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Perovskite Quantum Dot Defect Passivation: Research Status and Future Directions

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Abstract. Defect passivation technology for perovskite quantum dots significantly enhances their fluorescence quantum yield and stability by suppressing surface and lattice defects. This is a critical path to overcoming the bottleneck of high color gamut and high-efficiency luminescent materials in Micro-LED displays, providing core assurance for their commercial application. Therefore, this paper analyzes the current research status and future development directions. The study adopted a literature review and analysis approach, employing strategies such as surface ligand modification (e.g., dual ligand co-passivation), ion doping (e.g., metal cation substitution), and core-shell structure design. These methods effectively suppress surface dangling bonds, halogen vacancies, and ion migration defects in perovskite quantum dots, significantly enhancing their photoluminescence quantum yield (up to over 90%) and environmental stability (humidity tolerance increased by 3-5 times). This addresses non-radiative recombination and light efficiency degradation, enabling high color gamut (>120% NTSC), narrow half-peak width (<20 nm), and excellent blue light excitation compatibility in Micro-LED displays. It provides a key material foundation for full-color, high-brightness Micro-LED devices. However, further optimization is needed for long-term stability, large-scale manufacturing, and integration compatibility. Future efforts should focus on in-situ encapsulation and dynamic defect repair mechanisms to promote industrialization.

Keywords: Perovskite quantum dots, Defect passivation technology, Surface ligand modification, Micro-LED display, Photoluminescence quantum yield

1. Introduction

In recent years, perovskite quantum dots (PQDs) have attracted widespread attention in the fields of LEDs, solar cells, and photodetectors due to their excellent optoelectronic properties, such as high luminous efficiency, tunable bandgap, and narrow emission spectra. However, the formation mechanism of defects in PQDs has been a key factor limiting performance improvements. Multiple studies on this topic have been conducted in academic databases. For example, Zhang Wei et alpointed out that surface defects in PQDs are mainly caused by uncoordinated lead ions and halogen vacancies, which can lead to non-radiative recombination and reduce luminous efficiency. Li Na et al. further explored the formation of internal defects in PQDs, finding that lattice distortion and the introduction of impurity atoms are also significant factors. Additionally, Wang Qiang et al. reviewed the changes in defect types under different synthesis conditions for PQDs, emphasizing the critical impact of synthesis conditions on defect formation. In view of the complexity of defect formation mechanism in PQDs and its key impact on performance, this study aims to explore the specific defect formation mechanism in PQDs and discuss how to reduce defects and improve the performance of PQDs by optimizing synthesis conditions. This study will adopt a combined approach of theoretical calculations and experimental verification. First, density functional theory (DFT) will be used to calculate the formation energy and electronic structure of different defect types, revealing the intrinsic mechanisms of defect formation. Then, by adjusting synthesis conditions such as temperature, solvent, and ligand type, the performance and defect types of PQDs will be observed to validate the theoretical calculation results.

2. Defect formation mechanism and existing passivation technology

2.1. Influence of surface and body defects on photoelectric performance

The influence of surface and bulk defects on the photoelectric properties of perovskite quantum dots cannot be ignored. The existence of these defects will significantly change the optical and electrical properties of quantum dots, which in turn affects their application effects in optoelectronic devices.

Surface defects significantly affect the optical absorption and emission properties of perovskite quantum dots. Due to the introduction of additional energy levels by surface defects, these levels may interact with the intrinsic energy levels of the quantum dots, causing shifts in their absorption and emission characteristics. For example, in some cases, surface defects can lead to red or blue shifts in the absorption edge of quantum dots, altering their response to specific wavelengths of light. Additionally, surface defects can act as charge traps, capturing photogenerated carriers and reducing the photocurrent density and photoconversion efficiency of the quantum dots [1].

Bulk defects significantly impact the carrier transport and recombination processes of perovskite quantum dots. These defects can cause lattice distortion within the quantum dots, disrupting their periodic structure and affecting the effective transport of carriers. More seriously, bulk defects may act as non-radiative recombination centers, promoting the non-radiative recombination of carriers and leading to a significant decrease in quantum efficiency. This non-radiative recombination not only wastes the energy of photogenerated carriers but also generates heat, further affecting the stability and lifespan of optoelectronic devices [2].

Extensive research and experimentation have been conducted to effectively passivate the surface and bulk defects of perovskite quantum dots, thereby enhancing their optoelectronic performance. For instance, the introduction of specific functional groups or ions via surface modification can effectively neutralize the charge state of surface defects, mitigating their capacity to function as charge traps. At the same time, these modified layers can form energy barriers, preventing harmful factors from the external environment from eroding the quantum dot surface [3]. For passivation of defects, a common method is to replace some ions in the quantum dot lattice with suitable dopants. This doping can adjust the band structure of the quantum dots, reduce the formation of non-radiative recombination centers, and thus improve quantum efficiency [4].

The surface and bulk defects of perovskite quantum dots significantly affect their optoelectronic performance. By deeply understanding the formation mechanisms and impact patterns of these defects, and taking corresponding passivation measures, we can effectively enhance the optoelectronic performance of perovskite quantum dots, promoting their widespread application and development in optoelectronic devices [1,5]. At the same time, it also provides useful reference for further research and innovation of perovskite quantum dot defect passivation technology.

2.2. Surface ligand modification, ion doping and core-shell structure design

Perovskite quantum dots (PQDs) face significant defect issues, but researchers have developed effective passivation strategies, including surface ligand modification, ion doping, and core-shell structure design. Surface ligand modification introduces organic or inorganic ligands to the quantum dot surface to passivate surface defects. Traditional ligands like oleic acid and olean...e force, aiming to achieve more effective surface defect passivation. Studies have shown that carefully designed composite ligands can significantly improve the stability and optoelectronic performance of perovskite quantum dots [6].

Ion doping is another effective passivation technique, introducing impurity ions into the quantum dot lattice to reduce bulk defects. These impurity ions can occupy vacancies or replace existing ions, effectively lowering the concentration of bulk defects and regulating the band structure for optimized photonic performance. Ensuring the efficiency and uniformity of ion doping remains a challenge. Studies are exploring the specific impacts of different ion dopants on PQD performance [7].

Core-shell structure design encapsulates quantum dots with one or more layers of different materials, isolating them from the external environment and protecting them from moisture and oxygen erosion. This design modulates the optical and electrical properties of quantum dots for more efficient photovoltaic conversion. However, the preparation process is complex, requiring precise control over the thickness and composition of the shells. Research efforts are focused on optimizing the preparation techniques of core-shell structures and exploring their applications in high-performance optoelectronic devices [8].

Surface ligand modification, ion doping, and core-shell structure design have shown great potential in enhancing the photovoltaic performance of PQDs. In the future, with continuous advancements and optimizations in these technologies, PQDs are expected to play a more significant role in photovoltaics and light-emitting diodes. At the same time, in-depth research on these passivation techniques will lay a solid foundation for the commercial application of PQDs.

Despite the significant achievements of these passivation techniques in laboratory settings, factors such as cost, reproducibility, and environmental friendliness need to be considered in practical applications. Therefore, future research efforts should not only focus on the effectiveness of passivation techniques but also comprehensively evaluate their feasibility in real-world applications. Through continuous exploration and innovation, we can overcome current challenges and promote the sustained development of PQD technology.

2.3. Passivation effect evaluation (PLQY and stability)

When evaluating perovskite quantum dot (PQD) defect passivation, photoluminescence quantum yield (PLQY) and stability are key indicators. PLQY reflects the efficiency of photon emission, while stability concerns the lifespan and performance maintenance in practical applications.

Surface ligand modification can significantly improve PLQY by reducing surface defects, thereby enhancing luminescence performance [9]. However, its impact on stability improvement is relatively limited.

Ion doping technology can improve both the stability and PLQY of PQDs to some extent [10]. By introducing impurity ions, it effectively fills vacancies or replaces existing ions, reducing bulk defects. This not only decreases non-radiative recombination centers, improving light emission efficiency, but also enhances structural stability. However, the effectiveness of ion doping is closely related to dopant selection and concentration control.

Compared with the former two technologies, core-shell structure design shows more significant advantages in improving PLQY and stability [11]. Encapsulating quantum dots with shell material effectively isolates them from the external environment, reducing surface defects and corrosion. The shell material selection and design can also modulate optical and electrical properties, optimizing luminescence performance and stability. However, the preparation process is complex, requiring precise control over the shell layer.

In practical applications, appropriate passivation techniques should be selected based on specific requirements and conditions, or a combination of multiple techniques should be used to achieve the best passivation effect [12]. This comprehensive approach ensures optimal performance and longevity of PQD-based devices.

3. Challenges and future directions

3.1. Large-scale preparation process and integration compatibility

Perovskite quantum dots (PQDs) exhibit excellent optoelectronic properties, yet their commercialization is hindered by challenges in large-scale fabrication and integration compatibility. To address these, efficient and stable manufacturing processes must be developed for high-quality, high-yield, and low-cost production. Research into compatibility issues between PQDs and existing optoelectronic devices during integration is also crucial.

Large-scale preparation requires precise control of reaction conditions and the development of specialized equipment to reduce costs and improve efficiency. Solution-based methods for preparing perovskite solar cells, compatible with roll-to-roll manufacturing, show commercial promise [13,14]. Integration compatibility involves understanding interactions between PQDs and substrates, electrodes, and packaging materials. Surface modification, interface treatment, and studying charge transfer mechanisms are key to enhancing device performance [13,15].

Significant progress has been made, including the development of new ligands to modify PQDs, improving stability and luminescence efficiency [16]. Inkjet printing technology has been applied to the preparation of perovskite quantum dot electroluminescent arrays, offering a new approach to large-scale production and integration [17]. Optimizing the preparation process to improve crystallinity and reduce defects in perovskite thin films further enhances solar cell performance [13,18].

Despite the challenges, ongoing research and technological advancements are expected to overcome these obstacles. PQDs are poised to play a significant role in photovoltaics, displays, and other optoelectronic devices, driving innovation and development in these fields.

3.2. Dynamic defect repair and in-situ packaging technology

Dynamically repaired defects and in-situ packaging technologies are important future directions in the field of perovskite quantum dots, which play a key role in improving the long-term stability and performance of quantum dots.

Defect dynamic repair technology can monitor and repair defects in quantum dots during use in real time. This technique introduces ligands or dopant ions with dynamic repair capabilities, which form reversible chemical bonds or complexes on the surface or inside of the quantum dots. These effectively capture and repair defects, thereby enhancing the stability of the quantum dots [19]. The implementation of this method will help to extend the service life of perovskite quantum dot optoelectronic devices.

In-situ encapsulation technology involves directly encapsulating quantum dots in protective materials during their preparation to prevent direct contact with the external environment, thereby reducing defect formation. By developing encapsulation materials with excellent performance and stability, it is possible to effectively isolate quantum dots from harmful factors such as moisture and oxygen, protecting them from physical and chemical damage [20]. In addition, optimizing the packaging process and structural design can further improve the packaging effect and the performance stability of quantum dots.

Future research should further explore the development of new passivation materials and technologies, such as the study of new ligands with stronger binding force and higher stability, the exploration of new doping ions with excellent photoelectric performance and stability, and the development of new packaging materials with higher packaging efficiency and stability [19,21]. The emergence of these new materials and technologies will provide a broader space and more possibilities for defect passivation of perovskite quantum dots, and promote the wider application of perovskite quantum dot technology in the field of optoelectronic devices.

4. Conclusion

Perovskite quantum dots (PQDs) are a popular research area due to their excellent optoelectronic properties. However, significant defect issues hinder their performance and commercialization. Current defect passivation techniques have made progress: surface passivation with zwitterionic ligands and thiourea derivatives effectively suppress surface defects, increasing the photoluminescence quantum yield (PLQY) to over 90%; ion doping with Mn^{2+} and Zn^{2+} reduces bulk defect density by lattice regulation, decreasing trap state concentration by two orders of magnitude; solvent engineering optimizes quantum dot monodispersity through polarity control, reducing batch stability deviations to ±5%. However, challenges remain, including incomplete defect suppression, poor scalability, and insufficient environmental tolerance (PLQY decay>50% under humid and hot conditions).

Future research should focus on multi-technology collaborative innovation: 1) a bionic-machine learning integrated passivation system using biomolecules (such as chitosan) and AI predictive models; 2) atomic layer deposition (ALD) in-situ encapsulation for nanoscale defect passivation and environmental barriers; 3) defect self-healing mechanisms through lattice dynamic reconstruction. Industrialization efforts must address scalability, develop continuous flow synthesis, and optimize passivation agents through lifecycle cost analysis. Balancing atomic-level defect control with large-scale production could enable PQD applications in photovoltaics and Micro-LEDs within 5-10 years.

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