

Recent progress in Polymer Solar Cells: Breakthrough Efficiency of 14.64% by optimizing PSC device operation in NIR.

Scientists at the Department of Polymer Science and Engineering, Zhejiang University have presented a family of near-infrared nonfullerene acceptors (NIR NFA, T1-T4) with fluorinated regioisomeric A–A π –D–A π –A backbones for constructing efficient single-junction and tandem PSCs with photon response up to 1000 nm.

The study "Near-Infrared Electron Acceptors with Fluorinated Regioisomeric Backbone for Highly Efficient Polymer Solar Cells.", led by Zhejiang University professors Chang-Zhi Li (corresponding author), Hongzheng Chen and Fang-Xiao Chen (first author), and the South China University of Technology professor Hin-Lap Yip, have found that the tuning of the regioisomeric bridge ($A\pi$) and fluoro (F)-substituents on a molecular skeleton strongly influences the backbone conformation and conjugation, leading to the optimized optoelectronic and stable stacking of resultant NFAs, which eventually impacts the performance of derived PSCs.

With the rapid development of new electroactive molecules, the polymer solar cells has experienced fast breakthrough over the past few years. The promising virtue for PSCs is their functional tunabilities stemming from the chemical versatility of organic semiconductors, and which can make PSCs produced in large quantities, the price of PSCs is relatively low, and have stretchy characteristic. For instance, the recent development of near-infrared (NIR) organics (bandgap, Eg < 1.4 eV) enables PSCs with strong NIR photon responsiveness and visible-range transparency, which are promising for constructing tandem and semitransparent PSCs.

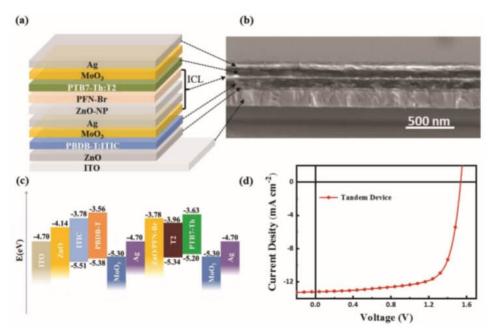


Figure. a) Schematic architecture and b) cross-sectional SEM image for tandem PSCs. c) Energy levels of each layer and d) optimal J–V curves of the tandem device under the illumination of AM 1.5G (100 mW cm⁻²). (Cited from the research)

Getting high efficiency from low-energy NIR is not easy!

Although considerable efforts have been devoted to developing NIR organic semiconductors PSCs based on NIR donor and fullerene acceptors usually show PCE lower than 10% and suffer from relatively low external quantum efficiencies (EQE). Encouragingly, the recent development of fused-ring nonfullerene acceptors (NFAs), such as IHIC, IEICO, ATT-2, BT-CIC, DTPCIC, and COi8DFIC, provides new opportunities, which enables PSCs to utilize NIR photons for achieving high short-circuit current (Jsc).



However, one of the challenges that NIR organics has been facing is to achieve NIR photon-toelectron conversion with high quantum efficiency and less energy loss in PSCs. Also, the access of optimal bulk heterojunction (BHJ) blend morphologies, which impacts largely to the overall performance of PSCs, is usually obtained via the trail-and-error processing, which is somehow impractical to scale up fabrication. So far, few as-cast PSCs yielded PCEs >8%, considering both fullerene-based and NFA-based devices. Hence there is a strong need to explore the structural design of NIR photoactive molecules that allow improvement of BHJ characteristics, such as charge mobilities and morphological domains, to eventually optimize PSC device operation, especially in the process of low-energy NIR photonto-electron conversion.

Breaking through the record!

The key is the new insights on structural design of NIR organics and devices. The team shows four new NIR NFAs with fluorinated regioisomeric A–A π –D–A π –A backbone, including IFIC-i-2F (T1), IFIC-i-4F (T2), IFIC-i-6F (T3), and IFIC-o-4F (T4) are developed for constructing efficient single junction and tandem PSCs. (Figure 1) This arrangement modulates the backbone rigidity and planarity as well as internal charge transfer of resultant IFICs, hence influences the optoelectronic and robust stacking properties. These four IFICs exhibit broad absorption (with Eg down to 1.27 eV), and fine-tuned energy levels. Interestingly, through with similar molecular formula, a significant increase of PSC performance can be observed from distal NFA, 7% (T4) to proximal NFAs with varied-F-atoms (T1-T3), up to 10.10% (T2), through the simple solution-cast with PTB7Th polymer.

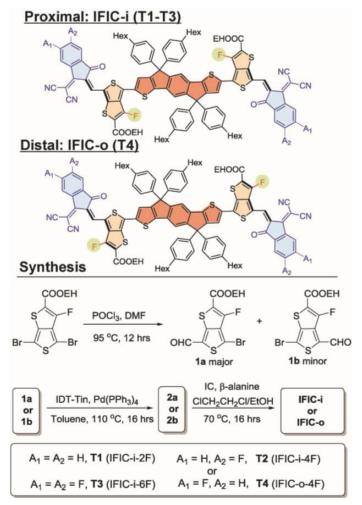


Figure. Chemical structures and the synthetic route for T1 (IFIC-i-2F), T2 (IFIC-i-4F), T3 (IFIC-i-6F), and T4 (IFIC-o-4F). (Cited from the research)



The optimal performance for T2:PTB7-Th-based PSCs can be further improved by proceeding with 1% 1-chloronaphthalene (CN) as the solvent additive, showing impressive PCE of 10.87% with high JSC of 24.85 mA cm-2, VOC of 0.65 V, and FF of 0.67. Interestingly, efficient tandem solar cells can be constructed by integrating NIR-absorbed IFIC-4F (T2): PTB7-Th subcell with mediate bandgap ITIC:PBDB-T subcell.

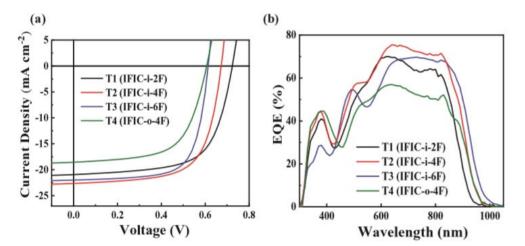
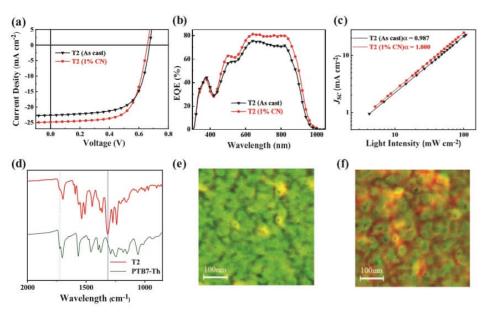


Figure. a) The J–V characteristics and b) EQE spectrum of the resultant PSCs for the inverted single junction PSC with NIR BHJs (PTB7-Th:T1-T4). (Cited from the research)

Together with careful optical simulation and device engineering, high PCE of 14.64% is achieved for the absorption range up to1000 nm, which is one new example among the best performing tandem PSCs to date. This study reveals new insights on the structural design of NIR organics and devices with improved photovoltaic performance.



(Cited from the research)



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The team uses <u>Enli Tech SS-F5-3A solar simulators</u> and <u>Si reference cell</u> in accordance with Enli Tech's filter technology (the calibrated report can be traced to NREL), as well as <u>QE-R solar</u> <u>cell quantum efficiency measurement system.</u>

The J–V curves of OSCs were measured with Keithley 2400, under AM 1.5G illumination at 100 mW cm⁻² irradiation using a Enli SS-F5-3A solar simulator, and the light intensity was calibrated with a standard Si solar cell with KG5 filter (made by Enli Technology Co., Ltd., Taiwan, and calibrated report can be traced to NREL). The EQE spectrum was measured using a QE-R Solar Cell Spectral Response Measurement System (Enli Technology Co., Ltd., Taiwan). For EQE of subcells in tandem devices, a third electrode was adopted for the measurement

It is a great honor and pleasure for Enli Tech can once again be involved in the research, and provide the high precision, fast and stable measurement system for the team. Enli Tech is looking forward to continuously providing you with the total solutions in material science, photovoltaic and semiconductor fields.

Reference :

<u>Near-Infrared Electron Acceptors with Fluorinated Regioisomeric Backbone for Highly</u> <u>Efficient Polymer Solar Cells.</u>

Fang-Xiao Chen, Jing-Qi Xu, Zhi-Xi Liu, Ming Chen, Ruoxi Xia, Yongchao Yang, Tsz-Ki Lau, Yingzhu Zhang, Xinhui Lu, Hin-Lap Yip, Alex K.-Y. Jen, Hongzheng Chen, and Chang-Zhi Li