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New amorphous small molecules—Synthesis, characterization and their application in bulk heterojunction solar cells

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ABSTRACT

We successfully synthesized a series of novel solution processible small molecules (2TAPM, 4TAPM and 2BTAPM) consisting of electron-accepting unit (2-pyran-4-ylidenemalononitrile) (PM) and electron-donating unit (Triphenylamine and different thiophene units). Differential scanning calorimetry (DSC) measurement indicates that these small molecules are amorphous. UV–vis absorption spectra show that the combination of PM with moieties having gradually increased electron-donating ability results in an enhanced intramolecular charge transfer (ICT) transition, leading to an extension of the absorption spectral range and a reduction of the band gap of the molecules. Both cyclic voltammetry measurement and theoretical calculations show that the highest occupied molecular orbital (HOMO) energy levels of the molecules could be fine-tuned by changing the electron-donating ability of the electron-donating moieties. The bulk heterojunction (BHJ) photovoltaic devices with a structure of ITO/PEDOT:PSS/small molecules:PC₇₁BM/LiF/Al were fabricated by using the small molecules as donors and (6,6)-phenyl C₇₁-butyric acid methyl ester (PC₇₁BM) as acceptor. Power conversion efficiencies of 1.76% and 2.47% were achieved for the photovoltaic devices based on 2TAPM:PC₇₁BM and 4TAPM:PC₇₁BM under simulated air mass 1.5 global irradiation (100 mW/cm²), respectively.

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1. Introduction

Photovoltaic devices based on organic semiconductors are evolving into a promising cost-effective alternative to the silicon-based solar cells due to their low-cost fabrication through solution processing, light weight, as well as excellent compatibility with flexible substrates [1]. According to theoretical models [2], devices based on these materials are predicted to reach a power conversion efficiency (PCE) close to 10%. Up to date, the highest PCE of the bulk heterojunction (BHJ) polymer photovoltaic devices has been up to 7.73% [3]. It can be seen that there is still a gap between the practical efficiency and the theoretical one. Therefore, it is critically important to design and synthesize new donor or acceptor materials for achieving higher PCE.

Generally, organic polymers possess the advantages of strong absorption ability, admirable solution processability, good film-forming ability [4] and tunable energy levels. However, the purification of polymers is one of the most difficult problems. For example, it is very difficult to separate the Pd-catalyst from the polymer [5]. As usual, a polymer is a mixture of molecules with different molecular weights. The impurity and relatively

high dispersity of molecular weight would significantly decrease the charge carrier mobility of polymers and further lead to relatively low fill factor (FF) and PCE in the resulting photovoltaic devices [6]. In contrast to polymers, small molecules have attracted more and more attention for photovoltaic applications due to their high purity, high charge carrier mobilities (15 cm²/V s) [7], solution processability, well-defined molecular structures and definite molecular weights.

Recently, profound progress has been achieved in the synthesis of new solution processible small molecules and corresponding photovoltaic applications [8–17]. Although the highest PCE of solution processed bulk-heterojunction photovoltaic devices based on small molecules has reached 4.4% [17], the mismatch between the absorption spectrum of small molecules and the solar spectrum is still one of the primary problems for improving PCE of photovoltaic device. Therefore, more attention is being directed to the design and synthesis of small molecules with donor–acceptor (D–A) structure [8,9,15–22]. The intramolecular charge transfer (ICT) from the donor moiety to the acceptor moiety inside a D–A molecule can efficiently extend the absorption spectrum of the molecule for better matching the solar spectrum. Moreover, the incorporation of electron-withdrawing moiety with different electron-donating moieties will bring different ICT degrees to the conjugated moieties and thus provide a means to tune their energy levels [27,23].

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It has been demonstrated that conjugated small molecules (such as oligothiophene) are usually apt to crystallize and, thus, are difficult to form a uniform film by solution process [25,26]. One effective way to increase the film forming ability of small molecules is to construct amorphous small molecules by introducing triphenylamine(TPA) into the structure [8–10]. The resulting amorphous small molecules possess isotropic optical properties and excellent film-forming ability, which increases the absorption cross section for the incident light as well as the charge transport efficiency through the active layer [27–29]. Furthermore, TPA possesses a high oxidation potential, and thus a high V_{oc} could be expected. Due to the advantages of TPA based small molecules, a series of amorphous small molecules have been synthesized and applied to the organic bulk heterojunction solar cell as donor materials in recent years [8–10,18,21,27–29]. Up to now, the highest PCE for this kind of small molecules has reached 2.39% [21].

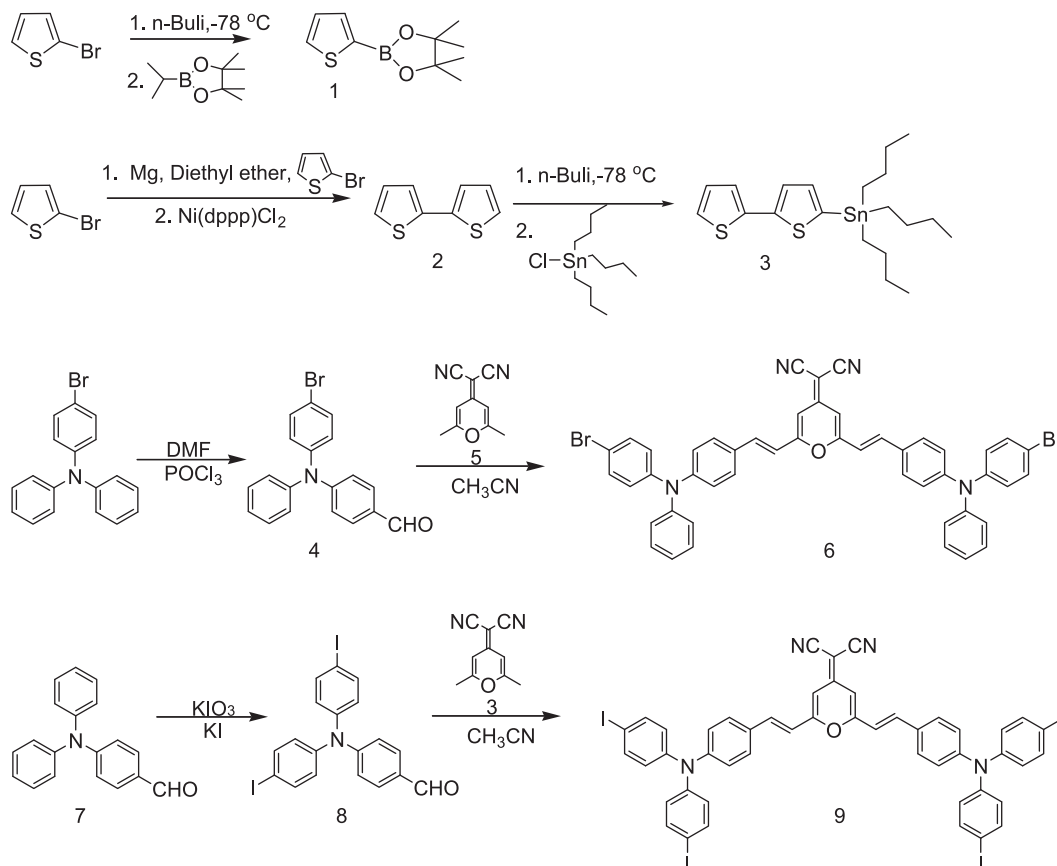
In this paper, we report three new solution processable D–A small molecules (2TAPM, 4TAPM and 2BTAPM) containing of 2-pyran-4-ylidenemalononitrile(PM) as electron-accepting moiety, triphenylamine and different thiophene units as electron-donating moieties. 2-pyran-4-ylidenemalononitrile is a strong electron-accepting group, which can increase the electron affinity and reduce the band gap of the conjugated system when combined with strong electron-donating moieties [8,9,23]. Triphenylamine was introduced into the molecule in order to increase the electron-donating ability, high-dimensionality and hydrotropy [30–32]. And thiophene units as well as the increased oligothiophene length can provide stronger light absorption and promote better π – π stacking/aggregation of small molecules leading to a small energy band gap and a broader absorption spectrum [28]. DSC measurement indicates that these small molecules are

amorphous. The normalized UV–vis absorption spectra showed that 4TAPM exhibited higher molar absorption coefficient and optical density ($70,900 \text{ M}^{-1} \text{ cm}^{-1}$ and $3.60 \times 10^{-3} \text{ nm}^{-1}$, respectively) than that of 2TAPM ($57,600 \text{ M}^{-1} \text{ cm}^{-1}$ and $2.18 \times 10^{-3} \text{ nm}^{-1}$). Both cyclic voltammetry measurement and theoretical calculations show that the highest occupied molecular orbital (HOMO) energy levels of the molecules could be fine-tuned by changing the electron-donating ability of the electron-donating moieties. The bulk heterojunction photovoltaic devices were fabricated by using small molecules (2TAPM or 4TAPM) as donor and PC₇₁BM as acceptor. A high short-circuit current density of 7.86 mA/cm^2 and PCE of 2.47% were achieved for 4TAPM:PC₇₁BM under simulated air mass 1.5 global (AM 1.5 G) irradiation (100 mW/cm^2). This PCE of 2.47% is among the top values for the solution-processed amorphous small molecule-based organic solar cells reported so far.

2. Experimental

2.1. Materials

All reagents and chemicals were purchased from commercial sources (Aldrich, Across, Fluka) and used without further purification unless stated otherwise. All solvents were distilled over appropriate drying agent(s) prior to use and were purged with nitrogen. Compound 2, 5 and 7 were synthesized according to literature procedure.[23,33,34] The synthesis routes and molecule structures (2TAPM, 4TAPM and 2BTAPM) are shown in Schemes 1 and 2, respectively.



Scheme 1. Synthetic routes of compounds.

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