Ternary solar cells with polymer donor and two nonfullerene acceptors

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I. INTRODUCTION

Using high-efficiency nonfullerene acceptors (NFAs) to replace fullerene derivatives and constructing ternary systems for all NFAs is an effective strategy to overcome the drawbacks of difficulties in tuning energy levels and absorption of fullerene. It is noted that third component has a strong effect on light absorption, energy level, and morphology of ternary blend film for all nonfullerene acceptors. Thus, a combination of two NFA in ternary blends is required reasonable optimization.

In this work, two nonfullerene acceptors IT-2Cl and IT-4Cl were employed as the third component to enhance light harvesting and modulate morphologies of the host binary systems composed by polymer donor PTB7-Th and ultra-low bandgap NFA acceptor 6TIC-4F. PTB7-Th: 6TIC-4F binary devices showed a PCE of 10.5% but with a relatively low open-circuit voltage (Voc) of 0.67V. Energy levels of IT-2Cl are lying between those of host systems, which facilitates energy gradient between host donor and acceptor. The absorption dip between two absorption peaks of PTB7-Th and 6TIC-4F could be compensated by IT-4Cl with absorption in ranges of 650-800nm, which benefits to enhance short-circuit current density (Jsc). Moreover, the incorporation of IT-2Cl or IT-4Cl could improve the morphologies of active layers. As a result, the addition of IT-2Cl increased the PCE of PTB7-Th: 6TIC-4F based devices from 10.5% to 11.4% with a higher Voc of 0.69V and a fill factor (FF) of 0.68. For optimal PTB7-Th: IT-4Cl: 6TIC-4F based device, PCE was increased to 11.3% with enhanced short-circuit current density (Jsc) of 25.7mA cm⁻² and FF of 0.68. This work would provide the guideline to fabricate high-efficiency ternary solar cells with two NFAs.

Figure 1. Chemical structures of PTB7-Th, 6TIC-4F, IT-2Cl and IT-4Cl

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II. RESULTS AND DISCUSSIONS

Table 1. Photovoltaic Parameters for Devices under Simulated AM 1.5 G Illumination at 100 mW cm⁻²

indimination at 100 m v cm					
	Ratio	$V_{oc}(V)$	J _{sc} (mA cm ⁻²)	FF	PCE(%)
PTB7-Th: 6TIC-4F	1:1.2	0.67	24.4	0.64	10.5
		(0.66±0.01)	(24.2±0.2)	(0.63±0.01)	(10.2±0.3)
PTB7-Th: IT- 2 Cl: 6TIC-4F	1:0.3:0.9	0.69	24.3	0.68	11.4
		(0.68±0.01)	(24.0±0.3)	(0.67±0.01)	(11.2±0.2)
	1:0.6:0.6	0.70	23.1	0.68	11.3
		(0.69±0.01)	(22.9±0.2)	(0.67±0.01)	(11.0±0.3)
	1:1.2:0	0.73	14.4	0.71	7.4
		(0.72±0.01)	(14.2±0.2)	(0.70±0.01)	(7.2±0.2)
PTB7-Th: IT- 4Cl : 6TIC-4F	1:0.3:0.9	0.65	25.7	0.68	11.3
		(0.64±0.01)	(25.5±0.2)	(0.67±0.01)	(11.1±0.2)
	1:0.6:0.6	0.65	23.8	0.68	11.1
		(0.64±0.01)	(23.5±0.3)	(0.67±0.01)	(10.9±0.2)
	1:1.2:0	0.64	16.2	0.71	7.4
		(0.63±0.01)	(16.0±0.2)	(0.70±0.01)	(7.1±0.3)







Figure 3. AFM height images of the binary and optimized ternary.

III. CONCLUSION

In conclusion, two nonfullerene acceptors IT-2Cl and IT-4Cl were selected as the third component to construct PTB7-Th: 6TIC-4F based ternary solar cells. By inserting IT-2Cl as the second acceptor materials, ternary devices show a cascading energy level and optimized morphologies. IT-4Cl not only exhibits complementary absorption to the PTB7-Th and 6TIC-4F, but also modulates the films morphologies. As a result, ternary solar cells containing IT-2Cl or IT-4Cl show enhanced PCEs of 11.4% and 11.3%, respectively, which are 9% and 8% improvement in PCE compared to PTB7-Th: 6TIC-4F binary devices. These results provide a rational guide for selection of NFA as the third component to prepare high-performance nonfullerene-based ternary solar cells.