Chinese Chemical Letters xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Chinese Chemical Letters

journal homepage: www.elsevier.com/locate/cclet

Review

Recent developments of di-amide/imide-containing small molecular non-fullerene acceptors for organic solar cells

He-Wei Luo [a], Zi-Tong Liu [b,*]

[a] Department of Material and Chemical Engineering, Zhengzhou University of Light Industry, Zhengzhou 450002, China
[b] Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

ARTICLE INFO

Article history:
Received 23 May 2016
Received in revised form 16 June 2016
Accepted 21 June 2016
Available online xxx

Keywords:
Diamide-containing small molecules
Diimide-containing small molecules
Non-fullerene acceptor
Organic solar cell
Donor-acceptor molecule

ABSTRACT

Non-fullerene organic solar cells have received increasing attentions in these years, and great progresses have been made since 2013. Among them, aromatic di-amide/imide-containing frameworks have shown promising applications. The outstanding properties of them are highly associated with their unique electronic and structural features, such as strong electron-withdrawing nature, broad absorption in UV–visible region, tunable HOMO/LUMO energy levels, easy modifications, and excellent chemical, thermal and photochemical stabilities. In this review, we give an overview of recent developments of aromatic di-amide/imide-containing small molecules used as electron acceptors for organic solar cells.

1. Introduction

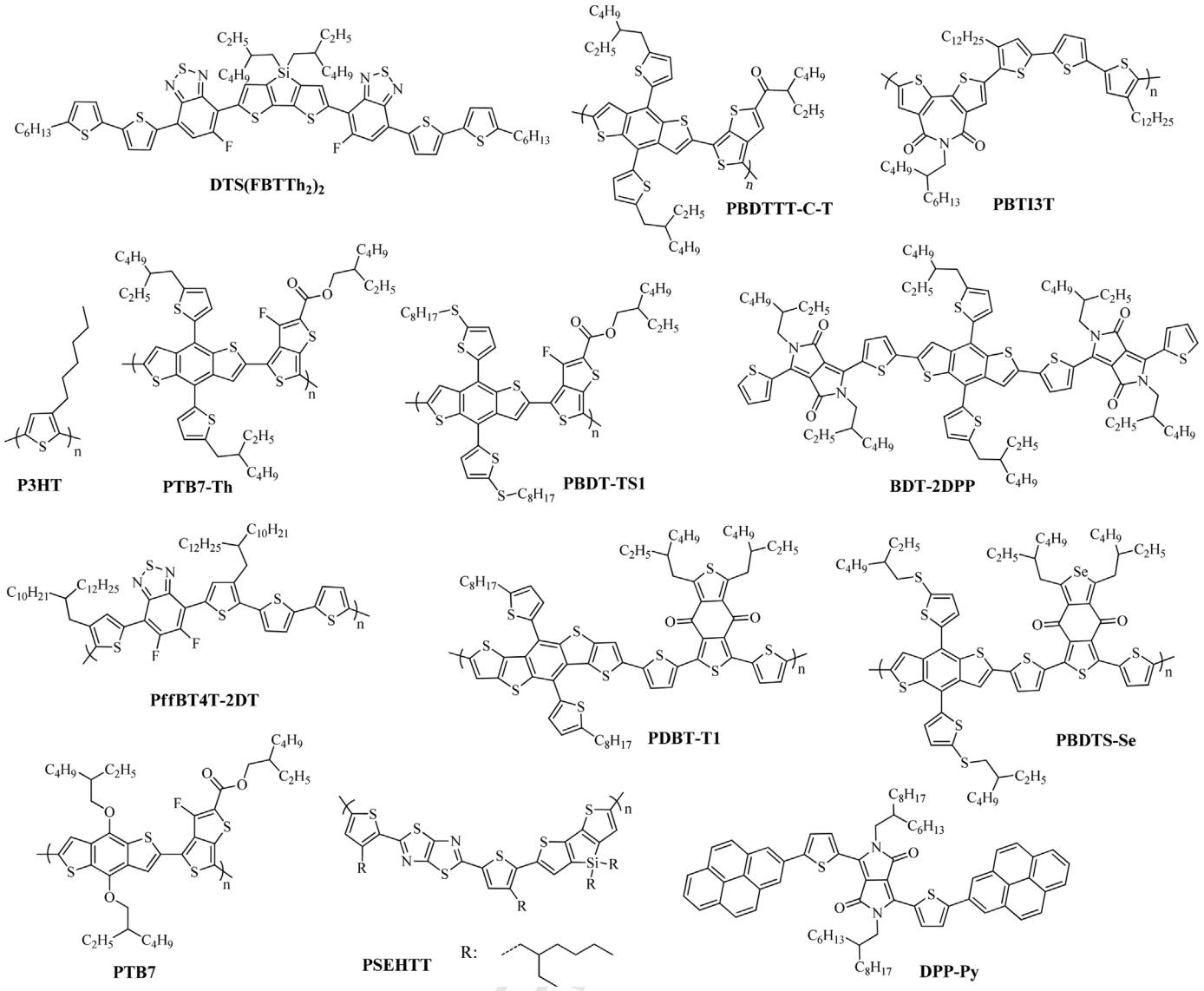
Solution-processed bulk heterojunction (BHJ) organic solar cells (OSCs) have received considerable attentions due to their low-cost, light-weight, flexibility and good compatibility with the roll-to-roll process for making large area devices [1]. Over the past ten years, extensive efforts have been focused on developing electron donor materials, such as low bandgap donor-acceptor small molecules, oligomers, especially polymers [2]. The bandgap, energy levels can be tuned, and absorption range can be broadened by varying the electron π-conjugated systems. Therefore high power conversion efficiencies (PCEs) above 10% have been achieved by blending the D–A polymers with [6,6]-phenyl-C_{71}-butyric acid methyl ester ($PC_{71}BM$) [3].

Compared to various of electron donor materials, the electron acceptors are still limited to fullerenes and their derivatives, particularly [6,6]-phenyl-C_{61}-butyric acid methyl ester ($PC_{61}BM$), $PC_{71}BM$ *etc.* [4]. However, invariable energy levels, limited absorption in the visible region, morphology instability, purity difficulty and high production cost have limited their further applications. Thus, non-fullerene organic acceptors have been widely studied during the past five years due to their diverse structures, tunable energy levels, good absorptions and ease of synthesis *etc.* [5]. High PCEs up to 11.21% has been achieved recently, which is comparable to fullerene-containing organic solar cells [6a].

Normally, non-fullerene organic acceptors should have broad and strong absorptions, suitable HOMO/LUMO energy levels, good solubilities and processabilities, and high electron mobilities. For this, conjugated electron push-pull structures are often used to construct non-fullerene acceptors, which could reduce the optical bandgap, extend the absorption and tune energy levels. For example, trifluoromethyl substituted or fluorinated pentacene derivatives, phthalocyanine drivatives, subphthalocyanine derivatives, quinacridone derivatives, imide derivatives and recently reported indacenodithieno[3,2-b]thiophene derivatives have been used as non-fullerene organic acceptors [5,6]. Among them, π-conjugated molecules with aromatic di-amide/imide-containing frameworks have shown promising applications, which have been widely studied in organic field effect transistors and donor materials in organic solar cells [7]. The outstanding properties of them are highly associated with their unique electronic and structural features, such as strong electron-withdrawing natures, broad absorptions in UV–visible region, tunable HOMO/LUMO energy levels, easy modifications, and excellent chemical, thermal and photochemical stabilities. In this review, we mainly focus on the recent developments of aromatic di-amide/imide-containing small molecules as electron acceptors for organic solar cells since 2013. The related electron donors including oligomers in this review, polymers are listed in Scheme 1.

* Corresponding author.
E-mail address: zitong_@iccas.ac.cn (Z.-T. Liu).

http://dx.doi.org/10.1016/j.cclet.2016.07.003



Scheme 1. Chemical structures of related electron donors in this review.

2. Aromatic di-amide-containing small molecular non-fullerene acceptors

Aromatic di-amide-containing conjugated materials usually possess planar and polar-ring structures, facilitating intermolecular interactions. Normally, the N-positions can introduce alkyl chains to fulfill the molecular solubilities. Additional electron π-motifs can be incorporated to tune the absorption intensities and ranges, energy levels and intermolecular interactions. The most commonly investigated non fullerene acceptors are based on diketopyrrolopyrrole (DPP) and isoindigo for the di-amide-containing conjugated molecules. Scheme 2 lists representative aromatic di-amide-containing small molecules reported in recent years, and Table 1 summarizes their non-fullerene OSC performances.

2.1. DPP-based small molecular non-fullerene acceptors

As a synthetic dye, DPP was first discovered in 1974 as a byproduct [8]. The excellent photophysical properties (molar extinction coefficient is up to 25,000 L mol^{-1} cm^{-1} in solutions), high thermal and photo stability have attracted more and more attentions since then. Nowadays, DPP and its derivatives have been widely investigated in organic semiconductors including field effect transistors [9] and solar cells [10], and even chemo/bio-sensors [11].

Normally, DPP-unit is end-capped with thiophenes, called dithienyl-DPP. It owns planar structure because of the hydrogen bonding between oxygen atoms in the DPP units and β-hydrogen atoms of the neighboring thiophenes, which can induce strong intermolecular interactions. The LUMO/HOMO energy levels of dithienyl-DPP is −3.4/−5.3 eV. To fulfill the condition of efficient exciton separations, higher LUMO energy levels above −3.1 eV of conjugated materials could only be used as electron donors (P3HT is normally used, see Scheme 1). For that, DPP is usually attached to another DPP unit or other conjugated units, which could not only lower the LUMO energy levels, but also extend the UV-vis absorption to longer wavelength. Thus the reported DPP-based non-fullerene acceptors are consisted of at least two DPP units [12–20]. According to the molecular configurations, they can be divided into linear, two-dimensional (2D) and three-dimensional (3D) structures. The structures are shown in Scheme 2 and the data are collected in Table 1.

Please cite this article in press as: H.-W. Luo, Z.-T. Liu, Recent developments of di-amide/imide-containing small molecular non-fullerene acceptors for organic solar cells, Chin. Chem. Lett. (2016), http://dx.doi.org/10.1016/j.cclet.2016.07.003