**Near-infrared Absorbing Acceptor Improves the Nanophase Segregation of Ternary Organic Photovoltaic Blend with a Performance of 12%**

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Introduction.

Non-fullerene acceptors (NFAs) with advantages of low open circuit voltage (Voc) loss, tunable energy levels and absorptions in visible and near-infrared (NIR) region are promising for high efficiency organic photovoltaics (OPVs). [1]

**Figure 1.** Structure of the material.

Aims.

The NFA was designed as a NIR-absorbing acceptor to study the blend film morphology of ternary OPV. The NFA was aimed to provide the complementary light harvesting and tailored the nanophase morphology for ternary OPV.

Methods.

We design and synthesis an A-D-A-configured molecule **PTTtID-Cl** (**Figure 1**). The strong ICT character enables the resulting material to have strong absorption in the range of 700–850 nm in CHCl3 solution, and red-shifted absorption centered at 881 nm was observed in thin film. We paired the low band-gap polymer PM7 and IT-4F, with PTTtID-Cl to explore their BHJ nanophase segregation and optoelectronic properties of ternary OPV.[2]

**Figure 2.** (a) *J-V* characteristics, (b) IPCE spectra of ternary devices

Results & Discussion.

 An optimized power conversion efficiency (PCE) of 12.0% (AM 1.5 G 100mW/cm2) was obtained with **PM7**:**IT-4F**:**PTTtID-Cl** ratio at 1:0.15:0.85 w/w. The 72% and 23% PCE improvement compared to **PM7**:**PTTtID-Cl**- and **PM7**:**IT-4F**-based binary device, respectively, are mainly caused by increased *J*sc and FF values (**Figure 2**). The higher *J*sc values of the device with ratio optimization than **PM7**:**IT-4F**-based binary device mainly resulted from superior photocurrents in the region of 750-900 nm shown in IPCE spectrum, which indicates the benefit of introducing NIR-absorbing **PTTtID-Cl**. **Figure 3** reveals the topology and phase images of binary and ternary blends. The rough surface morphology (RMS=15.9nm) and severe aggregation in **Figure 3f** imply the severe D/A segregation existing only in PM7:PTTtID-Cl blend. The severe D/A segregation might lead to low probability for exciton dissociation at D/A interfaces and high trap-assisted recombination in active layers, leading to lower low Jsc and Voc values for PM7:PTTtID-Cl-based devices, respectively. The smaller nanoscale phase segregation was observed for the PM7:PTTtID-Cl:IT-4F (1:0.15:0.85. w/w) ternary blend which exhibits the highest PCE compared with PM7:PTTtID-Cl and PM7:IT-4F binary blends.

**Figure 3.** Topology and phase images of **PM7**:**IT-4F**:**PTTtID-Cl** ratio at (a, d) 1:0:1, (b, e) 1:0.15:0.85 and (c, f) 1:1:0.

Conclusion.

The ternary OPV device with the best ratio of **PM7**:**PTTtID-Cl**:**IT-4F** = 1:0.15:0.85 (w/w) achieves a *J*sc of 19.6 mA cm–2, a *V*oc of 0.87 V, and a FF of 70.2% and a PCE of 12.0%. The optimized ratio of **PM7**:**PTTtID-Cl**:**IT-4F** = 1:0.15:0.85 (w/w) exhibits appropriate BHJ morphology with nanophase separation, expanded absorption region and lower dark currents which could contribute to higher values of *Jsc*, FF and thus higher PCEs.

**References**

[1] C.-K. Wang, B.-H. Jiang, Y.-W. Su, R.-J. Jeng, Y.-J. Wang, C.-P. Chen, K.-T. Wong, *ACS Applied Materials & Interfaces* **2019**, *11*, 1125-1134.

[2] C.-P. Chen, Y.-C. Li, Y.-Y. Tsai, Y.-W. Lu, *Solar Energy Materials and Solar Cells* **2018**, *183*, 120-128.