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ISSN

INTERNATIONAL
STANDARD
SERIAL
NUMBER

ISSN
2782-4365

Проверить
номер:



Научно-образовательный электронный журнал

ОБРАЗОВАНИЕ И НАУКА В XXI ВЕКЕ

Выпуск №62-5 (том 2)
(май, 2025)



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Международный научно-образовательный
электронный журнал
«ОБРАЗОВАНИЕ И НАУКА В XXI ВЕКЕ»

ISSN 2782-4365

УДК 37

ББК 94

**Международный научно-образовательный электронный журнал
«ОБРАЗОВАНИЕ И НАУКА В XXI ВЕКЕ». Выпуск №62-5 (том 2) (май,
2025). Дата выхода в свет: 02.06.2025.**

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Название публикации: «QUANTUM DOTS WITH IMPROVED QUANTUM YIELD»

Abstract

Quantum dots (QDs) are semiconductor nanocrystals exhibiting size-dependent optical and electronic properties due to quantum confinement effects. A key parameter influencing their performance in various applications is quantum yield (QY), defined as the ratio of emitted to absorbed photons. Improving QY is essential for enhancing the efficiency of quantum dots in applications such as bioimaging, photovoltaics, and quantum computing. This paper reviews the theoretical basis of QY in QDs, identifies factors affecting it, and explores recent strategies for its enhancement, including core/shell engineering, surface passivation, and doping.

1. Introduction

Quantum dots are zero-dimensional nanomaterials with unique optoelectronic properties, primarily governed by quantum confinement. Since their discovery in the 1980s, quantum dots have been extensively studied due to their tunable emission spectra, high brightness, and photostability. The quantum yield, a critical metric, determines the efficiency of their luminescence. Increasing QY is a central goal in materials science to broaden the commercial applicability of QDs.

2. Theoretical Background

2.1. Quantum Confinement Effect

Quantum dots typically range from 2–10 nm in diameter. When the size of the particle becomes comparable to the Bohr exciton radius, discrete energy levels emerge, similar

to those in atoms. This leads to size-dependent energy gaps, which allow emission tuning across the visible and infrared spectrum.

2.2. Definition of Quantum Yield

Quantum yield (QY) is given by:

$$\Phi = \frac{\text{Number of photons emitted}}{\text{Number of photons absorbed}}$$

A high QY implies efficient photon emission and is thus desirable in photonic applications. Low QY is generally due to nonradiative recombination pathways, which must be minimized.

3. Factors Affecting Quantum Yield

3.1. Surface Defects and Trap States

Surface atoms in QDs possess unsatisfied bonds (dangling bonds), which can form trap states that facilitate nonradiative recombination. This significantly lowers QY.

3.2. Crystal Structure and Phase Purity

The crystal structure (e.g., zinc blende, wurtzite) affects carrier mobility and recombination rates. Imperfections in the crystal lattice contribute to charge carrier trapping and reduced QY.

3.3. Core/Shell Architecture

Using a wide-bandgap shell (e.g., ZnS) around a core material (e.g., CdSe) confines charge carriers to the core and reduces surface recombination, increasing QY.

3.4. Ligands and Surface Chemistry

Organic or inorganic ligands stabilize QDs in solution and passivate surface states. However, improper ligand exchange may introduce new trap states or hinder charge transfer.

4. Strategies to Improve Quantum Yield

4.1. Core/Shell Engineering

Synthesis of QDs with a passivating shell significantly reduces surface defects. For instance, CdSe/ZnS core/shell QDs have shown QYs exceeding 70%.

4.2. Surface Passivation

Ligands such as trioctylphosphine oxide (TOPO) or thiol-based molecules are commonly used for surface passivation. Recent studies have used inorganic passivation (e.g., silica) for higher chemical stability.

4.3. Doping and Alloying

Doping with atoms like Mn^{2+} or Cu^+ introduces new energy levels that can enhance radiative recombination. Alloyed QDs (e.g., CdZnSe) exhibit better crystallinity and QY control.

4.4. Post-Synthetic Treatments

Chemical treatments such as photoactivation, thermal annealing, or shell growth in colloidal solutions have been employed to improve QY by reducing nonradiative decay pathways.

5. Practical Applications

5.1. Bioimaging

High-QY QDs are ideal fluorescent probes due to their photostability and brightness. Functionalization with targeting ligands allows imaging of specific cellular structures.

5.2. Light-Emitting Diodes (LEDs)

QDs with high QY are incorporated into display and lighting technologies to enhance color purity and efficiency.

5.3. Photovoltaics

Improved QY leads to higher absorption and charge carrier generation, critical for QD-based solar cells. Multiple exciton generation (MEG) is a promising mechanism linked to high-QY QDs.

5.4. Quantum Computing and Security

Single-photon emission from QDs with near-unity QY is essential for quantum cryptography and optical quantum computing platforms.

6. Challenges and Future Perspectives

Despite significant progress, challenges remain in achieving high QY under ambient and device-operating conditions. Future research directions include:

- Developing environmentally friendly QDs (e.g., InP, carbon dots)
- Integrating QDs into solid-state devices without loss of QY
- Scalable synthesis methods for commercial production

Advances in machine learning for materials design and in situ monitoring of QD formation may further accelerate QY optimization.

7. Conclusion

Quantum yield remains a cornerstone metric in evaluating the performance of quantum dots. Recent advances in synthesis, passivation, and structural design have significantly improved QY. Continued interdisciplinary research will pave the way for broader implementation of QDs in diverse technologies.

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