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Surface Engineering of CdTe Quantum Dots for Improved Optical Stability and QLED Applications: A Review

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Abstract. In the past several years, quantum dots (QDs) have gained considerable attention due to their unique properties and wide range of applications. Nevertheless, drawbacks and limitations of QDs still exist and affect their practical use. This review investigates surface engineering strategies that enhance optical stability and examines their application in quantum dot light-emitting diodes (QLEDs). It compares passivation mechanisms, advantages, and inherent limitations of organic ligand engineering (including small-molecule, long-chain, and multifunctional ligands) and inorganic shell engineering (including ZnS and CdS shells). It analyzes how these surface modifications impact optical stability, luminescent behavior, and QLED device performance. Furthermore, it discusses the significant challenges that researchers are facing, such as insufficient optical stability of CdTe QDs, long-term stability degradation, the complexity of regulating ligand–QD interactions, and the difficulty of balancing optical stability with charge transport. This review also clarifies the correlation between surface chemistry and optical stability of CdTe QDs, and outlines future research directions. It provides guidance for developing high-stability CdTe QDs for high-performance QLED applications.

Keywords: CdTe quantum dots, surface engineering, optical stability, ligand engineering, QLEDs

1. Introduction

In recent years, quantum dots (QDs) have attracted significant attention in optoelectronic applications because of their tunable optical properties and emission wavelengths, which cover the visible-light region. They also exhibit high photoluminescence quantum yields (PLQYs), excellent color purity, and outstanding optical properties, which have promoted their applications in advanced display technologies. Among these semiconductor quantum dots, CdTe quantum dots have been widely used and studied in optoelectronic and biomedical applications such as photovoltaic cells and biomedical tags because advances in synthesis enable researchers to obtain high-quality QD ensembles with narrow size distributions [1]. However, their further application is still restricted by insufficient optical stability, which mainly arises from surface defects and oxidation and is further aggravated by photodegradation.

In order to overcome these limitations, researchers have developed promising surface engineering strategies, including surface ligand engineering and inorganic shell engineering, which involve

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modifying the surface structure of CdTe quantum dots and passivating surface defects [2]. Previous studies have reported various surface modification approaches, including small-molecule ligands, long-chain organic ligands, multifunctional ligands, and inorganic shell modification, and demonstrated that surface chemistry can significantly affect the optical properties and stability [3, 4]. However, differences in ligand structure, surface interactions, and protection mechanisms can result in different effects on surface passivation, particle growth, photoluminescence, and long-term stability. Therefore, further research and analysis are required to find more efficient strategies for improving the optical stability of CdTe QDs for high-quality quantum dot light-emitting diode (QLED) applications.

This review focuses on surface engineering strategies for improving the optical stability of CdTe quantum dots and their applications in QLEDs. Through a literature review, it compares organic ligand engineering and inorganic shell engineering in terms of their mechanisms, advantages, and limitations, and evaluates how surface modification affects the optical stability of CdTe QDs and QLED performance. The main contribution of this review is to clarify the relationship between surface chemistry and optical stability and to highlight the challenge of balancing long-term stability with the electronic requirements of QLED applications.

2. Fundamentals of CdTe quantum dots and optical stability mechanism

2.1. Structure and optical properties of CdTe quantum dots

CdTe QDs are semiconductor nanocrystals with dimensions smaller than the exciton Bohr radius. This allows them to exhibit pronounced quantum confinement and distinctive optical properties. CdTe QDs generally exhibit a crystalline structure with a cubic zinc blende phase.

The quantum confinement effect gives distinctive, size-dependent optical properties in CdTe QDs, especially in their absorption and photoluminescence (PL) spectra. As the size of the nanocrystals increases, the quantum confinement effect becomes weaker, resulting in a decrease in the effective band gap. This leads to a shift in the excitonic absorption and PL emission peaks from shorter to longer wavelengths, indicating that the optical response depends on the particle size of the nanocrystals. Particle size distribution also affects the optical properties, so precise control of nanocrystal size is important for stable optical performance.

Due to their nanoscale dimensions, CdTe QDs have a high surface-to-volume ratio. This means that a relatively large proportion of their atoms are located at the surface compared to bulk CdTe. As a result, their optical properties are highly sensitive to changes in surface states. In addition, variations in particle size and size distribution can also alter the surface-to-volume ratio, thereby affecting the influence of surface defects and trap states on the optical properties of CdTe QDs. Moreover, surface defects and trap states can introduce additional energy levels within the band gap, capturing photogenerated electrons and holes in the process. These captured charge carriers may undergo non-radiative recombination rather than radiative recombination, resulting in energy loss and decreasing the PL quantum yield and PL intensity. Therefore, surface defects and trap states can have a significant impact on the optical performance of CdTe QDs.

2.2. Factors affecting the optical stability of CdTe quantum dots

The optical stability of CdTe QDs depends on their particle size, surface chemistry, and the surrounding environment. Surface chemistry can determine the interaction between surface ligands and surface atoms, thereby influencing surface defects and the PL behavior of QDs [5]. A previous

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study also showed that the type of thiol ligand can affect the growth kinetics, size distribution, and PL of aqueous CdTe QDs. For example, thioglycerol (TGH) and glutathione (GSH) showed different effects on QD growth. TGH exhibited stronger binding to the QD surface, which inhibited particle growth, whereas GSH promoted faster particle growth [3]. In addition, the thermal decomposition of thiol ligands during synthesis can result in a cadmium sulfide (CdS) shell, which can further change the surface structure and optical behavior of the QDs [3]. Ma et al. reported that laser radiation can break Cd-S bonds and detach thiol ligands, leading to QD aggregation and increased surface defects [6]. Thus, the effect of surface chemistry extends beyond the ligand itself and can also influence the structural characteristics of the QDs.

3. Surface modification strategies for improving the optical stability of CdTe QDs

3.1. Organic ligand engineering

Organic ligands are commonly used for the surface modification of CdTe QDs and can be classified according to their molecular structure and functional groups.

3.1.1. Small-molecule ligands

Small-molecule ligands are compounds with relatively low molecular weight and compact structures that allow their functional groups to coordinate with surface atoms of CdTe QDs. Their small molecular size also enables close interaction with the QD surface and facilitates passivation of surface defects [5].

In particular, MPA and TGA are two commonly used thiol ligands for aqueous CdTe QDs. Previous studies have found that the molecular structure of both MPA and TGA can influence the optical properties and growth behavior of CdTe QDs. Higher ligand coverage can provide more effective surface passivation, which may contribute to higher PL quantum yields (Φf) and stronger PL. Small-molecule ligands passivate surface trap states, suppressing non-radiative recombination and enhancing PL [3].

The influence of ligand modification was also reflected in the growth behavior and the size distribution of the particles. Silva et al. reported that despite differences in their molecular structures, MPA- and TGA-capped QDs exhibited comparable growth kinetics. However, TGA-capped QDs showed a broader size distribution at the beginning of the reaction. In contrast, MPA-capped QDs maintained a narrower particle-size distribution across the different synthesis times. The results suggest that MPA and TGA affect CdTe QD growth differently. This phenomenon may be caused by differences in the surface interactions between the ligands and surface atoms. Since particle size and particle-size distribution are closely related to the optical properties of QDs, controlling these characteristics through ligand modification may contribute to more consistent optical performance. Furthermore, Schneider et al. demonstrated that the optical properties of thiol-capped CdTe QDs can be affected by surface ligand chemistry and surrounding conditions [5]. The effectiveness of small-molecule ligands therefore depends on ligand structure, surface interactions, and environmental conditions.

3.1.2. Long-chain organic ligands

Long-chain organic ligands are another important class of ligands used to regulate the properties of CdTe QDs. Organic ligands can be classified according to their functional group, for example,

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ligands with long polyether chains, ligands with long polysiloxane chains, and the ligands with alkyl groups, such as oleic acid (OA). Compared with small-molecule ligands, their extended hydrocarbon chains can provide steric stabilization and influence the interactions between QDs and the surrounding environment [7]. The long chains provide steric hindrance between QDs, helping to reduce particle aggregation and maintain colloidal stability.

For CdTe QDs, long-chain organic ligands such as amines, phosphonic acids, and phosphine oxides can influence growth and surface stabilization. Studies on hexadecylamine (HDA), hexyl phosphonic acid (HPA), and trioctyl phosphine oxide (TOPO) showed that CdTe QD stability was associated with surface stabilization by HDA or HPA, and that removing HPA prevented quantized growth, indicating that the ligand environment affects the formation of QDs with specific sizes [8]. Hassinen et al. also demonstrated that tetradecylphosphonic acid and oleylamine form a mixed ligand shell of tightly bound phosphonate and amine ligands, which changes the surface chemical environment of CdTe QDs [9]. However, this ligand layer can also hinder charge transfer across the interface, because it affects the electronic coupling between the QDs and adjacent materials. Long-chain ligands can improve stabilization but may reduce charge transfer efficiency.

3.1.3. Multifunctional ligands

Multifunctional ligand engineering refers to the use of surface ligands that can simultaneously provide multiple functions, such as surface passivation, colloidal stabilization, biocompatibility, and further functionalization. Glutathione (GSH) is a representative multifunctional ligand for CdTe QDs. Its thiol group can bind to Cd atoms located on the QD surface, while its other functional groups can interact with the surrounding environment and biomolecules [10].

For CdTe QDs, the interaction between the thiol of GSH and the QD surface can contribute to surface passivation by reducing the surface trap states and improving the PL performance. Meanwhile, the GSH layer can act as a protective barrier, limiting the release of toxic metallic ions and providing an additional application in biology. Chen et al. demonstrated that GSH-capped CdTe QDs have relatively low toxicity [10]. Furthermore, GSH-capped CdTe QDs showed good water solubility and could readily link with biomolecules, which extends their applicability in aqueous biological environments [10]. Cell viability remained above 80% even after 24 hours of incubation at the tested concentration [10]. Studies have reported that GSH-capped CdTe/CdSe core-shell QDs have good dispersity, tunable near-infrared (NIR) emission, and biocompatibility. Additionally, after conjugation with RGD peptides, these QDs can target tumor cells, showing that GSH functionalization provides a method for biomolecular modification [11].

3.2. Inorganic shell structure modification

Inorganic shell modification is an effective strategy for improving the optical stability of CdTe QDs by depositing a semiconductor layer around the CdTe core to form a core-shell structure. Compared with ligand modification alone, a shell of a higher-band-gap semiconductor can provide both surface passivation and physical protection, especially in the type-I core-shell structure, which can reduce the influence of environmental factors, such as oxygen and water molecules, by separating the optically active CdTe core from the surrounding environment [12]. Moreover, the shell can passivate cationic and anionic surface defects, reducing non-radiative recombination on surfaces and improving the fluorescence properties of the QDs [12]. However, the efficiency of the protection depends on the integrity of the shell. If the shell has not grown completely and the bare core remains

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exposed, photoactivation and photocorrosion can still occur under prolonged irradiation [13]. Hence, effective protection depends on complete shell coverage.

3.2.1. ZnS

Zinc sulfide (ZnS) is an important shell material for CdTe QDs. Patra et al. demonstrated that controlled deposition of a ZnS shell can significantly enhance the fluorescence brightness and photostability of CdTe QDs. Compared with MPA-capped CdTe QDs, ZnS-capped CdTe QDs with a two-monolayer ZnS shell showed minimal changes in emission intensity and maintained a stable emission peak during prolonged illumination. In contrast, MPA-capped CdTe QDs initially exhibited photoactivation, followed by a strong emission quenching and a blue shift. The results suggest that the ZnS shell improves surface passivation and provides better protection of the CdTe core against photoactivation and photocorrosion [13].

3.2.2. CdS

Previous research has found that increasing the thickness of the CdS shell can reduce the rate of PL degradation in CdTe/CdS QDs under irradiation. Researchers also proposed that photooxidation involves a three-stage mechanism: oxidation of anion vacancies, oxidation of exposed core regions, and slow oxidation of the core through oxygen diffusion in the shell. Therefore, a thicker CdS shell may provide better protection for the CdTe core by decreasing the time that the CdTe core is directly exposed to the surrounding environment and increasing the barrier for oxygen diffusion. However, a CdS shell can only slow the process rather than completely prevent long-term photooxidation. Moreover, an overly thick shell can also lead to a decline in fluorescence intensity under specific conditions. An excessively thick shell may also alter the carrier-confinement regime and spatial distribution of electrons and holes, which can reduce the probability of radiative recombination under certain structural conditions [14].

4. Applications of surface-engineered CdTe quantum dots in QLEDs

4.1. Applications in QLED emitting layers

Due to the special optical and surface properties of QDs, QD light-emitting diodes (QLEDs) have become a popular choice for next-generation displays and solid-state lighting. As emissive materials, II-VI semiconductor QDs, such as CdTe QDs, can offer tunable emission wavelengths, which which make them suitable for emitting layers of QLEDs. In a QLED, electrons and holes are injected into the QD emitting layer, where they combine and generate electroluminescence. Therefore, high-efficiency carrier injection, transport, and recombination within the QD layer are essential for QLED operation [15].

Pidluzhna et al. demonstrated that CdTe/CdS core-shell QDs, synthesized in an aqueous medium and stabilized with thioglycolic acid, are widely used in light-emitting devices. The CdTe/CdS QDs act as the emission layer and are used to produce light-green electroluminescence. The EL spectrum differs from the PL spectrum. The main EL band at 530 nm is attributed to the emission of the CdTe core, while the other EL band at 595 nm is caused by the recombination of electrons in the CdS conduction band with holes in the CdTe valence band. This means that these CdTe/CdS core-shell QDs are able to create multi-channel electroluminescence involving different recombination pathways within the core-shell structure.

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4.2. Enhancement of QLED device performance

The successful application of CdTe QDs in QLEDs not only depends on their favorable optical properties, but also on efficient charge transport and recombination within the emissive layer. Lin et al. demonstrated the potential of type-II CdSe/CdTe core-shell QDs in deep-red QLEDs. This study reported that these QDs achieved relatively high external quantum efficiencies, which demonstrated their potential for efficient electroluminescence in QLED applications [16].

Surface ligand engineering can further enhance the performance of CdTe-based QLED devices. Feng et al. demonstrated that chloride treatment of CdTe/CdSe type-II QDs improved the performance of NIR QLEDs. For a device with a PL peak at 788 nm, the peak EQE increased to 7.2%, a 26.3% improvement over the untreated device, and the maximum radiant emittance increased by 24.5% [17]. The improved device performance was attributed to chloride treatment of the QD surface. The treatment enhanced charge transport, reduced carrier accumulation, and promoted radiative electron–hole recombination within the QD layer [17].

5. Discussion

5.1. Challenges

5.1.1. Stability and surface chemistry challenges

Despite the surface ligand engineering and inorganic shell engineering developed in recent years, the long-term optical stability of CdTe QDs remains a challenge. One major issue is the degradation of QDs during prolonged storage and exposure to light. Wansapura et al. found that CdTe QDs stored in water or buffer solutions degraded rapidly, especially under light exposure and elevated temperatures [18]. Buffer storage provided only limited improvement, and significant degradation still occurred during long-term storage.

5.1.2. Complexity of controlling ligand-QD interactions

Another difficulty is the complexity of controlling ligand-QD interactions. Previous experiments have shown that the PL and colloidal stability of CdTe QDs undergo pH-dependent changes following TGA and MPA functionalization. These characteristics are influenced by the pKa values of the ligand functional groups, the ligand shell, and the overall ligand concentration. Therefore, to achieve stable colloids and optimal PL properties, multiple factors such as concentration and surface coverage still need to be carefully regulated [5].

5.1.3. Trade-off between photostability and charge transport

Inorganic shell engineering can improve optical stability but cannot completely prevent photooxidation. Long-term irradiation of CdTe/CdS core-shell structures can result in PL loss and a blue shift due to photooxidation. Their optical stability depends on both the thickness of the CdS shell and the Cd/Te ratio. Furthermore, the type of ligand can affect QD growth, quantum yield, and core-shell formation. For example, GSH-capped CdTe QDs are able to form a thicker CdS shell, which shows improved photostability. However, an overly thick shell can also reduce the efficiency of charge transport.

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5.2. Future directions

Based on the challenges discussed above, future research should focus on improving the long-term stability of CdTe QDs, gaining better control over ligand-QD interactions, and finding a balance between the protective effect of the inorganic shell and the requirements for charge transport.

5.2.1. Improving long-term optical stability

New surface modifications need to resist degradation efficiently over the long term. Because the stability of CdTe QDs is affected by light exposure, temperature, and other external factors, optical properties measured only at the initial stage cannot represent long-term stability. Longer-term stability tests under different irradiation, temperature, and storage conditions are therefore necessary. Different ligands and shell structures should be compared under the same conditions to identify strategies for maintaining the optical properties of CdTe QDs over a long period.

5.2.2. Optimizing the interaction between ligands and QDs

The combination of ligands at optimized ratios is a promising route to better optical properties. Verheles et al. demonstrated that combining MPA and N-acetyl-L-cysteine (NAC) can produce synergistic effects. MPA provided efficient passivation during the early stage of QD growth, while NAC provided better long-term optical stability. When the MPA:NAC ratio was 1:2, the resulting QDs had a narrow size distribution and a quantum yield of up to 66%, while maintaining stable luminescence under long-term irradiation. Even after irradiation with a 405 nm laser for 29 hours, the quantum yield varied by only 1–3% [19]. These results indicate that optimizing ligand combinations and ratios can improve both passivation and long-term stability.

5.2.3. Balancing shell protection and charge transport

For inorganic shell engineering, the key issue is to balance optical protection and charge transport. Shells with different thicknesses, compositions, and structures should be explored to provide sufficient protection while maintaining the electrical and optical properties required for practical QLED applications.

6. Conclusion

Because of the outstanding optical properties of CdTe QDs, they have become promising materials for optoelectronic applications, such as QLED displays. However, their optical instability, particularly during long-term storage and light exposure, remains an important limitation for practical applications. To solve this issue, researchers have investigated various surface engineering strategies to improve surface passivation, colloidal stability, photoluminescence, and photostability. Previous studies have shown that these strategies can effectively regulate the surface properties and optical stability of CdTe QDs. However, the results have also shown that relying on a single modification may have limitations in enhancing optical stability and surface properties. Moreover, researchers have found that combining different ligands can further improve optical stability and other properties.

This review is based on secondary research, and no primary experiments were conducted. Future studies should therefore focus on systematic long-term stability tests and coordinated optimization of ligand chemistry, surface properties, and core-shell structures for practical QLED applications.

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