Electron-deficient core fused-ring based non-fullerene acceptor enables over 15% efficiency in single junction organic solar cells

With the support from the National Natural Science Foundation of China and National Key Research & Development Project of China, the research team led by Prof. Zou YingPing (邹应萍) at the College of Chemistry and Chemical Engineering, Central South University, reported a new nonfullerene acceptor Y6 with a fused-ring structure containing electron-deficient benzothiadiazole core, which made a breakthrough in single junction organic solar cells (OSCs) with power conversion efficiency (PCE) of 15.7%. The study was published in *Joule* (DOI:10.1016/j.joule.2019.01.004).

Organic solar cells are promising to access flexible, lightweight and semi-transparent photovoltaic devices. Recently, *n*-type organic semiconductors (*n*-OS) have attracted great attention as acceptors in OSCs, due to their easily tuned absorption and electronic energy levels in comparison with fullerene acceptors. In order to further enhance the performance of OSCs, the team reported the introduction of benzotriazole into the central core to form an electron-deficient-core-based fused structure (DAD) for adjusting the optoelectronic properties of the resulting molecules in early 2017. Following the above strategy, they further introduced stronger electron-withdrawing benzothiodiazole (BT) instead of benzotrizole as central core and applied thienothiophene (TT) instead of thiophene as the end group of the central fused ring, to obtain a new acceptor Y6. Such a design is beneficial for increasing electron mobility and broadening the absorption range. Besides, the central core of Y6 is attached to alkyl side chains on the nitrogen atoms at the same side to avoid over-aggregation of molecules, while maintaining an effective intramolecular contact for charge transport. Y6 based OSC without extra treatments showed a high PCE of 15.3% using PM6 as polymer donor. After optimizing the morphology, a record efficiency of 15.7% was achieved with both conventional and inverted devices, respectively measured at the Institute of Chemistry, Chinese Academy of Sciences (Prof. Li's research team) and South China University of Technology (Prof. Yip and Prof. Cao's research team).

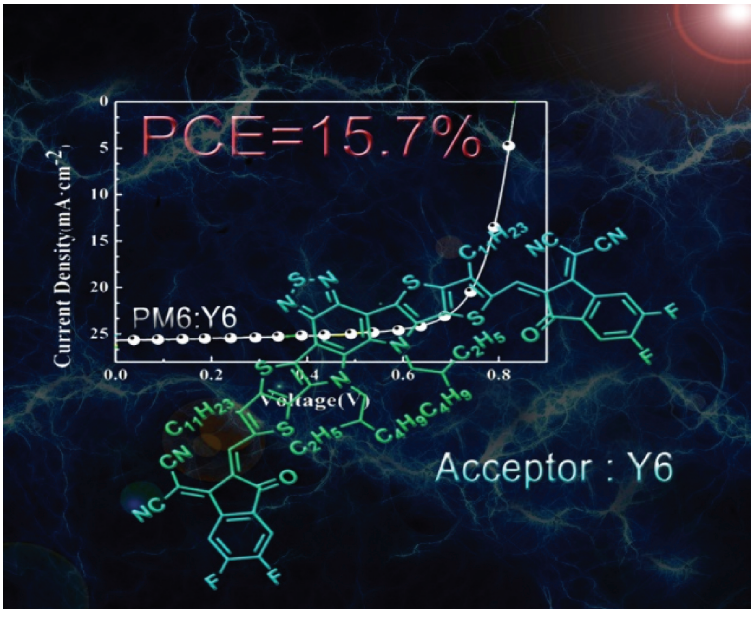

Figure Molecular structure and photovoltaic performance.

The results demonstrate highly encouraging development of new non-fullerene acceptors for enabling high performance OSCs. The electron-deficient-core-based fused ring acceptor reported in this work opens a new door in the molecular design of high-performance acceptors for the future OSC applications.