Advances in Quantum Dot-Sensitized Solar Cells

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Abstract: Quantum dot-sensitized solar cells (QDSSCs), as the third generation photovoltaic devices, have become an important direction to break through the efficiency limit of traditional silicon-based solar cells by virtue of their high theoretical efficiency (~44%), low preparation cost, and wide spectral absorption range. This paper focuses on the latest research progress of the four core components of QDSSCs (photoanode, quantum dot sensitizer, electrolyte system, and counter electrode materials). By modifying black titanium dioxide and heterostructured composite photoanodes (e.g., TiO2@ZnO, g-C3N4@TiO2), the photoelectron transfer efficiency of photoanodes has been significantly improved, with the highest photoelectric conversion efficiency (PCE) of 9.11%. The application of organic chalcogenide quantum dots has led to a PCE exceeding 18%, while novel deposition techniques (e.g., CLIS/DA method) have enabled the more conventional ZCISe quantum dot cell to exceed 17% PCE, while improving its stability. Solid/quasi-solid electrolytes (e.g., polysulfide gels, Ce-doped LaMnO3) effectively solve the problem of volatilization and corrosion of liquid electrolytes, and improve PCE by 33%. High entropy sulfide and metal-organic framework derived pairs of electrode materials further optimized the catalytic performance and cell efficiency. Although the lab efficiency is close to 8%, the long-term stability (thousand-hour test limit) and scale-up production of QDSSCs are still key challenges.

1 INTRODUCTION

Driven by the global energy structure transition and carbon neutrality goals, solar energy has become a core solution to alleviate fossil energy dependence and environmental pollution. Currently, traditional silicon-based solar cells dominate the solar photovoltaic (PV) market, but their photovoltaic conversion efficiency is close to the theoretical limit (~29%), and their production suffers from difficulties in the production of high-purity monocrystalline silicon feedstock, as well as high energy consumption for production.

Quantum dot sensitized solar cells (QDSSCs), as the third generation of solar cells derived from dye-sensitized solar cells (DSSCs), are characterized by a simple manufacturing process and relatively inexpensive raw materials. Moreover, quantum dots (QDs), with their quantum-limited-domain effect, size-dependent energy band tunability, and multi-exciton generation (MEG) properties, can achieve efficient absorption of the full wavelength of the solar spectrum, which results in a theoretical upper limit of the efficiency of quantum dot-sensitized solar cells as high as about 44%, which is much higher than the S-Q limit of 33.7% for single-junction cells. In recent years, with the increasing research on QDSSC, its laboratory efficiency has been increased to more than 18%, showing great potential for application. However, this efficiency still falls short of that of single-junction silicon-based cells, and its stability, flexibility, and environmental toxicity need to be improved urgently.

The main direction of research on QDSSCs lies in the targeted optimization of each structure of QDSSCs, and this paper will outline the research progress of QDSSCs in terms of each core component in the QDSSCs assembly respectively, and by summarizing the latest and advanced research results, this paper aims to provide researchers with the ideas to advance the QDSSCs from the laboratory to industrialization.

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2 STRUCTURE AND PRINCIPLE OF QDSSCS

As shown in Figure 1, the main structure of QDSSCs consists of quantum dots, photoanode, electrolyte and counter electrode. Among them, quantum dots are a nanoscale semiconductor material with a size-dependent energy band structure, which can be tuned in size to achieve precise adjustment of light absorption or emission wavelength. As the main absorbing structure of sunlight, quantum dots produce electron-hole pairs after absorbing light energy. The photoanode is the electrode that absorbs light energy and injects photogenerated electrons into the external circuit, often composed of semiconductors such as TiO_2, which assumes the function of electron generation and transmission in photoelectrochemical devices and is a good loading platform for quantum dots, and accepts photoelectrons generated by the QDs, and then transmits the photogenerated electrons to the counter electrode via the conductive glass and the external circuit. The counter electrode is used to receive electrons from the external circuit and catalyze the reduction of oxidized species in the electrolyte, thus closing the circuit and keeping the system running. The photogenerated holes are transferred to the electrolyte, which is the ionic conductor connecting the photoanode to the counter electrode and is responsible for transporting ions to maintain charge balance and complete the redox cycle. Finally, the electrolyte accepts electrons from the external circuit through the counter electrode and is reduced, thus completing the battery cycle.

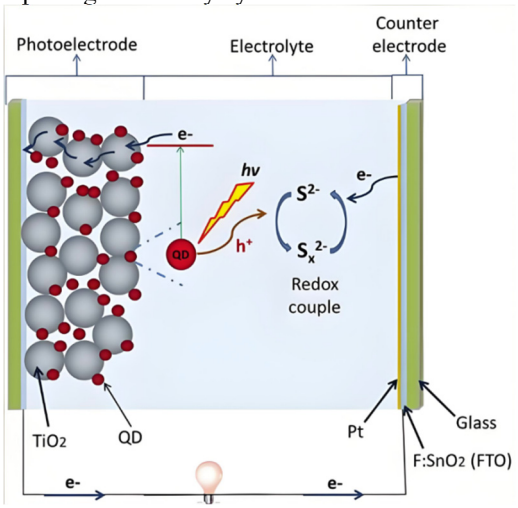

Figure 1: Schematic structure of quantum dot sensitized solar cells (QDSSCs) (Photo/Picture credit: Original).

3 PERFORMANCE AND OPTIMIZATION OF QDSSCS

The core performance indicators of QDSSCs cover photoelectric conversion efficiency (PCE), open-circuit voltage (Voc), short-circuit current (Jsc), fill factor (FF), and stability. Among them, photoelectric conversion efficiency (PCE) is the most important indicator for evaluating solar performance, reflecting the ability of the cell to convert light energy into electricity. The open-circuit voltage determines the voltage output of the cell in the open-circuit state, while the short-circuit current is directly related to the number of photogenerated carriers, both of which together affect the output performance of the cell. The fill factor = (maximum output power) / (Voc × Jsc) reflects the cell output characteristics. In addition, stability is crucial for the practical application of QDSSCs, which determines the lifetime and reliability of the cell, which can be effectively improved by means of adopting antioxidant quantum dots and encapsulation technology.

3.1 Photoanode

In QDSSCs, the ideal photoanode should have more attachment sites for quantum dots, lower compounding rate of photogenerated electrons, and excellent electron injection and transfer capability. Among them, TiO2, as a wide bandgap semiconductor, is still the most widely used photoanode material due to its excellent chemical stability, non-toxicity, low cost and relatively fast electron transfer rate (Akash, Shwetharan & Kusuma, 2022). The current research on TiO2 mainly lies in the further doping or compounding of TiO2 nanomaterials with different morphologies that have been explored.

Black titanium dioxide possesses higher photocatalytic activity due to its abundant oxygen defects and Ti3+. Jiang et al. (2024) and Yao et al. (2022) conducted studies on black TiO2 nanoparticles for the fabrication of photo-anodes for QDSSCs, respectively, where Jiang et al. (2024) used the black TiO2 produced by hydrogenation reduction as the photo-anode to achieve the FF and short-circuit current density (Jsc) obtained an enhancement of about 30%, which led to an enhancement of the final PCE by about 71% to 5.3% when all other conditions remained unchanged. On the other hand, Yao et al. (2022) prepared black TiO2 for the assembly of QDSSCs by modifying TiO2 of different crystal types under femtosecond laser, and the PCE of QDSSCs assembled with rutile TiO2 was as high as 9.11%,

which is 2.27 times higher than that of the pristine TiO2 QDSSCs, by laser-modifying rutile TiO2 to black TiO2 in ethanol. Regarding the composite TiO2 materials, Li et al. investigated the TiO2 heterostructure composite photoanodes, Li et al. (2024) fabricated hexagonal nanopillar array photoanodes with TiO2-coated ZnO heterostructure and TiO2 nanorods with g-C3N4@TiO2 heterostructure, which resulted in a higher PCE of QDSSCs compared to simple ZnO nanopillar array photoanodes and TiO2 photoanodes, respectively. anodes resulted in 25% and 17% enhancement in PCE of QDSSCs, respectively, and increased the stability of the photoanodes (Li et al., 2024). The above studies show that TiO2 has the advantages of good photocatalytic performance, chemical stability, non-toxicity and environmental protection, and low price, which is widely used in the fields of wastewater treatment, air purification, and photocatalytic hydrogen production. However, it only responds under ultraviolet light, and the photogenerated electrons and holes are easy to compound, which limits its catalytic efficiency. Through metal/non-metal doping, noble metal deposition, semiconductor composite, dye sensitization and other modification means, it can effectively broaden the light response range, enhance the electron separation ability, and significantly improve the photocatalytic activity. Modified TiO_2 materials also exhibit excellent visible light catalytic ability and cyclic stability. Future development directions include enhancing visible light utilization efficiency, developing multi-component synergistic modification technology, enhancing material stability and reusability, exploring green and low-consumption synthesis processes, as well as in-depth study of photocatalytic reaction mechanisms, etc., in order to achieve more efficient and wider environmental and energy applications.

3.2 Quantum Dot Sensitizers

The optimization of quantum dot sensitizers for QDSSCs mainly lies in the optimization of the design of the quantum dots themselves and the optimization of the quantum dot deposition method. Aqoma et al. (2024) designed a type of perovskite-based CQDs (PQDs) based on organocation cationic groups with a narrower bandgap, and adopted a ligand-exchange strategy based on ammonium iodide to enhance the surface passivation effect of PQDs by replacing long-chain oleyl ligands to improve their photovoltaic performance and long-term stability. A ligand exchange strategy was employed to enhance the surface passivation of the PQDs by substituting long-chain oleyl ligands to improve their photovoltaic properties and long-term stability. The QDSSCs assembled with such organic PQDs obtained the highest PCE of up to 18.1% in the laboratory so far and had a photostability of 1200 h. Wang et al. (2025) deposited water-soluble ZCISSe QDs on TiO2 nanorods substrates by first using a once-capped ligand-induced self-assembly chemical deposition method (CLIS method), and then on this basis by direct deposition method (DD method). The oil-soluble ZCISSe QDs were deposited on the substrate by direct deposition (DA method), which increased the quantum dot loading. Meanwhile, in this device, the photoanode is passivated by the quantum dots themselves, so the device can reduce the introduction of surface engineering reagents, lower the fabrication cost of the device, and effectively suppress the undesired charge complexation at the photoanode/electrolyte interface, as well as improve the stability of the device. The QDSSCs obtained by this method of deposition obtained a PCE of up to 17.01%, which is the highest efficiency among the existing liquid junction QDSSCs. Quantum dot sensitizers in QDSSCs have the advantages of tunable bandgap, wide range of light absorption and multi-exciton generation, which can significantly enhance the photoelectric conversion efficiency. Its performance can be further enhanced by optimizing the quantum dot structure and deposition method. In the future, novel quantum dot material design, surface-interface engineering optimization and scalable deposition process can be used to achieve high-efficiency, low-cost and long-term stable QDSSCs.

3.3 Electrolyte System

The liquid electrolyte in conventional QDSSCs faces common problems such as volatilization, leakage and corrosion. For the electrolyte system of QDSSCs, the current research hotspot is to improve the long-term stability of the battery and reduce the encapsulation requirement of the battery by switching to solid-state or quasi-solid-state electrolytes for QDSSCs (Prajapati et al., 2020). Wang et al. (2025) combined traditional polysulfide electrolytes with sodium alginate, and obtained quasi-solid-state polysulfide gel electrolytes. ZCISe QDSSCs assembled with them obtained a PCE of 8.85%, which is 6% higher than the PCE of liquid polysulfide under all other conditions being equal, and they are 3.2 times more stable than the liquid polysulfide electrolyte QDSSCs, as well as being more environmentally friendly. The

same research team fabricated quasi-solid polysulfide electrolytes by spin-coating Ce-doped LaMnO3 hole-transporting materials on semiconductor photoanodes, drying them, and then immersing them in polysulfide electrolyte (Wang etl al., 2025). The PCE of the assembled QDSSCs reaches 9.14%, which is 33% higher than that of the same standard liquid electrolyte QDSSCs, and the lifetime is 5% higher, and the QDSSCs show significant stability advantages over the liquid electrolyte QDSSCs in other aspects. Current research focuses on the development of solid or quasi-solid electrolytes, aiming to improve environmental adaptability and packaging simplicity. For example, quasi-solid polysulfide electrolytes can be constructed by introducing sodium alginate gels or $LaMnO_3$-doped hole-transporting materials, which can significantly enhance stability and environmental friendliness while improving PCE. The future development direction should focus on the design of quasi-solid-state or solid-state systems with high conductivity, low cost, and scalability.

3.4 Counter Electrode Materials

The main role of the counter electrode is to collect the electrons from the external circuit and transfer them to the electrolyte by catalytic reduction oxidation of the electrolyte. Ideal electrode materials should satisfy the following properties: 1) simple and low-cost preparation process; 2) good electrical conductivity and high catalytic activity; and 3) excellent chemical stability in the electrolyte environment. Wang et al. (2025) prepared high-entropy metal sulfide nanoparticles with the composition of (CdCuCoMnZn)Sx by the solution method and coated them directly on the FTOs by using screen-printing technique. The QDSSCs assembled in this way had an open-circuit voltage of 0.665 V and a high FF of 0.49, and the electrocatalysts were obtained by cyclic voltammetric stability test to have better electrochemical stability than other sulfide electrocatalysts, demonstrating the potential of high-entropy polysulfides as a pair of electrode materials for QDSSCs. Zhang et al. (2025) on the other hand, annealed ZIC-64 organometallic metal by high temperature framework, and then attaching MoS2 by vapor deposition to make the base material of the counter electrode, and finally depositing it on the mesoporous carbon supported by titanium mesh to produce a high-performance counter electrode. The QDSSCs assembled with the counter electrodes made of this material and ZCISe have a PCE of up to 16.39% and an excellent filling factor of up to 0.735.

The counter electrode plays a key role in QDSSCs to collect electrons and catalyze the reduction of electrolyte, and excellent counter electrode materials need to be highly conductive, catalytically active, chemically stable, and cost-effective. Nevertheless, the current non-precious metal catalytic materials still have limitations such as insufficient electrical conductivity, unstable catalytic sites, and complicated device preparation processes, which affect their promotion in commercialization. Future development should focus on the construction of multifunctional composite structures, the precise regulation of catalytic activity centers, the development of scalable and low-cost preparation processes, and the exploration of materials that take into account high performance and environmental friendliness, in order to promote the industrialization of highly efficient, stable, and sustainable QDSSCs.

4 CONCLUSION

Quantum dot-sensitized solar cells are the most competitive third-generation solar cells in the energy market due to the low cost of raw materials as well as the simplicity of the fabrication process, and their research history breaks the stereotype that semiconductor photovoltaic devices require high-purity, high-quality semiconductors. Currently, a variety of quantum dot-sensitized solar cells with photovoltaic conversion efficiencies of 16% or more have been fabricated in the laboratory, with efficiencies much higher than those of commercially available, inexpensive thin-film solar cells and polycrystalline silicon semiconductor cells, and the structures and theories of the various components have been matured.

As far as the present situation is concerned, the initial exploration of the marketable and industrialized production of QDSSCs based on ZCISe and organic chalcogenide quantum dots is ready to start. However, the stability test experiments of QDSSCs in the current research are limited to the thousand-hour level, and in the future, it is necessary to combine multi-scale simulation modeling techniques (e.g., first-principle calculations and device-level degradation simulations) to predict the degradation mechanism of the material interfaces and the environmental tolerance, and to provide theoretical guidance for the long-life design, in order to carry out simulation prediction of the stability of

QDSSCs for years or even decades of use. Simulation prediction.

Looking ahead, QDSSCs have the potential to shine in new application scenarios such as flexible electronics, building-integrated photovoltaics, and low-light environment energy systems. Their low-cost and easy-to-prepare characteristics also allow QDSSCs to provide energy security for people in poor production conditions, such as in disaster areas and on other planets.

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