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The challenges of using block copolymers for organic solar cells and identifying the most suitable approaches

Zefeng Huang

University of Warwick, Coventry, United Kingdom, CV4 7AL

U2096611@live.warwick.ac.uk

Abstract. For organic solar cells, a variety of materials are employed, including homopolymer donors and D-A copolymer donors. Organic solar cells are made from Pb (or Sn) halide perovskites, although they have some flaws. A mineral that resembles salt and is present in Pb perovskites quickly dissolves in moisture or water. It may have an impact on your health. The instability of Sn halide perovskites prevents them from becoming suitable. Perovskites are extremely vulnerable to oxidation on their own. Therefore, organic solar cells require a new substance. The usage of block copolymers as a component in organic solar cells is the main topic of this article. The quantum efficiency of organic solar cells will increase by modifying the block copolymer's shape and choosing the right material.

Keywords: block copolymers, organic solar cells, use of organic solar cell.

1. Introduction

This research mainly focuses on the area of the organic solar cell, and three main approaches to using block copolymers are discussed. As technology developed, conventional fuel sources are few, and using them produces hazardous byproducts whose effects are already detrimental to the environment and the global economy [1]. By designing different block copolymers, it can increase the total device efficiency of organic solar cells [2]. Firstly, A renewable resource is needed to improve this situation. It is widely acknowledged that sunlight is the most plentiful source of renewable energy that is also carbon-neutral. Secondly, Block copolymers for photovoltaics are used because of their lightweight [3], Mechanical flexibility and tunability of the photovoltaic function [4]. Thirdly, currently, commercially available conventional PV devices are mainly using silicon technology and can achieve 20% power conversion efficiency or more. Bulky modules and high production costs restrict their general use and can prevent them from being implemented at the scale required to significantly displace fossil fuels.

By studying how the block copolymers are used to combine the organic solar cells, the quantum efficiency can break out of the original limit. For the future development of organic solar cells, block copolymers are a suitable material for solving long-term stability and efficiency problems in organic solar cells.

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2. Literature review

One route for direct solar energy generation is Photovoltaic. Photovoltaic is based on a semiconductor. Electronic structure in the semiconductor can delay electron-hole recombination which gives time for extraction of the electron to the external circuit.

In organic semiconductors, there is a hopping of charge carriers which is a thermally activated process. So as the temperature goes up, mobility goes up.

Quantum efficiency is basically how many electrons can be drawn out for every photon that goes in. It is based on the semiconductor's absorption coefficient, the efficiency of electron-hole separation and the efficiency of electron and/or hole carrier extraction to the external circuit.

When electrons are excited from the valance band to the conduction band, vacancy is formed in the conduction band. Then there is an electric field that is used to separate that electron from the hole. They are oppositely charged and have large coulomb interactions between them.

The cathode has a much lower value of work function than the anode. When the light comes in, it forms an exciton, an electron and a hole and they are associated with each other. The exciton has to diffuse to the organic heterojunction. Exciton then splits at the organic heterojunction, forming free electrons and holes. Transport of holes will occur in the donor phase, whereas that of electrons will occur in the acceptor phase. It moves by a concentration gradient and a built-in electric field. charge extraction for the external circuit.

According to Figure 1, incident photons (i) excite electrons from the HOMO to the LUMO of the donor material, (ii) produce excitons (iii), and (iv) move the donor material across the donor material to the donor-acceptor interface (v), where (iv) excited electrons (excited electrons) separate from their bound holes to the LUMO of the acceptor. Steps (v) and (vi) involve the free electrons and holes moving through the acceptor and donor materials and onto the cathode and anode, respectively. A current is produced by the electrons and holes moving continuously through the apparatus.

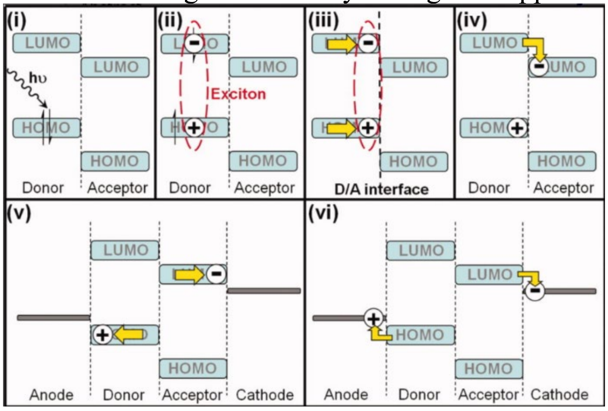

Figure 1. The theory of photovoltaic systems [5].

Block copolymers (BCP) are macromolecules made up of two or more covalently linked homopolymer chains or blocks [6]. Using block copolymers for organic solar cells has some advantages. Cheap raw materials are associated with lightweight, flexible equipment easy to process and have inherent installation efficiency compared to other materials [7] What is most importantly, BCPs create nanostructures that are inexpensive and rapid to apply across vast surfaces, making it possible to make large-area organic photovoltaic (OPV) cells at a low cost. BCPs are well-suited for solution-based processing techniques. The difference between BCP lithography and other high-resolution patterning techniques (such as electron beam lithography) is well illustrated when lithography is all at a bottleneck.

3. Three main ways to use block copolymers for organic solar cells

3.1. Block copolymers as active materials

The acceptor material was placed on top of the donor material in the bilayer structure used to create the initial organic solar cells. The performance of this device was significantly constrained by excitation losses [8]. One classic modern type of organic solar cell is called body heterojunction (BHJ). It involves a hybrid donor-acceptor active layer, and this layer has a high structural disorder due to the dependent on the random phase separation of the components [9]. Because of this, numerous structural domains are frequently too big, too tiny, sinuous, or discontinuous, which leads to poor carrier mobility, charge recombination, or loss of excitability. In theory, the self-assembly of BCPS can produce highly regular nanoscale structures in idealised forms [10]. Over the past 30 years, the power conversion efficiency (PCE) had broken records of 16% [11]. Modern OSCs have a PCE, although it is still much lower than other solar technologies like c-Si and calcium titanite cells [12]. The wide band gap (WBG) polymer donors and fused ring electron acceptors (FREAs) have recently been developed in an effort to enhance device performance. Recently, Two D-A copolymers were created, 2-(benzo[c][1,2,5] thiadiazol-4-yl)-4H-cyclopenta [2,1-b:3,4-b']dithiophen-4-one (CPDTOBT) and 2-(2-(benzo[c][1,2,5]thiadiazol-4-yl)-4H-cyclopenta[2,1-b:3,4-b']dithiophen-4-ylidene)malononitrile (CPDTNBT).It was been proved that the copolymer exhibits high charge transport capacity and promising photovoltaic properties with PCE up to 9.5%. CPDTNBT molecules with >C double bonded C-(C triple bonded N)2 bridge positions lead to strong intramolecular D-A interactions to produce improved charge carrier mobility and PCE. The construction of an acceptor1-acceptor2 (A1-A2) architecture of polymer donors using two "pull" electron-deficient units (A1 and A2) was an innovative method of producing BHJ [13–14].

Another method is the synthesis of donor/acceptor rod coils BCP. One D-A rod-coil BCP was synthesised by coupling polystyrene (PPV) blocks with flexible coil blocks consisting of polystyrene (PS) backbones, acceptor C60, Hazdiioannou et al [15]. By enhancing the BHJ nanoscale structure, grafting of the molecules demonstrated that the rod-coil BCP may be employed to somewhat increase solar performance. But the problem is partial grafting of fullerenes onto such BCPs significantly affects the self-assembly of the polymer through the growth of fullerene nanocrystals [16].

3.2. Rod-block copolymer photovoltaics

Block copolymers that are fully conjugated may be made without the need for lateral chromophores, their related problems with graft density, or their dependence on intermolecular charge transfer. The absence of live polymerization methods for creating completely conjugated materials, however, creates a new set of difficulties. [17, 18] Step-growth polycondensation polymerization is often required for the generation of completely conjugated materials. In the majority of polycondensation reactions, the catalyst is not linked to a particular growth chain but rather connects the reaction components at random, resulting in a wide range of chain lengths. But it still works in some cases. In 1996, the first completely conjugated block copolymer was created. [19] Then, an all-conjugated block copolymer with donor and acceptor blocks was created in 2006, 10 years after the first described system, for application in organic photovoltaics [20]. The latest invention of the block copolymer P3HT-b-PFTBTT was reported in 2011 by Mulherin et al [21]. The PFTBTT block was coupled via an AB-type Stille of fluorene-dithiophenobenzothiadiazole monomer and then end-capped with P3HT-Br. 42% of the material was free PFTBTT by weight; however, the inter-block coupling process was ineffective and resulted in a combination of block copolymer products and homopolymer impurities.

3.3. Amphiphilic block copolymers

This type of block copolymer was designed to solve the problem of using chlorinated and aromatic solvents when improving organic solar cells. The latest technic was completed by Suzuki condensation from the P3HT-Br macroinitiator, and hydrophilicity was formed by the partial incorporation of tetramethylene glycol (TEG) into the fluorene unit of the acceptor block [22]. The resulting block copolymers, P3HT-b-PF interrupter Tributyltin compound and P3HT-b-PF interrupter T6BT [23]. The increasing chemical differences between the donor, acceptor, and block copolymer in these materials enable for the development of straightforward purification techniques that can isolate block copolymer products. These materials do exhibit better solubility.

3.4. Block copolymers as structure directors

Use the unusual molecular and assembly properties from block copolymers to improve the performance of organic and even hybrid organic-inorganic photovoltaic devices [24, 25]. For example, when using Phenylenediamine to exchange performance of polythiophene/C in 60PV devices in the blends section, perylene crystallizes into domains larger than the exciton diffusion distance, and mixtures of polythiophene and circumference produce inefficient devices. By acting as a compatibilizer and lowering the interfacial tension between the individual nanostructured domains, BCPS can assist solve this issue by stabilising the structural domain size and bringing it closer to the exciton diffusion scale.

3.5. Block copolymers as both active materials and structure directors

Instead of replacement of organic receptors with nanocrystals [26], the nanocrystals are added to a conventional organic donor/acceptor mixture and this approach has reported over 100% EQE [27, 28]. The challenge of this is the nanoparticles will aggregate at the same time, especially during annealing. The way to solve this was to place BCP selectively [29]. A triple block copolymer was designed by Gatt and Cohen to achieve not only hole transport but also nanoparticle binding and electron transport. The long-chain carbazole and dinitrophenyl derivatives serve as hole and electron transport materials, while the short centre block is intended to bind passivated CdSe quantum dots. These components are based on norbornene. The interaction between the polymer and the nanoparticles effectively inhibits the aggregation of the latter [30]. Recently, a new block copolymer called PM6-b-PTY6 was designed, and its backbone contains both donor PM6 and Y6 chains. It has been demonstrated that using this block copolymer as a bulking agent enhances the power conversion efficiency and long-term durability of benchmark non-fullerene solar cells based on high-efficiency PM6:Y6.

Overall, there was a particular method that need to be considered. That was the Calcium titanate solar cells made from calcium titanate polymer passivation [31]. The challenge is to avoid backward energy transfer by fine-tuning the alignment of the band gap with the other layers of the device. [32, 33] Because the charge generation and charge transfer balance is likely to be considerably influenced by the geometric feature size and form. The outstanding performance of PPC-based polymeric chalcogenide solar cells was made by Han et al [34]. exhibited high stability of up to 20.06% through the formation of Lewis adducts between PPC and chalcogenide. Suitable block copolymers containing donor and acceptor behaviour as well as PQDs not only have the benefits of BHJ and PQDs solar cells, but also a wide range of properties [35, 36]. Due to the phase separation, the composites are well-suited as active layers. According to the reports, the inclusion of nanoparticles within the 2P3HT-P2VP BCP of TiO affects the geometry of the block and increases PL quenching, therefore demonstrating a significant increase in charge separation efficiency. Additionally, the addition of BM modifies the mechanical characteristics of PC71 polymer blends, and an adjusted doping ratio guarantees improved mechanical stability and polymer crystallinity. With a final PCE of 16.0%, PCBM was also seen to function as a dopant to fine-tune the chalcogenide grain formation process. So, the formation of vertical volume heterojunctions will facilitate near-perfect charge transport, and PQDs can serve as effective sites for charge separation [37]. It can be assumed that PQDs at the base sequence interface can enhance charge separation and transport. No specific experimental reports have focused on integrating PQDs in block copolymers to create bulk heterojunction solar cells with highly ordered nanostructures. But maybe in the future.

4. Conclusion

Block copolymers have active layers made of a single material, providing a stable morphology that is critical in the industry. However, this is not the best. Because the efficiencies currently described for high-performance OPV active layers are not met by the technology. This disparity is evidently caused by the fact that polymers already present in block copolymers frequently choose synthetic accessibility above OPV performance. But Chalcogenide materials have proven to be promising candidates for the fabrication of BCP composites and it is worth considering a variety of composite fabrication methods to overcome the limitations of chemistry and thermodynamics for future uses. Also, for many different uses, Composites made of BCP-PQDs will be thought of as flexible, incredibly durable materials with effective optoelectronic capabilities.

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