Optimizing Research on Solar Cell Semiconductor Materials in Optoelectronic Materials and Devices

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Abstract. Organic solar cells are considered to be a promising new generation of optoelectronic devices. Electrode materials are one of the most important parts of organic solar cells and have a direct impact on battery performance. The research of organic electronics is mainly concentrated in the field of organic semiconductors, and the research and development of related materials and devices have made rapid progress, including organic light-emitting diode display technology, organic thin film transistors, organic solar cells, organic memories, organic sensors, organic lasers, etc. A large number of research results have been obtained in the research of related organic semiconductor materials and devices. The paper analyses some common solar semiconductor battery materials, and prospects the application of the above-mentioned materials in solar cells in the future.

Keywords. Solar cells, semiconductor materials, optoelectronic materials, optoelectronic devices.

1. Introduction
Solar cell is a device that uses photovoltaic effect to convert light energy into electrical energy. Since the Bell Laboratory produced monocrystalline silicon solar cells in 1954, as people continue to develop new energy fields, the types of solar cells are also constantly expanding. According to the standard of materials, solar cells can be roughly divided into three generations: the first generation is silicon-based solar cells (based on monocrystalline silicon, polycrystalline silicon and their composites with amorphous silicon). This type of cell photovoltaic conversion efficiency is high, the technology is mature, and it has been commercialized [1]. At present, the efficiency of the laboratory certified by the US Renewable Energy Laboratory (NREL) has reached 27.6%.

The second generation of thin film solar cells (including GaAs, cadmium telluride, CdTe, copper indium gallium selenium CIGS, etc.), this type of battery has high photovoltaic conversion efficiency and stable device performance. It is also the type of battery that the industry looks forward to. Some of the elements in the material are toxic or have scarce reserves, which restricts the promotion and use of large areas.

The third generation is a new type of solar cell, including dye-sensitized solar cells (DSSCs), perovskite solar cells (PSCs), organic solar cells, quantum dot solar cells, etc. Among them, PSCs evolved from DSSCs. At present, the highest photovoltaic conversion efficiency certified by NREL has reached 23.7%. "Improving the efficiency of solar cells and systems and reducing the manufacturing
cost of photovoltaic systems" is the perfect ideal in the photovoltaic industry, and it is also applicable to PSCs. In the traditional PSCs device structure consisting of FTO or ITO conductive glass/electron transport layer/perovskite light-absorbing layer/hole transport layer/counter electrode layer, when the perovskite light-absorbing layer absorbs incident light, free electrons are generated. At the same time, the same number of holes are generated. The generated electrons will enter the electron transport layer and the holes will enter the hole transport layer. However, not all electrons will completely enter the electron transport layer during this process, and some will recombine with holes and reduce the photoelectric conversion efficiency. Therefore, it is necessary to use a hole transport layer to block electrons from transporting to the hole transport layer, thereby enhancing the transport of holes and preventing the perovskite active layer and the electrode. Direct contact causes quenching, so as to make more electrons move toward the electron transport layer as much as possible, so that the photoelectric conversion efficiency is improved [2]. In order to further reduce costs, the application of carbon materials with the advantages of low price, stable chemical properties, and work function matching with perovskite materials in the PSCs hole transport layer has become a hot research topic.

2. Photovoltaic effect theory and measurement methods
Photovoltaic effect is the result of carrier transmission and redistribution in semiconductors caused by light. Surface photovoltaic is a method to analyze the related properties of semiconductor materials by measuring the surface photovoltage (SPV) caused by photovoltaic effect. Taking the surface-depleted n-type semiconductor as an example, according to the law of conservation of charge, the surface net charge quantity \( Q_s \) should be equal to the net charge quantity \( Q_w \) of the space charge region. The magnitude of the surface potential \( V_S \) mainly depends on \( Q_s \) or \( Q_w \). As shown in Figure 1, under illumination with an energy greater than or equal to the forbidden band width \( E_g \), electrons transition from the valence band to the conduction band, generating photo-generated carriers (electron-hole pairs) on the surface of the semiconductor [3]. Under the action of separation and transfer, the photogenerated electrons migrate to the body and the photogenerated holes migrate to the surface, which reduces the surface electron density and the surface energy band bending, thus causing the changes of \( Q_s \) and \( V_S \).

![Figure 1](image)

**Figure 1.** When the energy is greater than \( E_g \), the carriers in the semiconductor are separated under the electric field.

Under light with energy less than \( E_g \), as shown in Figure 2, the most common situation is the transition of electrons from the surface state to the conduction band and the transition of holes from the surface state to the valence band, which also causes the changes in \( Q_s \) and \( V_S \). Therefore, conceptually speaking, in the absence of light and light, the change in surface potential is called surface photovoltage. It can be expressed as

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SPV = V^*_S - V_S
\]
Figure 2. Excitation of bound electrons and holes when light with energy lower than $E_g$

Where: $V_s'$ refers to the surface potential after illumination; $V_s$ refers to the surface potential before illumination; SPV is the surface photovoltage. The surface potential and work function can be linked together. When the semiconductor has a surface state, then

$$W = \mu + x - qV_s'$$  \hspace{1cm} (2)

In the formula: $W$ refers to the work function of the sample; $x$ is the electron affinity; $q$ is the electric quantity of the electron; $\mu$ is the distance between the conduction band and the Fermi level. From equation (2), it can be seen that the change of surface potential corresponds to the change of work function, namely

$$qSPV = W' - W$$  \hspace{1cm} (3)

Where: $W'$ is the work function after illumination; $W$ is the work function before illumination. From equation (3), it can be seen that the change of the surface work function is also equal to the surface photovoltage. In the experiment, the method based on the metal/insulating layer/semiconductor (MIS) structure or the method based on the Kelvin probe is usually used to measure the change value of the surface work function of the object, and then the surface photovoltage is obtained. The MIS structure method is suitable for studying the body energy level, and can also determine the position of the surface energy level, but it cannot study its dynamic parameters [4]. The Kelvin probe method has high measurement sensitivity and is suitable for studying the position and dynamic parameters of surface energy levels. Compared with the MIS structure method, the Kelvin probe method has higher noise level and lower transient resolution, which is suitable for studying long-term transitions.

3. The basis of quantum structure materials and devices

When the size of a certain dimension of the material is small enough to be comparable to the De Broglie wavelength of the electron or the exciton Bohr radius, the movement of electrons and holes in this direction is restricted, and compared with the body, the electron loses this direction. The above degree of freedom, such systems are called low-dimensional systems, and because these low-dimensional systems exhibit the characteristics of quantization, they are called quantum structures. Figure 3 schematically shows the structure of bulk materials and low-dimensional materials and their density of states distribution diagram [5]. Low-dimensional systems include 2-dimensional, 1-dimensional, and 0-dimensional systems, which confine electrons in one direction, two directions, and three directions, respectively, resulting in low-dimensional superlattices and quantum wells, quantum wires, quantum dots, etc. structure. In the low-dimensional system, the locality and coherence of electrons are enhanced, the quasi-continuous energy band of the macroscopic solid disappears, and discrete energy bands or energy levels appear, which makes the low-dimensional system of light, heat, electricity, magnetism and other physics the nature is different from the bulk material. Many novel physical properties are constantly revealed in these systems, so the research of low-dimensional systems has been paid more and more attention in recent years.
The quantum size effect means that when at least one of the three-dimensional scales of the microstructure material is equivalent to the De Broglie wavelength of the electron or the Bohr radius of the exciton, compared with the bulk material, the electron loses the degree of freedom in this direction, and the electronic state appears. The quantization distribution shows the phenomenon that the electronic energy level near the Fermi level changes from quasi-continuous to discrete energy level or the energy gap becomes wider. Taking the CdTe exciton characteristics in the quantum well structure as an example, the quantum size effect is briefly explained below. Figure 4 shows the theoretical calculation results of exciton binding energy and exciton Bohr radius in CdTe quantum well structures with different well widths [6]. It can be seen that as the width of the infinite potential well decreases, the quantum size effect becomes more obvious, the exciton binding energy increases, and the exciton Bohr radius decreases. When the well width is less than 5nm, the exciton binding energy will be greater than the room temperature ionization energy (26meV). In addition to the obvious quantum size effect of the exciton effect, the band gap of semiconductors also increases as the size of the material decreases. Due to the introduction of quantum effects, the magnetic, optical, acoustic, thermal, electrical and superconducting properties of quantum structures will all be affected differently by quantum size effects.
4. Application and characteristics of electrode materials

Electrode materials are a key component of organic solar cells and play a decisive role in the performance of the battery. Currently widely used electrode materials can be classified into two categories, namely indium tin oxide electrode materials and non-indium tin oxide multilayer electrode materials.

4.1. The development of indium tin oxide transparent conductive oxide film

Since Baedeker first discovered that cd0 film has both transparent and conductive properties in 1907, transparent conductive oxide (TcO) film has formed three major systems with indium oxide, tin oxide and zinc oxide as the main material [7]. Among them, indium tin oxide (ITO) Transparent conductive film has become a mainstream commercial product due to its excellent characteristics such as low resistance, high transmittance, and easy etching. It is widely used in flat panel display technology, solar cells, touch screens and other fields.

At present, the application of indium tin oxide conductive film is relatively wide and mature, and industrial production has been realized in the United States, Japan and other countries. In China, although the average annual production volume has increased relatively substantially, it still lags behind developed countries due to a late start [8]. Indium is a rare metal on the earth, and as its use continues to grow, the price will become more and more expensive. At the same time, the surface resistance of IT0 will increase significantly when the cyclic bending moment exceeds the minimum bending radius (<10mm), resulting in cracks and affecting the quality of OSCS. Therefore, there is a need to develop alternative new electrode materials.

4.2. Not to give up indium tin oxide multilayer electrode

In order to make OSCS a competitive technology, it is necessary to reduce its price to the greatest extent, but most of the current organic solar cells rely heavily on indium tin oxide, and its price will be due to the strong demand of the industry and the relative scarcity of indium. It remains high and even has an upward trend. To this end, it is necessary to develop and research different electrode materials, such as conductive polymers, carbon nanotubes, graphene, silver nanowires, metal grids and metal thin films, to replace ITO. These new electrodes mostly use a multilayer structure, usually containing three layers of oxide/metal/oxide (OMO), and this multilayer design can provide organic solar cells with high transmittance and conductivity. From the structural analysis, the reason why its transmittance is higher than that of a single-layer metal is mainly due to the strong optical interference in the three-layer stack structure. Compared with ITO, another advantage is that the multilayer structure can help resist the generation of cyclic bending moments.

5. Conclusion

Future research needs to establish an accurate electrical analysis model of the interface between the perovskite and the carbon material, master the assembly and process technology of the enhanced carbon material and the perovskite layer, and explore new types of carbon materials and composite materials. Accelerate the development of carbon materials in PSCs Research and application are more conducive to the promotion and development of PSCs. At the same time, carbon materials may become an indispensable element in PSCs in the future. I believe that in the future, carbon materials will make a great contribution to PSCs entering and applying to public life.

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