RESEARCH HIGHLIGHTS

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Nonfullerene acceptors based on perylene monoimides

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Nonfullerene organic solar cells (NF-OSCs) have become a research hotspot, and the device efficiency has been constantly updated[1–14]. The efficiency of binary and ternary solar cells has exceeded 18%[15–17] and 19%[18], respectively. In the early study of OSCs, the development of organic acceptors lagged behind that of organic donors. In addition to the common fullerene acceptors $PC_{61}BM$ and $PC_{71}BM$, there is growing interest in developing new electron acceptors. The two fullerene acceptors were derived from C_{60} and C_{70}, which were chemically modified to improve the solubility. Later, Li *et al.* developed a C_{60} derivative ICBA[19] and a C_{70} derivative $IC_{70}BA$[20]. Compared with $PC_{61}BM$ and $PC_{71}BM$, the lowest unoccupied molecular orbital (LUMO) levels of these two acceptors increased by 0.17 and 0.19 eV, respectively. This is conducive to the increase of open-circuit voltage (V_{oc}). At present, the development of fullerene acceptors is limited, the reason are as follows: (1) they show weak absorption in the visible region, which is not conducive to the full use of sunlight; (2) it is difficult to improve the absorption by the chemical modification; (3) difficult chemical synthesis and high cost; (4) it is difficult to control the morphology, and the aggregation easily takes place in thin films. The advantages of fullerene acceptors are also obvious, e.g., (1) fullerene acceptors can accept and transport electrons in three dimensions due to their delocalized LUMO; (2) high electron mobility. Perylene diimides (PDIs) have been widely used in biological imaging, and they are widely-studied non-fullerene acceptors. PDIs have many advantages, such as high electron mobility and high electron affinity[21]. In 1986, C. W. Tang of Kodak prepared two-layer OSCs by depositing copper phthalocyanine (CuPc) as the donor and perylene tetracarboxylic derivative (PV) as the accepter in vacuo, achieving a power conversion efficiency (PCE) of 1%[22]. PDI-based devices were made by solution processing, and the aggregation yielded micron-sized crystals. When the acceptors were blended with donors, large domains formed[23]. Since exciton diffusion length and life were limited, the domain size should be well controlled.

The solar cell parameters consist of V_{oc}, short-circuit current density (J_{sc}) and fill factor (FF). PDIs have two drawbacks: (1) the low LUMO level leads to low V_{oc}; (2) PDIs with rigid planar structure tend to form excessive aggregations, affecting the formation of uniform films. Thus, lifting LUMO level and constructing non-coplanar perylene monoimides (PMIs) to improve V_{oc} and the morphology are effective strategies. PMI-based nonfullerene acceptors and the photovoltaic performance are summarized in Fig. 1 and Table 1. In 2015, a nonfullerene acceptor PMI-F-PMI with a fluorene core and two PMI arms was reported. It presented a lift-up LUMO level around −3.54 eV, which matches well with that of P3HT donor to yield high V_{oc}. P3HT:PMI-F-PMI solar cells gave an efficiency of 2.3%, with a V_{oc} of 0.98 V, a J_{sc} of 5.61 mA/cm^2, and an FF of 42.0%[24]. Later, Li *et al.* used a polymer donor PTZ1, obtaining a PCE of 6.0%, with a V_{oc} of 1.30 V, a J_{sc} of 7.0 mA/cm^2, and an FF of 63.5%[25]. The favorable morphology, efficient exciton dissociation, balanced carrier mobilities, and reduced charge recombination also contributed to the increase of V_{oc}.

It is important to understand the effect of different aromatic core on the photovoltaic performance. In 2022, Scharber *et al.* developed a non-planar acceptor PMI-FF-PMI, consisting of two PMI units bridged with a dihydroindeno[1,2-b]fluorene unit. PMI-FF-PMI:D18 solar cells gave a PCE of 5.34%, with a V_{oc} of 1.41 V, a J_{sc} of 6.09 mA/cm^2, and an FF of 60.9%[26]. The 1.41 V V_{oc} is the highest record for solution-processed OSCs so far. Though producing a high V_{oc}, the cells presented a relatively large nonradiative voltage loss ($\Delta V_{oc}^{non\text{-}rad}$) of 0.25 V, which mainly resulted from the enhancement of spontaneous carrier generation and the decrease of charge carrier in CT state process[27]. More recently, Trimmel *et al.* developed three PMI dimers by changing the substitution position (para, meta or ortho) on the benzene ring. Compared with P-pPh-P and P-mPh-P and P_3Ph, P-oPh-P showed better solubility and device efficiency. With introducing two alkyl chains or alkoxy chains onto the benzene ring in P-pPh-P, three new PMI dimers were obtained, namely P-MePh-P, P-HexPh-P, P-DeOPh-P. P-HexPh-P and P-DeOPh-P with long chains exhibited higher crystallinity than P-MePh-P, and P-DeOPh-P with alkoxy chains presented a favorable face-on orientation as indicated by GIWAXS, which is beneficial to charge transport. As a result, PBDB-T:P-DeOPh-P cells offered a PCE of 3.17%, with a V_{oc} of 1.00 V, a J_{sc} of 7.46 mA/cm^2, and an FF of 43.0%[28]. Tuning the linking units is a simple approach to develop high-performance PMI-based acceptors.

In short, the V_{oc} and PCE for NF-OSCs can be enhanced *via* tailoring the molecular structures of NFAs and donors. In order to regulate the morphology of the blends, different aromatic cores were introduced into PMI-based acceptors. The LUMO energy levels should also be tuned to match that of

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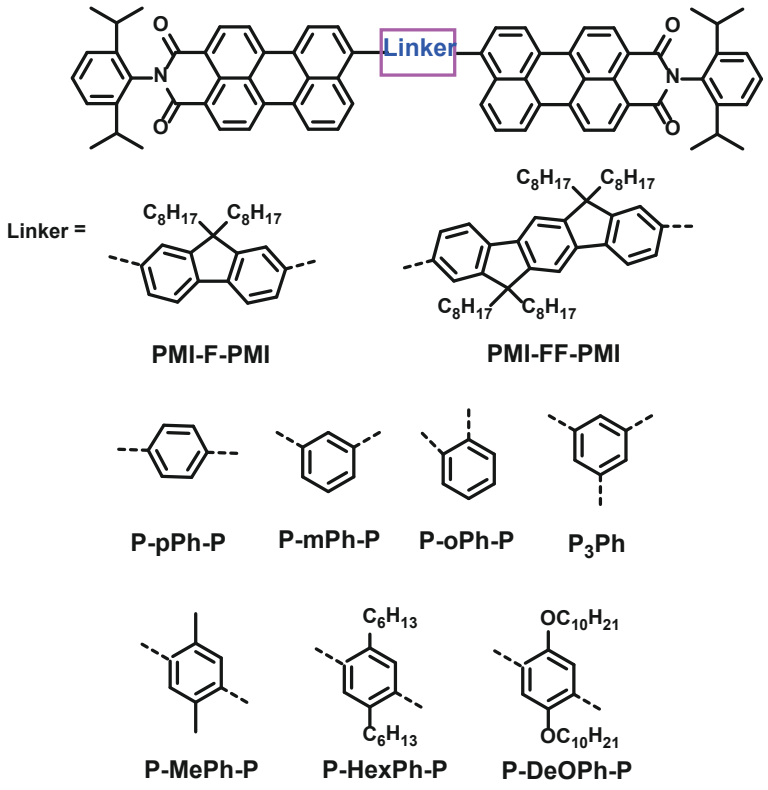

Fig. 1. The chemical structures for PMI-based non-planar acceptors.

Table 1. Materials energy levels and the performance for solar cells.

PMI acceptor			Polymer donor			V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)	Ref.
Name	LUMO (eV)	HOMO (eV)	Name	LUMO (eV)	HOMO (eV)					
PMI-F-PMI	–3.54	–5.74	P3HT	–2.74	–4.76	0.98	5.61	42.0	2.30	[24]
	–3.42	–5.50	PTZ1	–3.34	–5.31	1.30	7.0	63.5	6.0	[25]
PMI-FF-PMI	–3.74	–5.80	D18	–3.58	–5.62	1.41	6.09	60.9	5.34	[26]
P-oPh-P	–3.97	–6.38	PBDB-T	–3.41	–5.21	1.04	2.62	40	1.08	[28]
P3-Ph	–4.13	–6.22				0.69	1.70	46	0.54	
P-HexPh-P	–3.85	–6.40				1.12	9.97	46	2.02	
P-DeOPh-P	–3.92	–6.31				1.00	7.46	43	3.17	

the donors.

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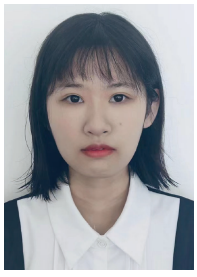

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