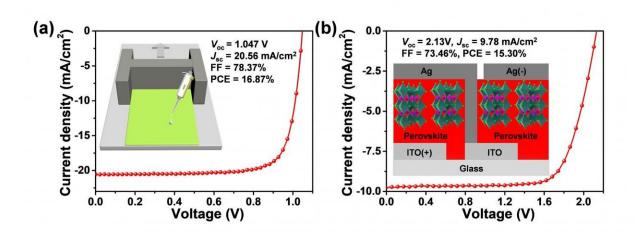


Organic small molecule hole-transporting layers toward efficient p-i-n perovskite solar cells

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Pero-SCs based on blade-coated BDT-TPA-sTh HTL and MAPbI3 active layer: (a) J-V curves in the reverse-scan direction; inset: schematic illustration of blade-coated HTLs. (b) J-V curves of a 1-cm2 pero-SC module in the reverse-scan direction; inset: schematic illustration of device-structure of modules. Credit: Science China Press

Perovskite solar cells (pero-SCs) show great potential in photoelectric fields due to high power conversion efficiency (PCE), simple processing technology, low fabrication cost, etc.. Recently, the highest certificated PCE of pero-SC has reached 25.2%, which shows great promise for



commercialization. Coming research will focus on the fabrication of efficient and modular pero-SCs to further promote the commercialization of pero-SCs.

In p-i-n planar pero-SCs, the hole-transporting layers (HTLs) have an important influence on the growth of perovskite crystals, hole transporting ability and device stability. Therefore, developing efficient and stable HTL materials suitable for large-area processing will play a crucial role in large-area modular pero-SCs. In addition to the matched energy levels, stable chemical properties and good reproducibility, the HTL materials suitable for large-area processing should also have high hole-mobility and good wettability with the perovskite precursor solution.

Although the device based on

poly(bis(4-phenyl)(2,4,6-trimethylphenyl)amine) (PTAA) as organic HTLs can achieve a PCE exceeding 22%, the poor wettability of the perovskite precursor solution will hinder the preparation of large-area modules. Up to now, new organic HTL materials in large-area devices have been rarely reported. Therefore, it is urgent to develop highly efficient and high-hole-mobility HTL materials that are compatible with large-area processing in p-i-n planar pero-SCs.

Very recently, Prof. Yaowen Li at Soochow University and co-authors designed a π -conjugated small-molecule HTL material BDT-TPA-sTh with a symmetric structure by rationally selecting the planar BDT core, TPA terminal groups, as well as conjugated 2-ethylhexyl-thienyl side chains.

The conformation and stacking model of the resultant BDT-TPA-sTh was directly observed by X-ray crystallography measurements from its single crystals. The pronounced planarity with parallel-displaced π - π and additional S- π supramolecular interactions between neighboring



molecules contributed to an improved hole-mobility. In addition, the marginal solubility of BDT-TPA-sTh in the perovskite solution enabled inverse diffusion into the perovskite films, which could be used to further passivate the uncoordinated Pb_2^+ ion defects by Lewis-base S-atoms in BDT-TPA-sTh without damaging the under-layer HTLs.

The p-i-n planar pero-SCs using BDT-TPA-sTh without dopant as the HTL not only realized a high PCE (20.5%) and improved moisture stability, but also demonstrated its feasibility for fabricating large area devices through the blade-coated technology. They believe that this HTL design concept through supramolecular interactions and inverse diffusion will pave the way for designing HTL materials of perovskite-based optoelectronic devices. Their work would provide a significant step in designing interface materials toward high performance, large area and printing p-i-n planar pero-SCs, and thus would be interesting to a wide readership for the perovskite-based opto-electronic community.

More information: Rongming Xue et al, Dopant-free hole transporting materials with supramolecular interactions and reverse diffusion for efficient and modular p-i-n perovskite solar cells, *Science China Chemistry* (2020). DOI: 10.1007/s11426-020-9741-1

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