Reduced energetic disorder enables over 14% efficiency in organic solar cells

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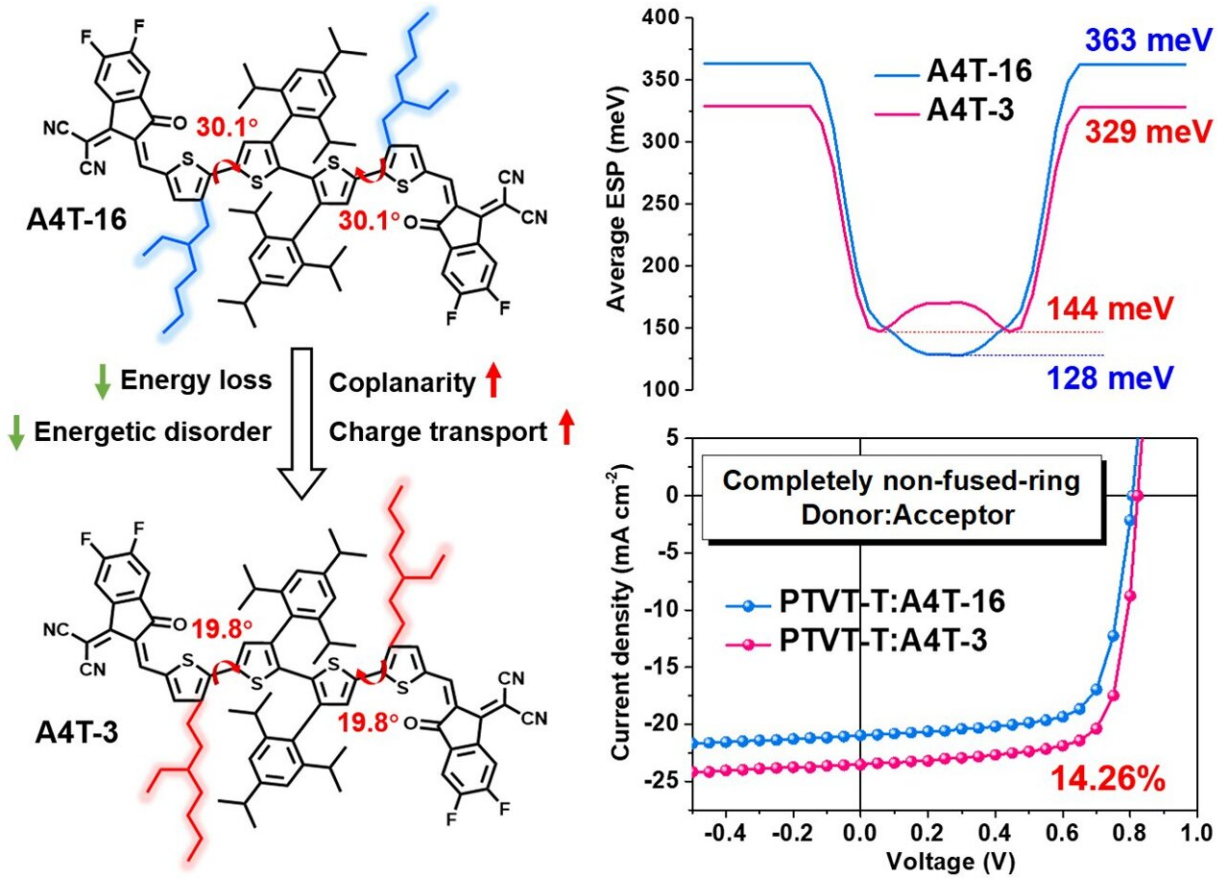

The more planar molecular structure of A4T-3 enabled it with lower energetic disorder and reduced energy loss, thus higher photovoltaic performance of the PTVT-T:A4T-3-based device. Credit: Science China Press

Non-fused-ring organic photoactive materials have attracted broad attention in recent years due to their low synthetic cost. Different from the rigid coplanar structure of fused-ring molecules, the easily rotated conformation of non-fused-ring molecules could lead to the different energetic disorder, which greatly affects the intramolecular electron transport and thus the device performance.

Recently, Prof. Shaoqing Zhang replaced the 2-ethylhexyl side chain of A4T-16, an efficient completely non-fused-ring acceptor reported previously, with 3-ethylheptyl to synthesize a new acceptor A4T-3. By contrast, the 3-ethylheptyl substituent had a smaller steric hindrance effect, enabling A4T-3 with a more planar structure.

The temperature dependent mobility results suggested that A4T-3 exhibited lower intramolecular energetic disorder than A4T-16, resulting in a more uniform surface electrostatic potential distribution. Therefore, A4T-3 showed a smaller barrier for intramolecular electron transport and a higher electron mobility.

Meanwhile, the lower electrostatic potential of the end group made A4T-3 have smaller intermolecular interaction with the donor, which could reduce the non-radiative energy loss of the corresponding device. When the non-fused-ring polymer, PTVT-T, was used as the donor material, the photovoltaic performance of A4T-3-based device is comprehensively improved in comparison with A4T-16, with a power conversion efficiency of 14.26%.

Notably, this is the highest value for organic solar cells where both the donor and the acceptor are completely non-fused-ring materials. The cost evaluation showed that the material cost of PTVT-T:A4T-3 combination was much lower than other high-performance combinations, revealing the great potential of completely non-fused-ring photoactive materials for application-oriented OSCs.

The research is published in the journal *Science China Chemistry*.

More information: Chenyi Yang et al, Reduced energetic disorder enables over 14% efficiency in organic solar cells based on completely non-fused-ring donors and acceptors, *Science China Chemistry* (2022). DOI: 10.1007/s11426-022-1449-4

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