

Bright future of polymerizing small-molecule acceptors in realizing high performance all-polymer solar cells

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All-polymer solar cells (all-PSCs) are prepared with a sandwich device structure based on a binary blend of a polymer donor and a polymer acceptor (Fig. 1), and have attracted intensive research attention as a potential renewable photovoltaic technology [1,2]. As compared to the PSCs with small molecule acceptors (SMAs), all-PSCs show pronounced advantages of superior mechanical flexibility/stretchability and improved device stability [3,4]. Thus, they are more attractive for the applications in wearable and portable electronics. After the first report of the all-PSCs in 1995 using cyano-substituted polyphenylenevinylene as the polymer acceptor [5,6], researchers have focused their efforts on the design of new polymer acceptors, such as rylene diimide [7], B←N bridged bipyridine [8], and cyanobenzothiadiazole-based polymer acceptors [9]. However, before 2017, the power conversion efficiency (PCE) of the all-PSCs was limited by the weak absorbance of the polymer acceptors in the near-infrared region [10].

In 2017, Zhang et al. [11] from Institute of Chemistry, Chinese Academy of Sciences proposed a strategy of polymerizing small-molecule acceptors (PSMAs) to construct new-generation polymer acceptors with narrow-band-gap SMAs as the key building blocks copolymerized with different aromatic linking units (Fig. 1(b)). This strategy can inherit the merits of strong absorption from SMAs and potential advantages of good film forming ability, mechanical flexibility and high stability for polymers [2]. Thus, PSMAs hold tremendous potential for all-PSCs, and most importantly, it breaks the major bottleneck limiting all-PSCs, i.e., poor absorptivity in the near-infrared region [1].

Inspired by the advantages of PSMAs, intensive works

from different groups on designing new PSMAs were carried out, and great progress has been made in the all-PSCs. Generally, the PSMAs are designed with an A-D-A or A-DA'D-A SMA backbone (see Figs. 1(c, d)) copolymerized with a suitable conjugated linking unit (see Fig. 1(e)). For example, the extension of the conjugation of central D-unit of the SMA from tetracyclic core to pentacyclic core, usually results in the PSMAs with slightly red-shifted absorption for a broad photo responsive range [12]. Notably, the success of the A-DA'D-A type Y6 and its derivatives as SMAs in PSCs [13–15], also triggered their use as building blocks to construct efficient PSMAs [16–19]. By replacing the common used linking unit of thiophene with benzodithiophene, bithiophene, selenophene [19], bridged BT and flexible chain tethered thiophene, photophysical properties of the PSMAs can be tuned. It is worth noting that the using of electron-deficient bithiophene imide, producing PSMAs with improved n-type characteristics and suitable low-lying frontier molecular orbital levels [20]. Despite the remarkable progress, regioisomeric issue of the polymer chain is a limitation for a higher device efficiency. Regioregular PSMA can be obtained by carefully purifying the SMAs terminal A unit, producing improved crystallinity and electron mobility of the polymer acceptors thus higher device efficiency [21–23]. The photovoltaic performance of the PSMAs can also be improved by molecular weight control of donors, stepwise optimization strategy and ternary blend. Notably, the ternary blend approach has resulted in the first example of the all-PSCs with efficiency over 17% [24]. Moreover, flexible all-PSCs are also constructed, showing excellent morphological and mechanical stabilities [25]. With these encouraging results, it is believed that higher device efficiency over 18% can be realized by constructing flexible PSMA-based all-PSCs. Also, the followings are suggestions for realizing real application of the PSMA-based all-PSCs.

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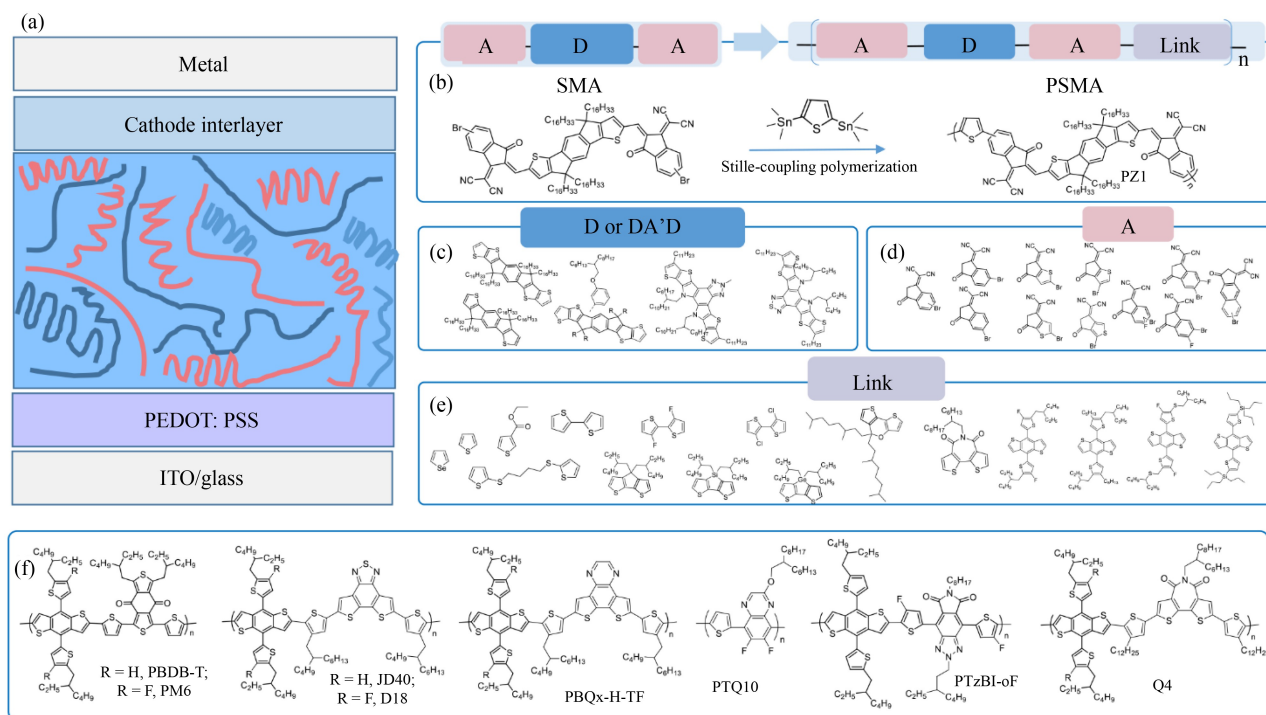


Fig. 1 (a) Device structure of all-PSCs; (b) schematic illustration of the strategy of PSMA along with (c–e) the building blocks used to construct PSMA; (f) typical polymer donors that working well with PSMA.

(1) The design of PSMA with a simple structure is greatly desirable to reduce the cost of their production. Previous studies highlighted the important role of proper molecular weights of PSMA in achieving high-efficiency all-PSCs. Thus, it is also desirable to develop greener and more effective synthetic routes to well control the molecular weights of PSMA. In general, the molecular structural diversity of polymer donors can provide more choices for device fabrication. In the PSMA-based all-PSCs, only a very few polymer donors are available. Typical examples are provided in Fig. 1(f), including benzodithiophenedione-based polymers (PM6 and PBDB-T), quinoxaline-based polymers (PTQ10 and PBQx-H-TF) [26,27], imide based polymers (Q4 and PTzBI-oF) [28,29] and benzothiadiazole based polymers (D18 and JD40) [30,31]. In addition, the pairing of the benzotriazole based polymer donors [32] with those newly developed PSMA is also very appealing to further increase their photovoltaic properties. Therefore, it is challenging and appealing to construct new polymer donors that can work well with the PSMA to realize higher PCEs.

(2) Single-component organic solar cells (SCOSCs) are under investigation with advantages of high stability and reduced complexity in device fabrication. With a PSMA approach, Min [33] and Ma [34] independently construct block copolymer based SCOSCs via a stepwise stille coupling reaction, producing high efficiency in the range 9%–11%. Higher morphological stability and lower energy loss were also observed in the reported SMOSC compared with the control binary blend devices.

However, the performance of the state-of-the-art SCOSC still lags significantly behind that of binary organic solar cells. Thus, under a PSMA approach, a lot of further efforts are necessary to develop tailor-made block copolymers with optimized donor/acceptor couples for SCOSCs. To realize a highly ordered film, a certainly high molecular weight of the individual blocks and a narrow molecular weight distribution are preferred. However, it is a great synthetic challenge using conventional synthetic methods to control weight distribution, such as Stille coupling reaction.

(3) Besides efficiency, mechanical robustness is crucial for the practical applications of all-PSCs in stretchable and wearable electronics. However, seldom efforts are made on the investigation of the correlations between the chemical structure of PSMA and the mechanical stretchability in the all-PSC devices [35]. Exploration of new chemical approach to design PSMA that can promote a high crack onset strain along with a suitable toughness in flexible device are highly desired.

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