Solar Active Layer Materials and Research Progress

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Abstract. Solar cell is an electrical device, which converts the light energy into electrical energy through the photovoltaic (PV) effect. It is an efficient way to alleviate global warming effect. This work explains the principle and the structure of OPV. There are mainly five layers of OPV and five steps of how OPV works. Besides, a brief review of the history of OPV's development is given in this work. As a matter of fact, the active layer is the most important part of the solar cell. It directly determines the conversion efficiency of solar cell. The stucture of active layer is shown in the paper as well. The active layer is divided into two main categories: organic and inorganic. The research progress of each type of active layer is illustrated in this work. A detailed description of the types of active layer of solar cell and the pros and cons of each type are given in this work.

Keywords: Solar cell; active layer; principle.

1. Introduction

With population growth and global industrialization, global warming is becoming a serious issue need to be cope with immediately. Last year, global average near-surface temperature 1.45 degrees celsius above pre-industrial average. As a result of global warming, the frequency of extreme weather and climate events is surging. The development of sustainable energy is facing serious challenges, and solar energy, as a clean and sustainable energy source, is gradually becoming an alternative to electricity production and fossil fuels. Currently, photovoltaic power generation is one of the main directions of China's energy transition, and photovoltaic technology is becoming a promising renewable energy technology and is being used to generate and provide sustainable energy. In 1839, the French scientist A.E. Becquerel discovered the photovoltaic effect, two pieces of platinum metal clicks inserted into an acidic solution, between the electrodes to produce a flow of electric current, from then on to open the door to the world of photovoltaics. By 1954, the United States made the first monocrystalline silicon solar cells, marking the birth of photovoltaic power generation technology. The PERC cell structure was first formally reported by Martin Green's research group at the University of New South Wales, Australia, in AppliedPhysicsLetter in 1989, when it achieved a laboratory cell efficiency of 22.8%. By 1999 its laboratory research PERC cells created a conversion efficiency of 25% of the world record. When it came to the second generation, there are various thin-film batteries, including cadmium telluride solar cells (CdTe), amorphous silicon thin film batteries (a-Si), copper indium gallium selenide solar cells (CIGS), gallium arsenide solar cells, nano-titanium dioxide dye-sensitized solar cells, etc. In the early 1960s, T.F. Goodrich developed amorphous silicon thin film solar cells for the first time. In the early 1970s, Soviet scientists invented CIGS solar cells. With the continuous deepening of research, solar energy conversion efficiency has been improved, the cost has been reduced, and the range of applications has been expanded. Third-generation solar cells: various super-stacked solar panels, thermal photovoltaic cells (TPV), quantum well and quantum dot superlattice solar cells, intermediate band solar cells, up-conversion solar cells, down-conversion solar cells, hot carrier solar cells, collision dissociation solar cells and other new concepts of solar cells. However, the conversion efficiency of solar panels is relatively low and the production cost is relatively high. This work gives an introduction of several genre of solar panels to make comparisons to each panel's advantages and disadvantages. This work will suggest each solar panel's potentials for further improvement in convertion efficiency.

2. Principle of Solar Panels

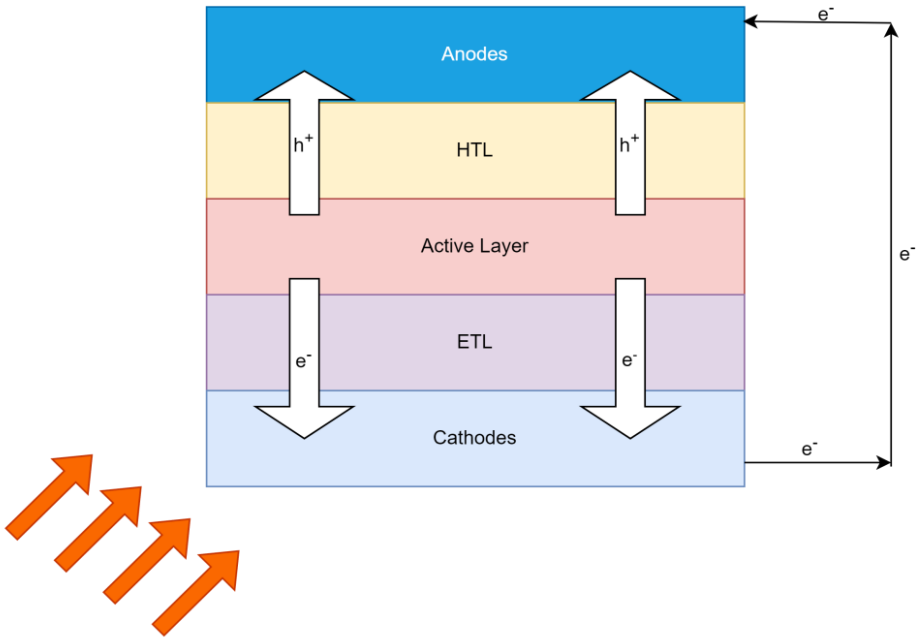

Fig 1. The principle of solar panel.

There are five layers (shown as fig.1) which are cathode, electron transport layer, active layer, hole transport layer and anode. The active layer is the most important part of an organic solar cell, where light is converted into electrical energy, and plays a decisive role in the energy conversion efficiency of the device. The electron transport layer is connected with cathode. It is required to have some requirements such as a high electron transport rate, a low hole transport rate, and a minimum unoccupied molecular orbital energy level close to or below that of the acceptor material, which can facilitate the movement of electrons toward the cathode electrode. And the hole transport layer connected with anode have the requirement such as a high hole transport rate, a low electron transport rate, and a HOMO energy level close to or higher than the HOMO energy level of the donor material is usually needed, which can facilitate the transport and collection of holes.

There are five steps of how solar panels convert light into electricity. To begin with, the first step is photon absorption and exciton generation. When the organic solar cell active layer material molecules absorb enough energy photons, the electron breaks through the energy level barrier(E_g), from the highest occupied molecular orbital energy level to the lowest unoccupied molecular orbital energy level, become excited electrons, and leave holes, forming electron - hole pairs. This requires the active layer material to have a high absorption coefficient and an absorption spectrum that matches the solar spectrum. The second step is exciton diffusion. The excitons diffuse into the donor-acceptor interface layer. The exciton needs to diffuse and transport to the interface between the donor and acceptor molecules for the next step of charge separation. Since electrons and holes exist to be compounded by means of radiative and non-radiative compounding, this causes loss of excitons and wastage of absorbed light energy. Furthermore, the third step is separation of excitons. When the exciton diffuses to the interface of the donor and acceptor molecules, the electrons will flow from the LUMO level of the donor molecule into the LUMO level of the acceptor molecule due to the LUMO energy level potential of the donor and acceptor, and the holes will stay in the HOMO energy level of the donor molecule. This will form free electrons and holes. Last, the forth step is charge transportation and collection. Under the effect of the internal potential energy difference of each layer of the organic solar cell, the separated electrons will be gradually transported from the acceptor material to the cathode electrode, while the holes will be gradually transported from the donor material to the anode electrode. The charge collected on the electrode can generate photovoltage and photocurrent to the external circuit. Since holes and electrons are highly reversible in the transport

process and are inevitably lost due to various defects, the addition of a suitable electron transport layer and a hole transport layer promotes the rapid movement of electrons and holes in the appropriate direction.

3. Active Layer Materials and Research Progress

3.1. Introduction of Active Layer's History

The active layer is mainly composed of donor and acceptor materials, which is an important part of realizing photoelectric conversion, and the material of the active layer has a decisive role in the overall performance of the battery. The energy difference between the LUMO energy level of the acceptor material and the HOMO energy level of the donor material determines the short-circuit current JSC and the open-circuit voltage VOC of the cell; the size of the respective phase regions of the donor and acceptor materials determines the efficiency of exciton diffusion, which in turn affects the separation of charges. Therefore, the study of active layer materials is of great significance to improve the PCE of organic solar cells. The active layer materials applied to solar cells are mainly divided into two categories: inorganic active layer materials and organic active layer materials.

There are three generations of inorganic active layer materials. The first generation was crystalline silicon cells based on silicon crystalline material. The second generation is thin-film solar cells represented by compounds such as cadmium telluride (CdTe). The third generation is a new generation of high-efficiency cells represented by chalcogenide solar cells.

Currently commonly used active layer materials for organic solar cells can be categorized into donor and acceptor materials. Among them, the receptor material can be divided into non-fullerene receptor and fullerene receptor, and the donor can be divided into polymer donor and small molecule donor.

3.2. Inorganic Active Layer Materials for Organic Solar Cells

The first generation was crystalline silicon cells based on silicon crystalline materials. The first practical p-n junction silicon crystalline solar cell was invented at Bell Labs in the United States in 1954. After decades of development, the silicon crystalline solar cell has become one of the most important photovoltaic devices. In 2018, Bullock et al [1]. Prepared a heterogeneous structure of the active layer with both monocrystalline silicon and non-monocrystalline silicon, and used TiOx material as a protective layer between the active layer and the cathode, obtaining a crystalline silicon cell with PCE=20.7%. However, the production of monocrystalline silicon solar cells requires the use of expensive high-purity monocrystalline silicon, and the processing process is complex, which limits the popularization of the use of silicon crystalline solar cells to a certain extent.

The second generation of thin-film solar cells is represented by compounds such as cadmium telluride (CdTe), which is a semiconductor material with an ideal band gap (1.45 eV) and a good light-absorbing ability, and it can be applied to the production of thin-film solar cells [2]. In 2017, the U.S. FirstSolar prepared a CdTe thin-film solar cell with a PCE = 21.5 % [3]. However, thin-film solar cells often use toxic elements such as Cd and Te, and the preparation of thin films requires expensive deposition equipment, which increases the cost of preparation and limits the scope of application.

The third generation is a new generation of high-efficiency batteries represented by chalcogenide solar cells (shown as fig.2). Calcitonite cells are the most rapidly developed class of inorganic solar cells in recent years, in 2009, when calcitonite cells were first reported, the PCE was 3.8%, and in 2017, the PCE of calcitonite cells was raised to 22.7% [4]. The active layer of the chalcogenide battery is mainly composed of crystals with the molecular formula ABX3, where a represents the anion, B represents the cation with a size smaller than A, and X represents the halogen ion [5]. The crystal structure of chalcogenide is shown in Fig. 2. Miyasaka's group [6] used two chalcogenides, $CH_3NH_3PBr_3$ and $CH_3NH_3PbI_3$, as sensitizers for the first time in 2009 to form a dye-sensitized solar cell. Ahli et al. [7] deposited a layer of chalcogenides on the surface of monocrystalline silicon to

form a bilayered heterostructure chalcogenide-silica tandem cell, and then used a layer of chalcogenides to form the active layer of chalcogenide-silica tandem cell-silicon crystal tandem cell, the device PCE reached 25.2%. However, the high manufacturing cost of chalcogenide crystals also limits its application scale.

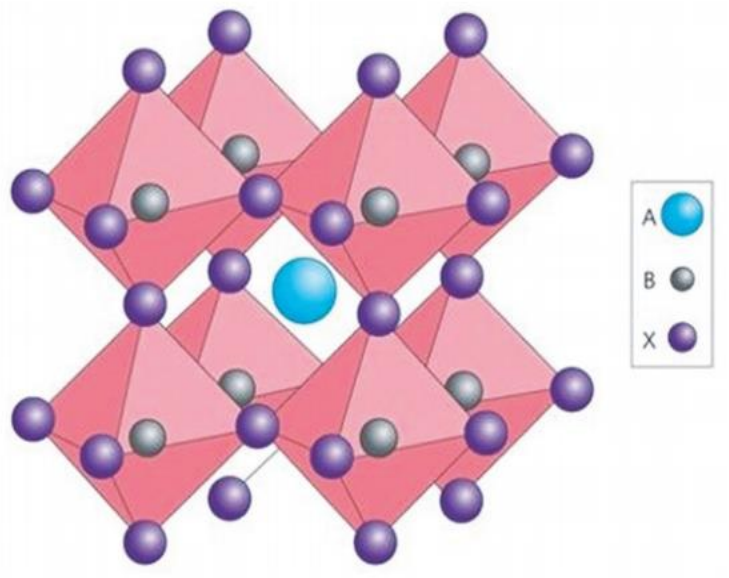

Fig 2. The structure of perovskite crystal [8].

3.3. Organic Active Layer Materials for Organic Solar Cells

Organic solar cells can be divided into two categories according to the active material: polymer solar cells and small molecule solar cells. The more desirable materials are required to have properties such as broad absorption spectra, suitable energy level structures, high carrier mobility, good solubility, and low HOMO and LUMO energy levels.

3.3.1. Polymer donor material

The development of polymer solar cells preceded that of small molecule solar cells, which have been studied since the 1990s, with relatively high types and conversion efficiencies.

In 1993, Wudl and Srdanow synthesized the poly (p-styrene-vinylidene-vinylidene)-based feedstock material MEH-PPV, which opened the way for the rapid development of organic polymer feedstock materials [9]. PPV materials are widely used in polymer photovoltaic materials because of their good photovoltaic properties. However, PPVs generally need to be modified instead of PPVs in order to have better performance. MEH-PPV is one of them, and there are also MDMO-PPV, CN-PPV and M3EH-PPV. However, PPV materials have low light absorption and hole transport properties, to compensate for this shortcoming, researchers have found polythiophene-based conjugated polymer donor material 3-hexylthiophene (P3HT). P3HT is characterized by high hole mobility, good solubility and simple structure. The efficiency of devices fabricated based on the P3HT/IC_{70}BA system has been reported to be 7.40% [10].

PPV derivatives and polythiophene-based donor materials have a wide band gap, and most of the energy of the solar spectrum is located in the near-infrared region, so the absorption of sunlight by these two materials is not up to the ideal state, and it is difficult to continue to improve the energy conversion efficiency. For this reason, the researchers proposed a molecular mechanism in which the electron-donating part (D) and the electron-deficient part (A) are alternately copolymerized. This structure, on the one hand, can improve the rigidity of the molecular main chain, which promotes the π-electron delocalization and thus reduces the material energy gap. On the other hand, the HOMO energy level can be regulated by the electron-donating part and the LUMO energy level by the electron-deficient part.

3.3.2. Small molecule donor material

Compared to polymeric donors, small molecule donor molecules offer advantages such as easy purification, well-defined chemical structure, molecular weight determination and excellent batch reproducibility, which are advantageous for future commercial applications. The first report of such donor was the small molecule donor D2 (fig.3) first synthesized by Walker et al. in 2012, whose all-small-molecule organic solar cells prepared by solution method showed the highest energy conversion efficiency PCE of 3.72% for fullerene system, while the energy conversion efficiency PCE of non-fullerene system was basically below 1% [11]. Many polymer donors can be prepared as small molecules by linking the polymerization units to the end groups, however, the reported energy conversion efficiencies PCE of organic solar cells containing small molecule donors are usually lower than those of the corresponding polymers, with only a few PCEs higher than 10%.

The current small molecule donors with high energy conversion efficiency are as follows: Li Yongfang et al. synthesised the receptor-donor-acceptor (A-D-A)-type small molecule SM1 (fig. 3) in 2017, which has a thiophene-substituted benzothiophene in its midst and is connected to the ester group end-group with a cyano substituent via a triplet thiophene π-bridge. It has high light absorption in the visible region and complements the absorption of the acceptor IDIC, resulting in an energy conversion efficiency PCE of 10.11% for SM1: IDIC devices [12].

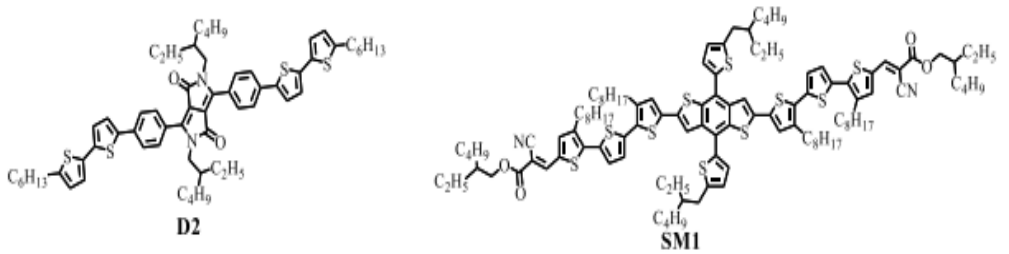

Fig 3. Small molecule donor material [13].

3.3.3. Fullerene-derived receptor materials

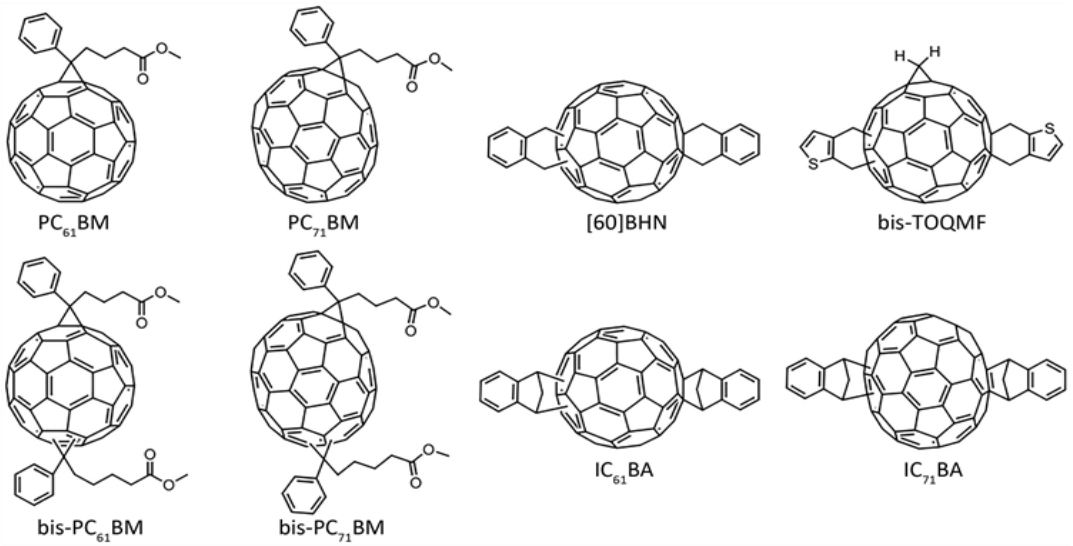

Fig 4. Fullerene-derived receptor materials [13].

Fullerene derivatives have been used as acceptor materials for 30 years, and their three-dimensional conjugated electronic structures are prone to exhibit better electron acceptance and photovoltaic transport properties. Since 1995, when Wudl et al. first reported the application of $PC_{61}BM$ **(**fig.4), a C_{60} fullerene derivative, in organic solar cells [14], this kind of structure has become very popular. Later on, researchers developed a series of receptor materials with similar

structures by modification, among which $PC_{71}BM$ (fig.4) reported by Hummelen et al. is the most famous. Comparison with $PC_{61}BM$ **(**fig.4) shows that $PC_{71}BM$ (fig.4) has a narrower bandgap and is red-shifted in light absorption, and the conversion efficiency of the device is correspondingly higher **[**15]. Of course, in addition to PCBM-like structures, some other fullerene derivatives of acceptor materials have also been developed and have shown good performance, Li Yongfang's group reported a group of fullerene derivatives based on the bis-indene addition $IC_{60}BA$, $IC_{70}BA$ (Fig. 4), the efficiency of the devices made of P3HT as the donor material reached 6.48% respectively [16], 5.44% **[**17]. While the efficiency of the cell fabricated based on PC61BM/P3HT is only 3.88%.

3.3.4. Non-fullerene acceptor materials

Non-fullerene receptor materials include polymers and small molecules, which can be classified into wide-bandgap non-fullerene receptors, medium-bandgap non-fullerene receptors, and narrow-bandgap non-fullerene receptors according to the energy level bandgap Eg.

In the research of non-fullerene receptor (NFA) based solar cells, the more successful ones so far include two main types. The first one is the aromatic diimide derivatives; the second one is the electron acceptors based on thick ring structures (FREAs).

In 2015, Xiaowei Zhan's group [18] synthesised ITIC-like molecules, which are ADA-type structural electron acceptors, to improve the PCE of batteries, of which the study of ITIC-like molecules is a hot topic at present. In Zhanshaowei's group [19] also modified ITIC by using the side chain conjugation strategy for the first time, and designed and synthesized the first two-dimensional conjugated thick ring electron acceptor material, ITIC2.

ITIC2 has a heptameric thick ring skeleton and conjugated side chains, and thus exhibits redshift and higher absorption, energy level and electron mobility than ITIC1, and the PCE of FTAZ: ITIC2-based OSC is 11.0%, which is much higher than that of FTAZ: ITIC1-based PCE (8.54%). The same group **[**20] also improved the heptabicyclic skeleton to a ninabicyclic one to broaden the absorption spectrum of the molecule and isomerized it to synthesize FNIC1 and FNIC2 with the same end groups and side chains, and the results showed that the PCE of the OSC based on PTB7-Th: FNIC2 was 13.0%, which was much higher than that based on PTB7-Th: FNIC2 (8.54%). Th: FNIC1-based OSC had a PCE of 13.0 per cent, much higher than that of PTB7-Th: FNIC1-based OSC (10.3 per cent).

4. Conclusion

Five steps of how solar cell convert light into electricity. As the decisive part of solar cells, the active layers are approximately divided into two main categories-organic and inorganic. There are mainly three generations of inorganic active layer. The organic active layer catagories are divided according to the active material.

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