



Properties of functional layers in inverted thin film organic solar cells



Saheed O. Oseni, Genene Tessema Mola*

School of Chemistry & Physics, University of KwaZulu-Natal, Pietermaritzburg Campus, Private Bag X01, Scottsville 3209, South Africa

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ABSTRACT

Thin film organic photovoltaic cell (TFOSC) is increasingly becoming an alternative solar energy converter and offering several potential advantages over inorganic molecules based devices. Tremendous research progresses have been made on the realization of TFOSC in the last two decades. Despite intensive research efforts towards reaching the required 10% power conversion efficiency (PCE) threshold, the device environmental stability and the constant requirement for high vacuum top metal electrode deposition still remain the major challenges. One of the encouraging findings in terms of alternative device architecture that caters for these challenges is the inverted device architecture of polymer solar cells. This review covers recent progress and approaches that have been achieved to improve device performance due to the changes in properties and structures of the constituent layers such as electrodes, active layers and buffer layers of the inverted organic solar cell.

1. Introduction

The introduction of silicon based solar cells made the generation of large scale useful electricity from solar energy possible. The foundation laid down for device preparation and characterization since the inception of silicon based solar cell has steadily been improved and employed in the development of new technologies [1,2]. However, the cost of device fabrication and industrial waste opens up the search for new materials as photon harvesting medium. The discovery of conducting polymer offered a new medium of solar absorber which has been driven by the demand for cleaner and more affordable energy sources. In the 1970s, the first organic molecules based solar cell (OSC) was fabricated using polyacetylene doped with halogens [3,4]. Since then a number of other conducting polymers and various device structures were tested to achieve environmentally stable and high performing thin film organic solar cell. Tang, in the 1980 s, presented the first bilayer organic photovoltaic cell [5], an idea borrowed from the concept of p-n junction. Later, more and more approaches were introduced into the field of organic photovoltaic (OPV) including the novel concept known as bulk-heterojunction design, dye-sensitized solar cells and recently a new generation of perovskite solar cells are under intense investigations [6–14].

The discovery of ultrafast electron transfer between donor and fullerenes in a blend of the molecules makes a new devices structure called bulk-heterojunction (BHJ) possible [10,12]. Despite the breakthrough that BHJ design has brought in terms of overcoming the challenges of the short exciton diffusion length and the efficient dissociation of photon-generated excitons at the donor/acceptor inter-

faces, the reported power conversion efficiency is still very low. This is due to poor charge transport properties of the conjugated polymers and energy loss during charge transfer process at the donor/acceptor (D/A) interfaces. However, significant progress have been achieved in terms of attaining high PCE by various investigators via different optimization approaches [1–20]. As early as the year 2000 s P-phenylene vinylene (PPV) based polymer solar cells were fabricated with PCE around 3% [15,16]. In spite of improved PCE in PPV based solar cells the molecule became less attractive for OSC because of its narrow optical absorption band and poor charge carrier mobilities. The introduction of poly (3-hexylthiophene) (P3HT) alongside the fullerene derivatives renewed the prospect of attaining higher PCE which ultimately leads to the achievement of large scale OSC device fabrication [17,18]. The use of clean room in device preparation and various mechanisms to control morphology of the active layer led to enhanced power conversion efficiencies between (4 to 5)% for P3HT:PCBM blend [18–23]. Generally, in TFOSC the device architecture and the choice of inter-layer material play an important role in the overall device performance. For instance, the interface instability caused by acidic nature of Poly(3,4 ethylenedioxythiophene):poly(styrenesulfonate) PEDOT:PSS [24] and the formation of insulating layer due to oxidation of hot metal atoms for cathode electrode reduces the performance of TFOSC [25]. In order to cater for these challenges, the inverted device architecture (IDS) was introduced with the view to improve interface stability so as to reduce photoactive layer degradation and increase device performance [26–30]. Since its introduction, in 2005, the inverted device structure has been given tremendous research attention because of its better power conversion efficiency, stability and compat-

* Corresponding author.

E-mail address: mola@ukzn.ac.za (G.T. Mola).

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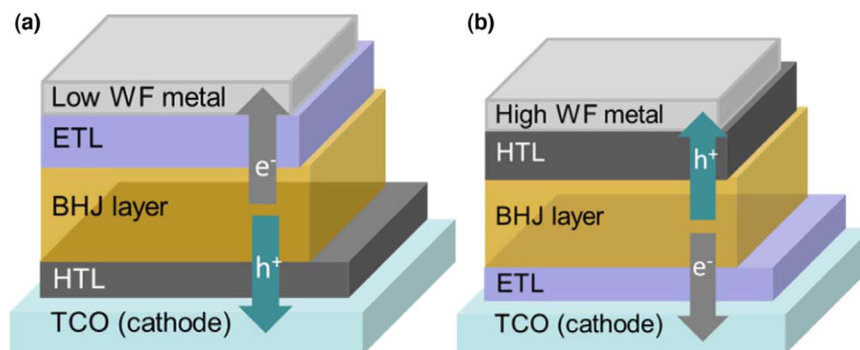


Fig. 1. General device architecture for (a) Conventional organic solar cell and (b) Inverted organic solar cells (Ref. [31]).

ibility with roll-to-roll manufacturing procedure compared to the standard device architecture.

This review focuses on the recent research progress on inverted polymer solar cells with a view of unveiling the developments achieved on the various layers of the device structure which include the electrodes, the photoactive layers and the buffer layers. Furthermore, the article discusses the different approaches that have been employed to enhance the effectiveness of each layer by way of improving the processes of light absorption, exciton dissociation, charge transport and collection.

1.1. Overview of inverted organic solar cell

Inverted thin film organic solar cell can be fabricated either on glass or flexible plastic substrates coated with transparent conductive metallic oxide (TCO). The term inverted is presumably used to refer the opposite directional flow of charges in the device compared to the conventional BHJ structure (see Fig. 1) [30]. However, the inverted structure offers a number advantages over the conventional one, for instance, it shows better device environmental stability under ambient condition because of the exclusion of low work function cathodes as well as acidic and corrosive hole transport buffer layer known as PEDOT:PSS. The later are often regarded as the main source of device instability in organic solar cells. The inverted structure also provides the possibility of re-positioning peak optical density of the incident light to the most photosensitive part of the device which allows better photon harvesting in the photoactive medium. Inverted structure creates better Ohmic contacts with active layer which allows efficient collection of photon-generated charges and improved device performance. The most efficient bulk-heterojunction organic solar cells reported so far were fabricated in inverted structure (see Table 1, 2 and 3).

The popular transparent conductive metal oxide, Indium tin oxide (ITO), can be used both as anode or cathode in the preparation of TFOSC depending on the nature of the device structure (Table 1). The ITO's work function that lie between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of most common conjugated polymer molecules which makes it a suitable electrode for fabrication of organic solar cell regardless of the device architecture [31]. Inverted device architecture employs ITO as the cathode while the conventional architecture uses it as an anode. Furthermore, low work function alkali compounds such as (TiO_x, ZnO etc) are used as cathode buffer layer in IDS as opposed to LiF layer in conventional structure. PEDOT:PSS is the mostly used and extensively reported anode buffer layer in the conventional architecture of the OSC(s). Similarly, the most common anode buffer layers in an inverted structure are (e.g. MoO₃, V₂O₅, or PEDOT:PSS etc.) (Table 3) followed by Ag or Al electrode for the fabrication of efficient and environmentally more stable organic solar cell [26,32,33].

2. Photoactive layer

The photoactive medium of a bulk-heterojunction organic solar cell is a critical component of the device for photons to charge carriers conversion through the process that involves light absorption, exciton generation, excitons diffusion into the interfaces leading to charge separation and transport. These constitute more than 90% of the overall processes of conversion of solar energy into useful electricity via TFOSC. It is to be noted that the photoactive layer of the bulkheterojunction design comprise of conjugated polymer donor and fullerene derivative acceptor molecules blend. However, the choice of the polymer molecules and fullerene derivatives in the preparation of BHJ need to satisfy certain criteria for effective generation and transportation of charges. Some of the factors that influence the choice of donor and acceptor molecules in BHJ design are the HOMO-LUMO levels of the molecules that need to match with the work-function of the metal electrodes. The optical absorption band of the donor molecules required to be wide enough to be able to absorb as much incident radiation as possible, especially, in high intensity emission regions such as visible and infrared wavelength ranges of the solar spectrum. High charge carrier mobility, well-tuned molecular energy levels, solubility in various organic solvents amongst others are the necessary conditions for organic molecules to serve as medium for solar energy conversion. Researchers have synthesized various types of conjugated organic molecules and fullerene derivatives for potential application as photoactive medium of TFOSC; some of the most known molecules are discussed in the following sections.

2.1. Donor conjugated polymers

The most popular group of conjugated polymer used in the preparation of organic solar cell are Polythiophenes, Thienothiophene and 2,1,3-Benzothiadiazole (BT). The polythiophenes and its derivatives are the main source of electron donor conjugated polymer that have attracted high research interest for photovoltaic applications. Among the polythiophene, P3HT molecules are often utilized in the fabrication of both conventional and inverted organic solar cells than any other conjugated polymer to date. P3HT has been intensively investigated by researchers because of it's stability in ambient environment, solubility in several organic solvents and the simplicity of its chemical structure allow computational modeling for detail investigations of the behavior of the molecule (see Fig. 2). As a consequence P3HT together with fullerene derivatives has been employed to produce efficient and stable inverted organic solar cell both on glass and flexible substrate [34–37]. Another major category of donor conjugated polymer that showed high overall performance in inverted OSC is the Thienothiophene derivatives. This is a system of low band gap polymers constituted by Benzo[1,2-b;4,5-b] dithiophene (BDT) and the thienothiophene (TT) alternating units. They found much application both in the conventional and inverted solar cells fabrication due to their tunable molecular energy levels, high hole mobility, impressive

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