

Outstanding Brightness and Long-term Stability for Quantum Dots in QLED and Color Conversion Application, Driven by Gradient Shell Engineering

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Abstract

Gradient-shell quantum dots (gs-QDs) show enhanced photoluminescence quantum yield (PLQY) and stability, making them ideal for quantum dot light-emitting diodes (QLEDs) and white light LEDs. We present a scalable synthesis for gradient giant-shell QDs, addressing Cd-based system limitations under RoHS regulations, showcasing their potential for sustainable optoelectronic devices.

Author Keywords

Quantum Dots; gradient shell, alloy; core/shell engineering; CdSe/CdS, CdSe/CdS/ZnS; CdSe/ZnSe/ZnS; RoHS compliant

1. Introduction

Quantum dots (QDs) have emerged as a transformative material in optoelectronic applications, particularly in quantum dot light-emitting diodes (QLEDs) and color conversion technologies. Their size-tunable emission, high color purity, and exceptional photoluminescence quantum yield (PLQY) and photostability make them ideal candidates for next-generation displays and lighting systems. However, achieving both outstanding brightness and long-term operational stability remains a critical challenge, primarily due to surface defects, lattice mismatch, and nonradiative recombination processes.

Recent advances in core/shell engineering, particularly the development of giant-shell QDs, have significantly improved the performance of QDs. Giant-shell QDs, characterized by thick shells surrounding the core, effectively suppress Auger recombination and enhance photostability under high excitation conditions. These 3D structures still show the quantum size effect due to the small size of the core, but the giant shell leads to enhanced stability and huge absorption coefficients in the blue while the reabsorption rate remains neglectable. However, the abrupt interface between core and shell materials in traditional designs often introduces strain and defects, limiting their efficiency and stability.¹

Gradient shell engineering addresses these limitations by introducing a gradual compositional transition between the core and shell materials. This design reduces lattice mismatch, minimizes interfacial defects, and optimizes charge carrier confinement. As a result, gradient-shell QDs

exhibit superior brightness, enhanced PLQY, and remarkable stability, making them highly suitable for QLEDs and color conversion applications.²

Based on this knowledge, we have developed a scalable, high-volume synthesis route for gradient giant-shell QDs,

designed to produce these advanced materials with precision and adaptability. Our approach ensures not only the highest quality standards but also the capacity to meet the demands of industrial-scale applications. More importantly, we have extended the principles of gradient shell growth to tackle one of the most critical challenges in the field: the growing restrictions on the widely used CdSe/CdS system due to its heavy metal content and contrary with RoHS regulations. By leveraging our expertise, we have successfully synthesized high-performance, RoHS-compliant giant-shell QDs that maintain exceptional optical properties while adhering to modern environmental and regulatory standards.

2. Results

To enable the production of suitable quantum dots (QDs) for various applications, Fraunhofer CAN has developed an automated synthesis method for gradient GSQD.

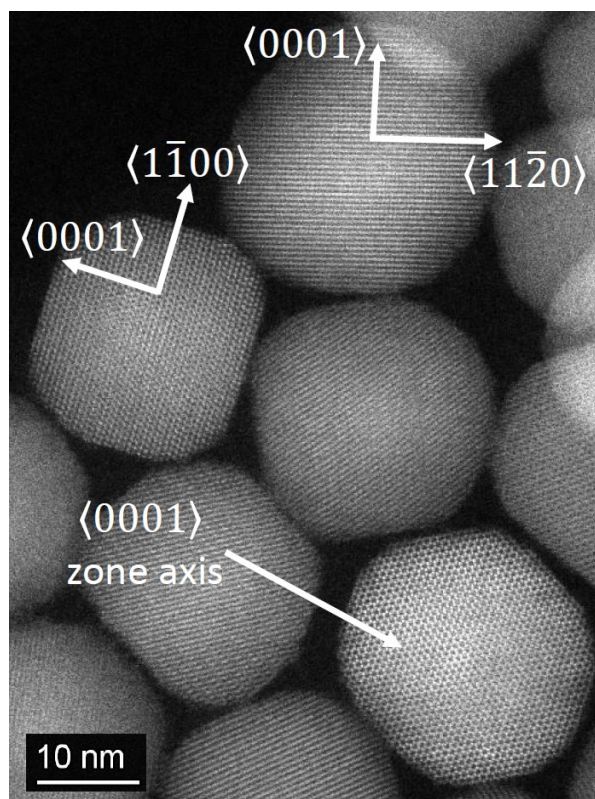


Figure 2. High-resolution transmission electron microscopy (HR-TEM) image of crystalline CdSe/CdSeS/CdS gradient giant-shelled quantum dots.

The diameter of the core particles can be adjusted between 1.6 and 5 nm, significantly affecting the band gap due to the size quantization effect.

A shell is then grown on this core, increasing the particle diameter up to 20 nm. The continuous addition of precursors facilitates defect-free shell growth with pronounced crystallinity (Figure 1).

The key for synthesizing such uniform and crystallin nanoparticles is the highly reproduceable automated semicontinuous synthesis procedure resulting in alloyed core shell transition regions. These slow transitions between the different crystal structures relax the crystal lattice mismatch over a wide account of atoms and lead to a non-tensioned lattice, validated with Raman spectroscopy and Small-Angle X-ray Scattering.

Raman Spectroscopy

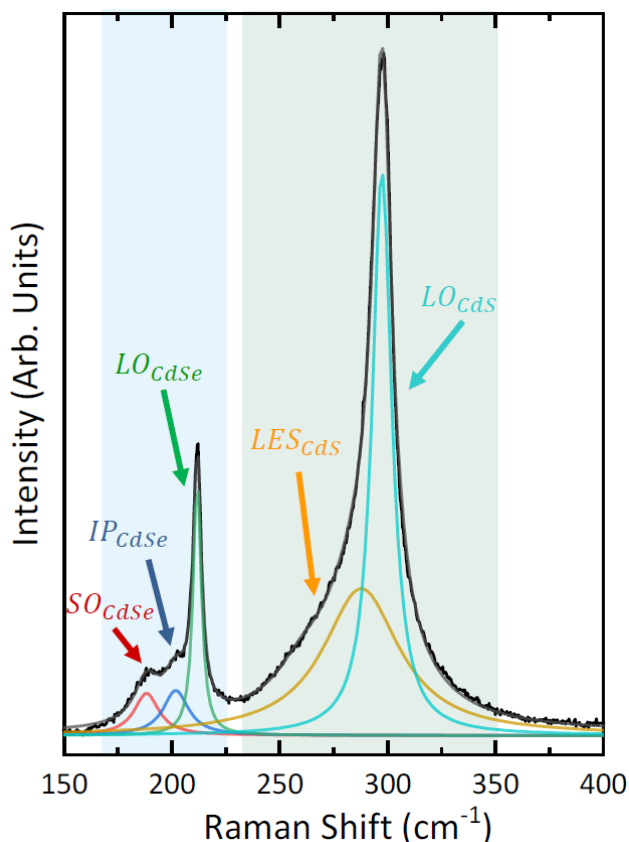


Figure 2. Raman spectra showing a high shoulder referring to an interface alloy mode.

Raman spectroscopy analyzes vibrational modes in materials, providing insights into their atomic structure and composition. In nanocrystals, Raman spectroscopy can detect size-dependent shifts in vibrational frequencies due to phonon confinement effects.

This allows for the assessment of strain, interface mixing, and the presence of alloying elements. The technique is non-destructive and can be used to probe different regions of heterogeneous nanocrystals by tuning the excitation wavelength.

Via Raman spectra of different synthesis procedure, we found the perfect settings for not tensioned Quantum Dots. A Raman spectrum of as designed gs-QDs is shown in figure 2.

Small-Angle X-ray Scattering

These findings were supported by the Data from SAXS measurements, suggesting a composition of the shell shown in figure 3.

SAXS provides information about the size, shape, and distribution of nanocrystals. SAXS measures the scattering of X-rays at small angles, which is sensitive to the nanoscale features of materials. It can reveal the size distribution and structural characteristics of nanocrystals, including the presence of alloying elements.

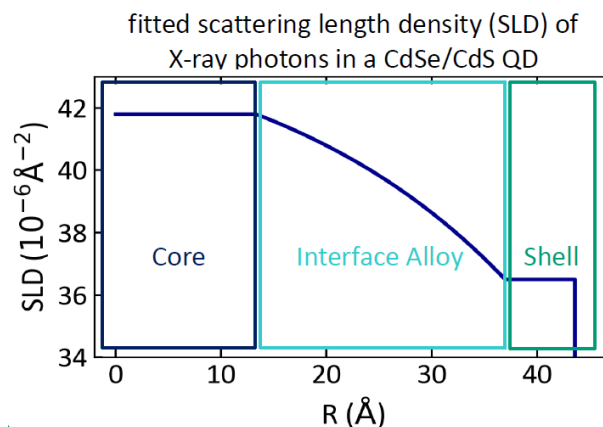


Figure 3. Suggested interface of the CdSe/CdS interface after interpretation of the SAXS Data.

The resulting giant shelled Quantum shows a quantum yield close to 1, absorption in the blue is high, while the reabsorption rate is low (figure 5). Stability measurements of these GSQDs prove that this shape is superior to 0D, 1D and 2D particles, especially concerning photoluminescence stability at high flux. However, the shell growth also results in a tremendous red shift of the emitted light compared to the core prior to shell growth. This effect makes the synthesis of red emitting GSQD favorable, while the synthesis of green emitting GSQD is a major problem. Fraunhofer CAN has solved this problem by adapting the intermediate layer between core and shell. So far, we were able to produce GSQDs with an emission between 530 and 635 nm in gram scale.⁴

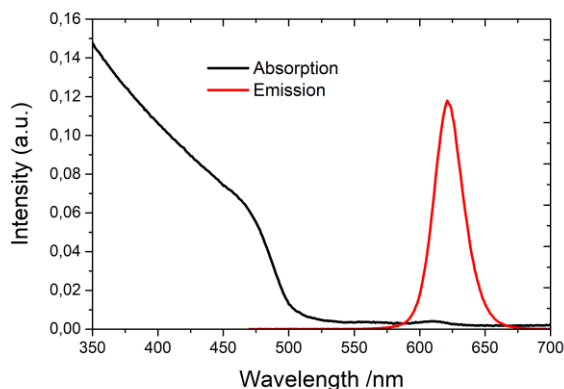


Figure 4. Absorption and emission spectra of a typical red emitting GSQD with gradient core/shell interface.

Based on these synthesis protocol we were able to adapt the procedure to more stable multishell materials with even higher stabilities like CdSe/CdS/ZnS. Other materials like InP/ZnSe/ZnS, CdSe/ZnSe/ZnS and other have also been realized. These materials exhibit enhanced stability and photoluminescence efficiency, making them suitable for various applications in the display and lighting markets. For example, as Light-Emitting Devices: InP quantum dots (QDs) with a ZnSe/ZnS shell have shown improved luminescence efficiency, making them viable for light-emitting diodes (LEDs). These QDs can achieve high photoluminescence quantum yields (up to 70%) and narrow emission peaks, which are essential for high-quality displays and lighting solutions.³

These advancements indicate a promising future for multishell quantum dots in enhancing the performance and efficiency of display and lighting technologies.

3. Impact

The controlled synthesis of a giant shell QD system in gram scale with excellent emission properties (QY and stability) in red and green allows moving on from using a QD sheet in the TV backlight to color conversion at a high flux. This is not

References

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4. Prior Publication

Previous talks at SID Display Week and IDW have significantly advanced the understanding of quantum materials, particularly in the area of elongated 1D quantum rods, where the focus was on their unique polarized emission properties [3,4]. Additionally, our work on CdSe/CdS giant-shell quantum dots (GSQDs) was presented in 2020 and 2022, showcasing their potential for high-performance optoelectronic applications. The cadmium-reduced GSQDs, which were first reported at IDW23, marked a major step in addressing the limitations of traditional Cd-based systems, improving photostability and emission properties for use in quantum dot light-emitting diodes (QLEDs) and color conversion technologies. The 2025 presentation will build on these advancements, introducing a more scientific, analytical approach to shell characterization and shell engineering, with a focus on optimizing the compositional gradient between core and shell materials. This presentation will highlight the impact of this approach on enhancing the optical properties, charge carrier dynamics, and long-term stability of GSQDs.