical gap NFAs based on a stronger electron-donating at the central core were carefully designed and synthesized for OPVs. Undoubtedly, it is a successful strategy to elevate HOMO level reducing the optical gap.

Benzotriazole-based conjugated molecules with unique luminescence properties are common building blocks for increasing the photo-luminescence quantum yield (PLQY) of the single

component. The high PLQY indicates efficient radiative recombination pathways, which may result in high electroluminescence yield of resulting devices. Hence, it attempts to introduce benzotriazole into the central core to form an electron-deficient-core-based fused structure (DAD) for adjusting the optoelectronic properties of the resulting molecules, aiming for small voltage loss and high performance in devices.

In this work, the team reported a certified high efficiency of single-junction OPVs based on two fused-ring NFA molecules (Y1 and Y2) consisting of dithienothiophen[3,2-b]pyrrolobenzotriazole (BZPT) group with non-halogenated dicyanomethylene derivatives (INIC or INTC). A simple design strategy of covalent nitrogen bridge with adjacent thieno[3,2-b]thiophene and benzotriazole makes it possible to delicately tune the optoelectronic properties of target molecules, resulting in an improvement of optical coverage of near-infrared region (NIR) spectrum. A commercial donor polymer PBDB-T35 is selected because of its negligible band offsets with Y1 and Y2. In spite of this small energetic offset, which results in relatively high EQE_{EL} (approximately 0.5×10^{-4}) and small voltage losses, charge separation is still efficient and offers decent short-circuit current density (over $22mAcm^{-2}$), resulting in PCEs of over 13.4% (13.42% for Y1 and 13.40% for Y2). These certified devices showed a 12.6% efficiency. This remarkable feature of the presented fused benzotrizole-based system serves as an inspiration to design next-generation NFAs for high-performance OPVs.

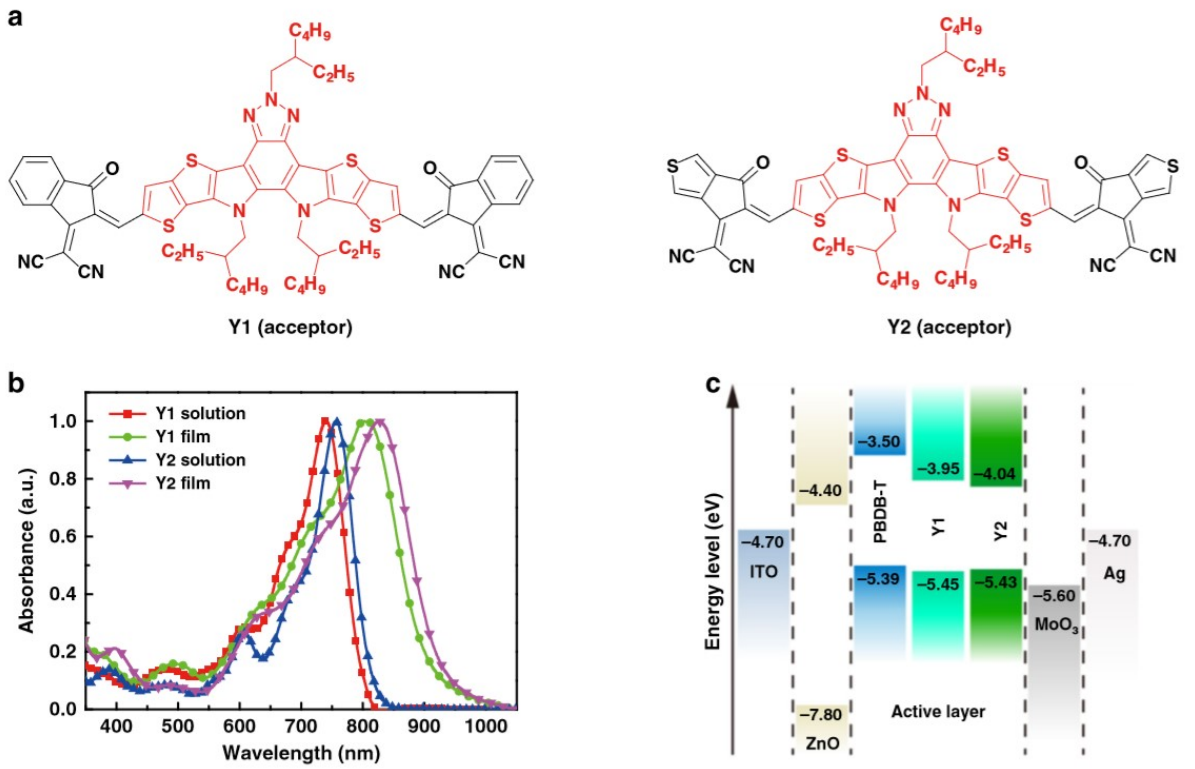

Fig. Molecular structure and properties. (a). Chemical structure of the acceptor molecules. (b) Normalized absorption spectra of the acceptors Y1 and Y2. (c) Energy diagrams of the materials used in OPVs.

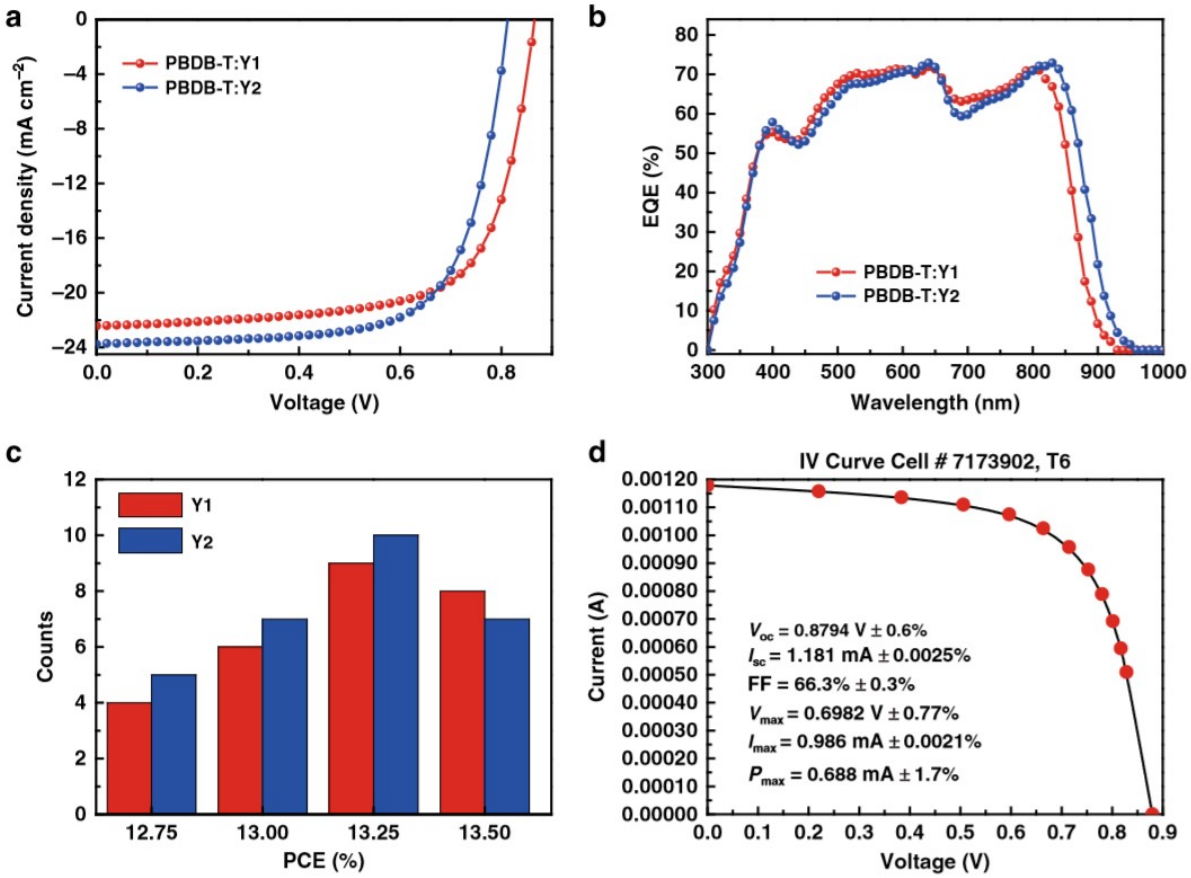

Fig. Photovoltaic performance. (a). The J-V curves of PBDB-T:Y1 and :Y2 blend solar cells. (b). The EQE curves of PBDB-T:Y1 and :Y2 blend solar cells. (c). Statistical diagram of efficiency of PBDB-T:Y1 and :Y2. (d). Current-voltage parameters of PBDB-T:Y1 certified device (0.0548cm^2 device area)

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