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Review

The impact of regiochemistry of conjugated molecules on the performance of organic electronic devices

Qi Cheng Zhang^{a,b}, Xiao-Zhang Zhu^{a,*}^a Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China^b University of Chinese Academy of Sciences, Beijing 100049, China

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ABSTRACT

Organic photovoltaics and field-effect transistors have attracted considerable attention due to the easy fabrication, low cost, light weight, and flexibility. Unsymmetrical conjugated building blocks are widely utilized for the design of new organic π -functional materials in order to achieve high-performance electronic devices, which has become a hot research topic in recent years. In this review, we summarized some typical organic π -functional materials with regioregular conjugated backbones with unsymmetrical electron-deficiency moieties and focused on the influence of regiochemistry on the final device performance.

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1. Introduction

During the last two decades, organic photovoltaics and field-effect transistors based on conjugated π -functional materials have attracted considerable attention due to their potential advantages of easy fabrication, low cost, light weight, and high flexibility [1]. For bulky-heterojunction organic photovoltaics (OPVs), rational design of donor materials in the active layer is recognized as the most effective way to push up power conversion efficiency (PCE). Generally speaking, the ideal donor material should have a suitable optical bandgap with a wide absorption in the visible and near-infrared region, the suitable highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels, a coplanar molecular structure with proper solubilizing substituents, which in combination can lead to a high open-circuit voltage (V_{oc}) [2], short-circuit current (J_{sc}), and fill factor (FF) [3,4]. Meanwhile, organic semiconductors also require suitable frontier orbital energy levels and proper packing mode for the realization of high-performance ambient-stable OFETs [5].

The regiochemistry of conjugated molecules have been confirmed to be crucial in the development of organic π -functional

materials. As regioregular polythiophenes, poly(3-alkylthiophene) (P3HT) as the most typical example, showed highly ordered thin-film morphology, people started to notice the important influence of regiochemistry on the performance of electronic devices about 25 years ago [6]. Indeed, regioregular P3HT exhibited better performance both in OPVs and OFETs than that of regiorandom counterpart [7]. Recently, it has been found that the introduction of some unsymmetrical conjugated building blocks into conjugated backbones may significantly improve the device performance [8]. Especially, the unsymmetrical electron-deficiency moieties could effectively regulate HOMO and LUMO energy levels and packing modes in thin films. In this short review, we will summarize some of the recent applications of unsymmetrical electron-deficiency moieties and the positive influence of structural regioregularity on OPV and OFET devices.

2. Unsymmetrical moieties related to nitrogen

For organic solar cells, the proposed “ideal” conjugated donor materials should exhibit a low HOMO energy level of -5.4 eV and a small bandgap of 1.5 eV [9] in order to better match the most commonly used electron acceptors, fullerene derivatives. Nitrogen atom has been frequently utilized to replace carbon atom of electron-deficiency moieties to optimize the photoelectric properties, which may help establish a comprehensive understanding

* Corresponding author.

E-mail address: xzzhu@iccas.ac.cn (X.-Z. Zhu).

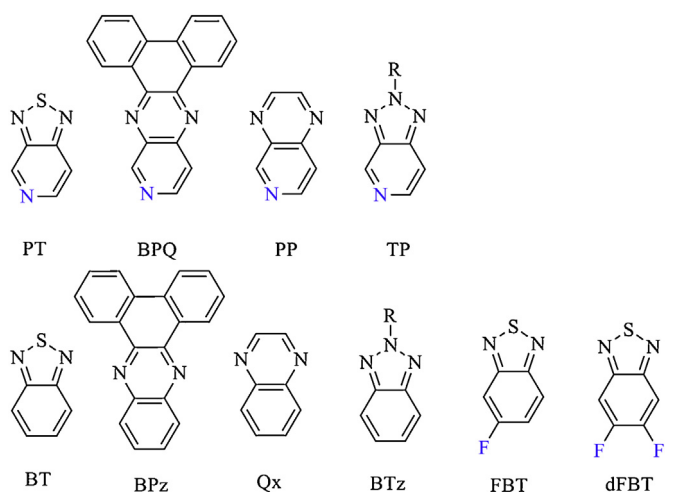


Fig. 1. Chemical structure of benzene- or pyridine-based electron-deficiency moieties.

on the structure-property relationships. By replacing the benzene ring of 2,1,3-benzothiadiazole (BT), dibenzo[*a,c*]phenazine (BPz), quinoxaline (Qx), and 2*H*-benzo[*d*][1,2,3]triazole (BTz) with

pyridine, [1,2,5]thiadiazolo[3,4-*c*]pyridine (PT), dibenzo[*f,h*]pyrido[3,4-*b*]quinoxaline (BPQ), pyrido[3,4-*b*]pyrazine (PP), and 2*H*-[1,2,3]triazolo[4,5-*c*]pyridine (TP) (Fig. 1) become more electron-deficiency moieties and can be utilized for the design of low-bandgap (LBG) materials with low HOMO energy level [8]. Compared to their benzene counterparts, those pyridine-based materials normally showed better PCEs. For instance, the PCE of **1b** [10] was significantly higher than that of **1a**, 6.7% vs. 0.18% [11], which can be attributed to its wider absorption band, better crystallinity, and higher carrier mobility. Similarly, compound **2b** showed a higher PCE, 3.15% than **2a**, 1.73% in a planar heterojunction device: ITO/C₆₀/donor/Di-NPB/Di-NPB:NDP9/NDP9/Au [12], which was attributed to the better stacking in the solid state. This phenomenon is also observed in polymer solar cells. Quite a few PT-based polymers have delivered considerably high PCEs. Compared with **3a**, 3.75%, regiorandom polymer **3b** exhibited slightly higher PCE 3.93% with the same device configuration [13]. C.-G Wu and co-authors discussed the difference of polymers **4a** and **4b** without/with nitrogen and found that **4b** had better planarity and stronger intermolecular stacking. Thus, the PCE of benzene-based polymer **4a** was 2.45% which is smaller than that of pyridine-based **4b**, 4.40% [14]. W. You and co-authors designed and synthesized three different PT-based polymers **5a**, **5b**, and **5c**, and the PCEs of 6.20%, 5.57%, and 6.32%

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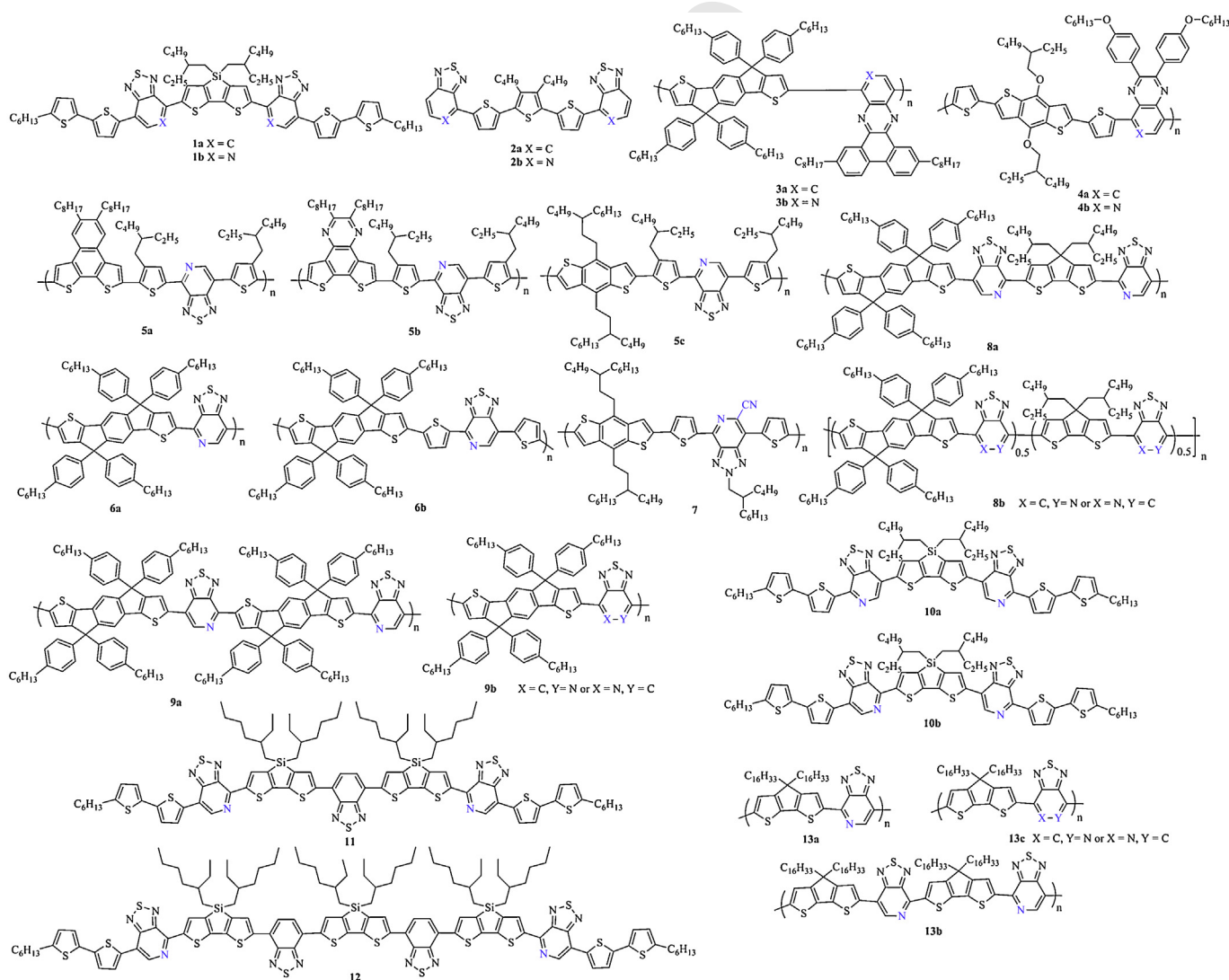


Fig. 2. Chemical structure of 1-13.

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