Proceedings of the 4th International Conference on Functional Materials and Civil Engineering
DOI: 10.54254/2755-2721/2026.37158

Influence of Quantum Confinement and Surface Modulation on the Luminescence Properties of Quantum Dots

Daqi Huang

School of Materials Science and Engineering, Hanshan Normal University, Chaozhou, China
19540572527@163.com

Abstract. The key performance indicators of conventional luminescent materials, such as luminous efficiency, emission full width at half maximum (FWHM), and operational stability, are progressively approaching their theoretical ceilings. And this hinders further performance improvement in application fields like high-efficiency lighting, ultra-high-definition displays, and high-sensitivity biological imaging. To address the requirements of these applications, including narrow emission FWHM, high quantum yield, and tunable emission wavelength, semiconductor luminescent nanocrystal systems like quantum dots, perovskite nanocrystals, and rare-earth-doped nanocrystals have been extensively investigated due to their potential for enhancing emission efficiency, spectral tunability, and optical stability. Accordingly, their luminescence properties can be precisely regulated through size engineering, composition engineering, and defect engineering. This paper examines relevant literature and investigates the luminescence mechanisms of semiconductor nanomaterials as well as their performance optimization. The results reveal that the three material classes differ significantly: quantum dots exhibit broad wavelength tunability; perovskite nanocrystals demonstrate high luminous efficiency but limited environmental stability; and rare-earth-doped nanocrystals provide narrow emission spectra with excellent color purity. In addition, the optimization of synthesis conditions and surface functionalization can further boost luminous efficiency and suppress non-radiative recombination. However, these materials still suffer from limitations including poor stability, poor uniformity during large-scale manufacturing, and heavy metal residues in certain systems.

Keywords: Semiconductor nanomaterials, quantum confinement, exciton effect, luminescence properties, quantum yield

1. Introduction

When semiconductor materials are reduced to the nanoscale, quantum confinement effects arise, converting the continuous energy bands into discrete energy levels [1]. Consequently, the band gap increases with decreasing particle size, hence allowing precise control over emission wavelengths. With the rapid development of low-dimensional nanomaterial synthesis and regulation technologies, material architectures have gradually evolved from bulk structures to zero-dimensional quantum dots, one-dimensional nanowires/nanotubes, and two-dimensional nanosheet systems [2, 3]. Their

© 2026 The Authors. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (https://creativecommons.org/licenses/by/4.0/).

DOI: 10.54254/2755-2721/2026.37158

optical properties are strongly influenced by the interplay among size, composition, and interfacial structures. At present, widely studied systems include II–VI and III–V quantum dots, metal halide perovskite nanocrystals, and single-walled carbon nanotubes, which hold significant application value in visible light emission regulation and near-infrared optoelectronic functions. Besides, the understanding of luminescence mechanisms, structure-property relationships, and application potential remains a key research focus. Thus, this paper explores the luminescence mechanisms and performance control of semiconductor luminescent nanomaterials, with focused analysis on how carrier recombination processes affect luminescence properties across various low-dimensional systems. It also compares and generalizes the structural characteristics and optoelectronic properties of representative materials, so as to provide guidelines for structural design, performance optimization, and application of such materials in luminescent and optoelectronic devices.

2. Regulation of luminescence performance by quantum confinement

2.1. Exciton localization and size-dependent effects

In semiconductors, photogenerated electrons and holes bind through Coulomb interactions to form excitons. Notably, the spatial scale of an exciton, characterized by its Bohr radius, represents a critical criterion for evaluating quantum confinement [4].

If the material size exceeds the Bohr radius, carrier motion is nearly unrestricted, and the energy level structure matches that of bulk materials. When particle size is equal to or smaller than the exciton Bohr radius, quantum confinement intensifies: carrier wavefunctions are spatially confined, and energy level discretization becomes prominent. The band gap expands with shrinking particle size, inducing a blue shift of the emission spectrum; conversely, particle size enlargement causes a red shift [5, 6]. Therefore, size variation acts as the primary factor governing energy level evolution and emission wavelength tuning.

Furthermore, when excitons are trapped by lattice defects or impurities to form bound excitons, their energy levels become lower than those of free excitons [5, 6]. As a result, this mechanism serves as an additional pathway for regulating exciton states. In indirect-bandgap semiconductors, defect-induced exciton localization partially relaxes momentum selection rule constraints, increases the probability of radiative recombination, and enhances exciton stability at room temperature, thereby improving photoluminescence performance [7].

2.2. Quantum dot shape effects on emission efficiency

The geometric morphology of quantum dots mainly modulates the spatial distribution of carriers and the overlap degree of their wavefunctions, thereby influencing the balance between radiative and non-radiative recombination.

For example, spherical quantum dots possess high structural symmetry and relatively few surface defects. Therefore, the strong wavefunction overlap between electrons and holes promotes radiative recombination, resulting in high luminescence efficiency [8]. In contrast, as the morphology evolves from spherical to rod-shaped structures, one-dimensional elongation induces spatial separation of carriers along the axial direction, increases the density of surface states, facilitates non-radiative recombination, and reduces luminescence efficiency. Moreover, the multi-exciton effect generated under high excitation affects luminescence processes. When multiple electron-hole pairs form within a quantum dot, Auger recombination occurs between excitons: energy dissipates as heat, radiative emission is suppressed, and fluorescence lifetime shortens [9]. Increased excitation intensity

DOI: 10.54254/2755-2721/2026.37158

elevates multi-exciton density and Auger recombination probability, hence aggravating the drop in luminous efficiency.

2.3. Material systems and variations in quantum confinement

Variations among semiconductor material systems lead to diverse quantum confinement behaviors, originating from discrepancies in exciton Bohr radii and carrier effective masses, and consequently affect their confinement-induced properties. II–VI quantum dots display strong quantum confinement, delivering a wide band gap and emission wavelength tuning range via size variation. However, their quantum efficiency and stability heavily depend on the quality of surface passivation. III–V quantum dots are more sensitive to diameter changes; their wavelength-size dependence follows the same trend as II–VI systems, yet the overall tuning amplitude differs [10].

In contrast to conventional semiconductor quantum dots, perovskite quantum dots feature high quantum yields, narrow full widths at half maximum (FWHMs) of emission, outstanding color purity, and flexible spectral tunability. Despite these advantages, their sensitivity to environmental factors, such as moisture, oxygen, and continuous light irradiation, poses severe challenges for long-term stability [11]. By comparison, carbon-based quantum dots exhibit favorable chemical stability and biocompatibility; but their luminescence arises from both interband transitions and surface-state-mediated radiative recombination. Thus, they typically suffer from broad emission linewidths, limited quantum yields, and restricted wavelength tunability.

3. Mechanisms of surface regulation for enhancing quantum dot luminescence efficiency and stability

3.1. Surface defects and non-radiative losses

Lattice termination at surfaces and lattice mismatch at hetero-interfaces generate coordination-unsaturated atoms, which form defect states and interface states within the band gap. These defect states act as primary carrier trapping centers: electrons and holes are preferentially captured during migration, then transition to the ground state through non-radiative relaxation pathways. Energy dissipates via lattice vibrations, inhibiting radiative recombination [8, 9].

As the density of defect states increases, carriers preferentially recombine through defect-mediated pathways, shifting the dominant recombination mechanism from radiative to non-radiative processes [9]. For nanostructures with large specific surface areas or heterojunction systems, trapping effects induced by interface states are amplified, making recombination behavior strongly dependent on surface defect distribution [8]. Accordingly, defect state density and trapping capacity determine the predominance of non-radiative recombination pathways.

3.2. Core-shell structure engineering and ligand modification

The epitaxial growth of a wide-bandgap semiconductor shell around a quantum dot core provides an effective strategy for modulating luminescence properties, mainly via improved carrier localization and suppression of surface-derived defects. In Type-I core-shell configurations like CdSe/ZnS and InP/ZnSe, both electrons and holes are spatially confined within the core region, resulting in enhanced electron-hole wavefunction overlap. Meanwhile, the shell layer passivates surface dangling bonds and reduces non-radiative recombination pathways, boosting quantum yield. For

DOI: 10.54254/2755-2721/2026.37158

instance, bare CdSe quantum dots exhibit a quantum yield of 20%–30%, which can be lifted to 50%–80% after ZnS shell deposition [12, 13].

On this basis, shell structure parameters further influence the distribution of interfacial defects. An overly thin shell fails to fully shield surface defects, while an excessively thick shell introduces new interfacial strain via lattice mismatch and modifies recombination pathways. Multilayer or gradient-composition shells are thus adopted to balance interfacial stress relaxation and defect suppression, optimizing luminescence performance. Unlike the spatial control enabled by core-shell structures, ligand functionalization mainly modulates the surface chemical environment and carrier transport behavior. Organic ligands such as oleic acid and oleylamine passivate surfaces via coordination bonds and improve colloidal stability. Short-chain thiol-containing ligands suit aqueous systems and enable surface state regulation; amphiphilic ligands realize oil-water phase transfer, broadening biological application prospects [11].

In comparison, inorganic ligands such as S^{2-} and halide ions bind to under-coordinated surface metal sites via ionic coordination, filling deep-level surface defects and thereby reducing the density of non-radiative recombination centers. Meanwhile, these ligands form short-range ionic bridging structures between quantum dots, reducing interparticle potential barriers and enhancing electronic wavefunction coupling. This boosts continuous carrier transport within thin films, benefiting charge injection and transport in electroluminescent devices.

3.3. Doping and alloying regulation for band structure modulation

Lattice doping introduces foreign atoms to locally perturb energy level structures, achieving fine band-edge modulation and triggering red or blue shifts of emission spectra. Meanwhile, local dopant centers alter the localized carrier distribution and recombination pathways, modifying radiative transition selectivity and affecting emission spectral width and color purity [14, 15]. Doping therefore primarily governs local electronic structures and recombination processes.

By comparison, alloying constructs a continuous lattice framework through the homogeneous incorporation of isovalent elements, enabling the overall regulation of electronic band structures and lattice distortion states. This process primarily involves lattice-scale compositional homogenization and structural reconstruction, where the reduced mismatch between bulk and surface structures suppresses defect formation tendencies, altering the probability of non-radiative recombination. In terms of structural stability, the continuous chemical bonding network formed through alloying enhances the overall lattice robustness, allowing the material to maintain more stable structural responses under light irradiation, thermal perturbation, and environmental exposure. Compared with single-component systems, alloyed materials generally exhibit more consistent optical behaviors [14].

4. Synergistic regulation strategies and functional device design

4.1. Multi-scale synergistic luminescence mechanism

The luminescence performance of quantum dots is governed by multiple factors, including size, morphology, and surface states, while a single regulation strategy is generally insufficient to achieve comprehensive optimization of the emission process [1]. Size effects modulate energy level structures via quantum confinement and determine emission wavelength. Morphology control and core-shell construction influence the spatial distribution of carriers, strengthen exciton localization,

DOI: 10.54254/2755-2721/2026.37158

and mitigate the impact of surface defects on recombination [8]. Surface ligand functionalization and doping act on interface states, passivating trap states to suppress non-radiative recombination.

These regulation methods correspond to three distinct dimensions: energy level structure, spatial confinement, and interfacial processes [1, 8, 9]. They form complementary modulation relationships in luminescence behavior and collectively determine the competition between radiative and non-radiative recombination.

4.2. Performance evaluation of quantum dot-based devices

Through synergistic modification of quantum dots, quantum dot light-emitting diode (QLED) devices have achieved remarkable improvements in optoelectronic performance, with external quantum efficiency (EQE) values exceeding 26% and peak luminance reaching 270,000 nits. Meanwhile, these devices exhibit excellent high-speed response capabilities, making them suitable for high-resolution display applications [16].

In white-light LEDs, quantum dots primarily improve the radiative recombination efficiency of the emissive layer, thus reducing energy losses, enhancing output stability, and delaying luminance degradation [1, 5]. In bioimaging applications, the high emission intensity and narrow spectral features of quantum dots improve signal discrimination, enabling clearer contrast between tumor tissues and surrounding background regions. In ratiometric fluorescent probe systems, variations in intensity ratios among different emission channels are utilized to reflect local environmental changes, thereby enabling lesion identification and facilitating the correlation analysis between imaging signals and functional responses.

4.3. Device stability and large-scale manufacturing limitations

Even after multi-layer structural and surface optimization, the practical application of quantum dot devices faces two major constraints: stability and scalable production. For environmental stability, erosion by water and oxygen triggers surface ligand detachment and lattice structural mismatch. Photothermal effects accelerate ion migration, multiplying non-radiative recombination pathways and reducing device luminescence persistence and operational lifetime [11].

In large-scale manufacturing, maintaining uniform heat and mass transfer within reaction systems remains challenging, resulting in non-uniform core-shell growth during scale-up processes [3]. Such inconsistencies can broaden particle size distributions, induce batch-to-batch variations in optical performance, and decrease overall production yields. To overcome these challenges, current research strategies are primarily directed toward two aspects. First, the development of low-toxicity or toxicity-free quantum dot systems, including cadmium-free and lead-free compositions, is being pursued to minimize potential environmental and biological concerns. Second, efforts are being made to extend the functional scope of quantum dots beyond their traditional role as light-emitting materials toward multifunctional platforms, including catalytic systems and photothermal therapeutic agents, improving their versatility for complex application environments.

5. Conclusion

The luminescence performance of quantum dots is jointly determined by their size, morphology, and surface states, fundamentally reflecting the synergistic regulation of emission processes by multiscale structural features. Among these factors, size primarily governs the electronic energy-level structure and emission wavelength range, morphology regulates carrier spatial distribution and

DOI: 10.54254/2755-2721/2026.37158

recombination pathways, while surface states directly control non-radiative recombination intensity and determine practical luminescence efficiency. Accordingly, various structural modulation approaches are not isolated from each other; rather, they cooperatively regulate the competition between radiative and non-radiative recombination pathways during the emission process. From the perspective of material design, performance optimization has gradually evolved from single-parameter regulation toward multifactor synergistic engineering, establishing systematic optimization strategies centered on structural design and interfacial modulation.

Future research efforts are expected to increasingly emphasize low-toxicity material platforms and multifunctional integration, coupled with precise exciton dynamics regulation and device architecture optimization to achieve improved device efficiency and response performance. From an application standpoint, balancing uniformity in large-scale manufacturing and long-term operational stability remains a challenge. Nevertheless, as understanding of material structural and interfacial mechanisms deepens, quantum dot systems will continue expanding their application boundaries in optoelectronic displays, biological imaging, and intelligent optical devices.

References

[1] Klimov, V. I. (2003). Nanocrystal quantum dots-From fundamental photophysics to multicolor lasing. *Los Alamos Science, 28*, 214-220.

[2] Prestopino, G., Orsini, A., Barettin, D., Arrabito, G., Pignataro, B., & Medaglia, P. G. (2023). Vertically aligned nanowires and quantum dots: promises and results in light energy harvesting. *Materials, 16*(12), 4297.

[3] Baig, N., Kammakakam, I., & Falath, W. (2021). Nanomaterials: a review of synthesis methods, properties, recent progress, and challenges. *Materials Advances, 2*(6), 1821-1871.

[4] Jones, A. P. (2025). Quantum confinement and carbon nanodots-A conceptual view of the origin of diffuse interstellar bands. *Astronomy & Astrophysics, 699*, A16.

[5] Li, Y., Li, T., Zhu, F., Yin, Q., Zhang, K., Li, R. A., & Wang, Q. (2026). Preparation of multicolor fluorescent silicon-doped carbon dots and the mechanism of controllable fluorescence. *Ceramics International*.

[6] Bastos, A. R., Dias, L. M., Fu, L., Pereira, R. F., de Zea Bermudez, V., André, P. S., & Ferreira, R. A. (2026). Tunable multicomponent emission from carbon nanomaterials for neuromorphic optical synaptic functions. *Optical Materials*, 118255.

[7] Chen, J., Xie, X., Li, S., Liu, Z., Wang, J. T., He, J., & Liu, Y. (2025). Stable localized excitons at room temperature via exciton–plasmon coupling in monolayer WSe2. *Applied Physics Letters, 127*(16).

[8] Gong, K., Beane, G., & Kelley, D. F. (2016). Strain release in metastable CdSe/CdS quantum dots. *Chemical Physics, 471*, 18–23.

[9] Efros, A. L., & Rosen, M. (1997). Random telegraph signal in the photoluminescence intensity of a single quantum dot. *Physical Review Letters, 78*(6), 1110.

[10] Xie, R., Battaglia, D., & Peng, X. (2007). Colloidal InP nanocrystals as efficient emitters covering blue to near-infrared. *Journal of the American Chemical Society, 129*(50), 15432–15433.

[11] Akkerman, Q. A., Rainò, G., Kovalenko, M. V., & Manna, L. (2018). Genesis, challenges and opportunities for colloidal lead halide perovskite nanocrystals. *Nature Materials, 17*(5), 394–405.

[12] Grabolle, M., Ziegler, J., Merkulov, A., Nann, T., & Resch-Genger, U. (2008). Stability and fluorescence quantum yield of CdSe-ZnS quantum dots—influence of the thickness of the ZnS shell. *Annals of the New York Academy of Sciences, 1130*(1), 235–241.

[13] Bertolucci, A. (2014). *Quantum dot/enzyme bioconjugation and investigation of optoelectronic properties*.

[14] Zhang, H., Yang, W., Lang, L., et al. (2026). Completely substituting anionic group to develop Eu^{3+}-doped tellurite oxides for precise optical thermometry and high-color-rendering white-lighting applications. *Ceramics International*.

[15] Wang, Y., Hajilouei, M., Jiang, Q., et al. (2026). Luminescent solar concentrators based on lanthanide bimetallic red-emitting metal-organic framework. *Inorganic Chemistry Communications*.

[16] Li, M., Li, R., Wu, L., Lin, X., Xia, X., Ao, Z., ... & Chen, S. (2024). Ultrabright and stable top-emitting quantum-dot light-emitting diodes with negligible angular color shift. *Nature Communications, 15*(1), 5161.