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Review

High efficiency small molecule-based donor materials for organic solar cells

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ABSTRACT

Organic photovoltaic (OPV) materials, especially small molecule donor materials (SMDMs) have enormous potential to revolutionize the solar energy sector. However, to be a viable alternative to the polymer donor counterparts, SMDMs must have high power conversion efficiency (PCE). A large number of different SMDMs have been reported, which have crossed the 10% threshold of the PCE for commercialization. In this review, we present the SMDMs that have been developed in recent years capable of generating moderate to high-efficiency photovoltaic devices. The steady rise in the variety of materials and PCE values in recent years, point to a bright future for SMDMs as solar energy materials.

1. Introduction

Solar energy is one of the most powerful alternatives to non-renewable fossil fuels. Unfortunately, we are unable to harness the full potential of the solar energy, partially due to engineering challenges and largely due to the lack of efficient photovoltaic (PV) cells, which convert sun light to electrical energy. Based on the solid-state electronic material system used, a PV cell can be divided into crystalline elemental (silicon), organic, thin-film (CIGS, CdTe, amorphous Si) or hybrid [1]. At present, the PV market is dominated (> 90%) by the crystalline, polycrystalline and amorphous inorganic materials based solar cells [2]. Despite the fact that these solar cells (SCs) have excellent light to electricity conversion ability, their high manufacturing cost, slow manufacturing, sensitivity to impurities, low-flexibility, etc. pose significant challenges to the industrial and individual consumers [3]. To overcome these challenges, organic photovoltaic (OPV) cells emerged as a promising alternative. Organic semiconductors are conjugated materials that conduct electricity when they reach sufficient number of alternating single and double bonds and have conductivity between a metal and an insulator (10^{-9} to $10^{3}\ \Omega^{-1}\ cm^{-1}$) [4]. Organic materials have several advantages over inorganic semiconductors like high absorption coefficient and broad absorption range, which can be tuned by chemical functionalization. The easy functionalization of organic semiconductors is a prime advantage that surpasses all advantages of inorganic semiconducting materials. The last decade witnessed a tremendous rise in the development of the OPVs with a high power conversion efficiency (PCE) [5] using organic donor material. Although the value is lower than their inorganic counterparts, it's sufficient for use, which is set at 10% [6].

Based on the type of molecular system used, OPV is divided into two classes: polymer-donor solar cells (PDSCs) and small molecule-donor solar cells (SMDSCs). Interestingly, the efficiency of SMDSCs have increased considerably from 0.001% in 1975 [7], through 1% in 1986 [8] to > 11.3% in 2017 [9,10], which is very close to the highest value obtained by any OPV cells (PDSCs ~ 13%) [11]. This incredible rise in performance has been possible due to several advantages offered by the SMDMs, e.g., synthetic ease, synthetic reproducibility with high purity, discrete molecular weight, well defined molecular structure, low weight and cost, mechanical flexibility, suitability for large area applications and high charge carrier mobility, etc. [12–14]. Considering the importance of this rapidly developing field, we present herein the progress made in recent years in the development of SMDMs for OPV. Fig. 1 depicts result generated by Web of Science when searched for the term "Organic Small Molecule Solar Cells" during the time interval of 2010–2017. A total of 553 articles have been published since the beginning of 21st century, which is still on the rise. Furthermore, citation related to this topic has also grown tremendously. Both PDSCs and SMDSCs have been reported in the literature. In the succeeding sections, attempts have been made to discuss progress made in the development of SMDSCs for OPV.

2. Performance parameters of solar cells (SCs)

There are many excellent articles and books which chronicles the structure and mechanism of PV devices [15–20]. We herein discuss briefly the performance parameters that are required for characterizing SCs. Generally, the OSCs are characterized under a 1000 W/m^2 light with the spectrum matching that of the sun on the earth's surface at an

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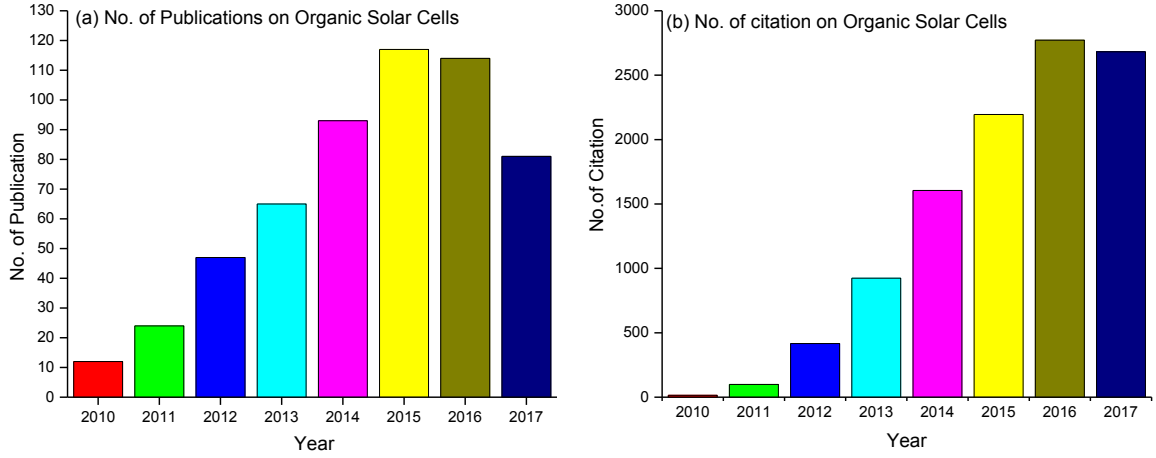

Fig. 1. Histogram showing the number of scientific publications contributing to the subject "Organic SC(s)" by the year. The period was **2010–2017** and the keyword was "Organic Small Molecule Solar Cells". Search done through ISI, Web of Science.

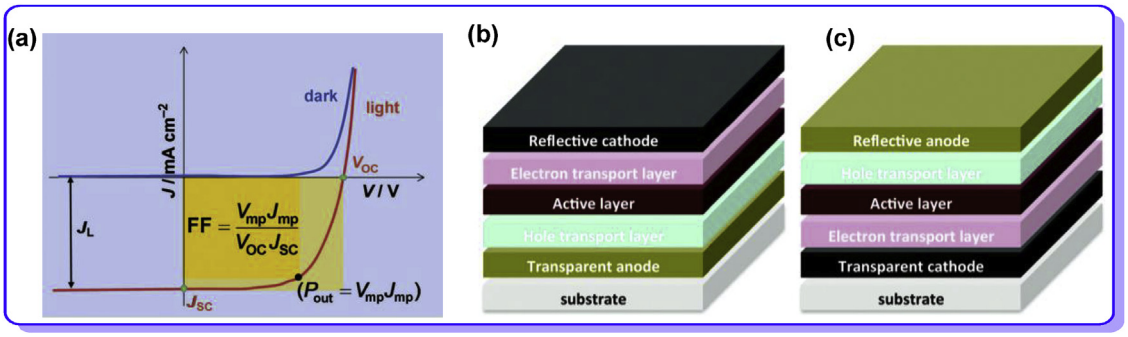

Fig. 2. (a) A typical current-voltage *J-V* characteristics of solar cells. (b) standard architecture of bulk-heterojunction (BHJ) and (c) inverted structure. Reproduced with the permission of Ref. [17] and [30].

incident angle of 48.2° (called the AM 1.5 spectrum) [21]. A typical current–voltage (I-V) curve of a SC in the dark and under illumination are shown in Fig. 2a along with the structures of standard PV cells (Fig. 2b and c). In the dark, there is almost no current until the forward bias for voltages is larger than the open circuit voltage (V_{OC}). Under illumination, the SCs start generating power which is recorded with a source meter. For characterization of any SC, the key parameter is the PCE, which is the ratio of the maximum electrical power (P_m) generated by the device to the total incident optical power (P_{in}) (equation (1)). P_{in} is given by the spectral intensity matching the sun's intensity on the Earth at an angle of 48.2° (equivalent to AM 1.5 spectrum) [22].

$$\eta_e = \frac{P_m}{P_{in}} \times 100 = \frac{V_{OC} \times I_{SC} \times FF}{P_{in}} \times 100 \quad (1)$$

The term V_{oc} in Eq. (1) is defined as the potential at which current is zero and depends on HOMO and LUMO energy level difference of the donor (D) and acceptor (A). Therefore, the V_{oc} of the SC can be increased either by reducing the HOMO level of the donor or increasing the LUMO level of the acceptor material. The second term in Eq. (1) J_{sc} is a maximum generated photocurrent density. As the band-gap of the material decreases, the value of J_{sc} increases and can be affected by the electron and hole transport efficiency of the active material [23]. The third term is the fill factor (FF) and is defined as the ratio of observed maximum power output to the theoretical power output. Maximum power output is given by P_m (= I_m x V_m), and the theoretical output is the product of J_{sc} and V_{oc}, therefore, the FF can be defined by Eq. (2).

$$FF = \frac{J_{MP} \times V_{MP}}{J_{SC} \times V_{OC}} \quad (2)$$

The FF suggests how swiftly the charges can be removed from the cells and in an ideal case the value is 1.0. There are a number of factors that can affect the FF of SCs and they often interact in intricate ways. The series resistance (R_s), parallel resistance (R_{sh}) are two other important factors that affect the FF and performance of SCs. The physical phenomena governing J_{sc} [24,25] and V_{oc} [26–28] have been well documented. However, factors affecting the FF is still not so clearly understood [29].

3. SMDMs–based photovoltaics

Several reviews have chronicled the progress made on SMDMs–based PV cells [30,31]. Herein we have reviewed only very recent articles with moderate to high PCE.

3.1. Oligothiophene-based SMDMs

During the literature survey, we noted that most of SMDMs are based on electron-rich thiophene units, supporting the importance of this heterocyclic core in materials science. Sulphur containing heterocycles such as simple thiophene, fused and non-fused oligothiophenes, and their derivatives are commonly employed as electron-donor units. The electronic properties and bulk-heterojunction (BHJ) SC parameters of some recently reported oligothiophene based SMDMs are summarized in Table 1. The results indicate that structurally simple SMDM molecules are potential candidates as donor for achieving highly efficient OSCs. Liu et al. [32] reported an oligo-thiophene (n = 7) based small donor **1** (Chart 1) composed of 3-octylthiophene as the central donor decorated with 3-ethylrhodanine at the periphery. The electron withdrawing nature of 3-ethylrhodanine created a strong donor-acceptor (D-A) interaction within the oligomer, leading to absorption in