

Optical Performance of Quantum Dots and Their Applications in Biomedical Imaging

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Abstract:

Quantum dots are nanomaterials which have attracted significant focus over the past few years because of their singular optical features. They have shown great potential in the field of bioimaging. This study delves into the photonic properties of quantum dots which include good luminescence stability and broad excitation spectra. Besides, the emission wavelength can be precisely controlled. These properties make them an excellent choice for bio-imaging. The usage of quantum dots in live organism imaging, such as pinpointing cell boundaries, tracking intracellular molecular dynamics, and early disease diagnosis, indicate the immense potential of quantum dots in biomedical realm. Through modifications on the surface of quantum dots, targeted imaging can be realized, which greatly improves the specificity and sensitivity of imaging. Nonetheless, the biosafety and long-term in vivo behavior of quantum dots still need to be further investigated. Overall, the light-based attributes of quantum dots have brought breakthroughs in bio-imaging technology. In addition, it would foretell a bright future for quantum dots in the biomedical field.

Keywords: Quantum dots; optical properties; surface modification; bioimaging.

1. Introduction

In the field of bioimaging, in recent decades, quantum dots (QDs) have become a focal point. QDs are related to biomolecules at the molecular level due to their extremely small physical scale. In addition, this leads to higher detection specificity and sensitivity [1]. Meanwhile, the specific surface area is increased for nanoparticles when being compared to bulk materials. Therefore, the surface modification by reagents can easily be achieved. The properties such as biocompatibility and solubility can be changed easily. Because of all these advantages, they are being used in a wide range of applications [2, 3].

Bio-imaging is an important research tool to understand the internal structure of organisms [4]. With the development of various advanced imaging methods, people are able to obtain real-time, quantitative, in situ, in vivo and highly sensitive biological information of living organisms, which lays the foundation for the rapid development of modern life science research. Present bio-imaging techniques encompass fluorescence imaging (FI), magnetic resonance imaging (MRI), computed tomography (CT), and photothermal imaging (PTI) [5-7]. These imaging methods are generally associated with the disadvantages of high radiation, certain hazards to the human body, high

cost, and complicated operation. Optical imaging, especially bio-imaging using QDs, has been well acknowledged to have high imaging stability in living organisms, low harm to tissues, and low cost of imaging equipment. Therefore, the purpose of this paper is to discuss the application of QDs in bioimaging.

2. Optical Properties and Surface Modification

2.1 Optical Properties of Quantum Dots

Quantum dots have many singular characteristics. The particle diameter of QDs is between 2 and 10 nanometers. Besides, QDs also have the tunable composition, remarkable yield and accurate chromaticity. These attributes have propelled their utilization across a broad range of biomedical applications, with a special emphasis on bio-imaging techniques. Their main attraction can be attributed to the tunable optical properties. In small quantum dots, the separation between electron energy levels is relatively easy due to the fact that they do not have a semicontinuous form of energy between electrons. Instead, the quantisation effect intensifies as the spatial constraints on their movement shrink, resulting in a shift from continuous energy bands to discrete energy states [8]. The

bandgap energy required is higher when the quantum dot is smaller. This leads to a heightened energy level of the emitted photon, accompanied by a reduction in the emission wavelength. When the excitation energy of quantum dots exceeds the bandgap, electrons can transition from the valence band to the conduction band, generating holes within the valence band. As the size of the nanocrystals shrinks to the scale of a few nanometers, an increase in the band gap will occur, fixing the energy levels at quantized different values. This intriguing effect is known as quantum confinement.

Compared with conventional organic fluorescent dyes, quantum dots have many advantages, such as high luminescence, narrower luminescence spectral range, and wider UV-visible absorption spectra. Electron-hole pairs exhibit a characteristic peak in the broad quantum dot UV-visible absorption spectrum. The energy corresponds to the band gap, which is called the first exciton peak. The intensity of this peak is determined by the elemental composition in QDs [9]. For example, CdS and CdSe quantum dots fluoresce in the visible range. In contrast, CdTe quantum dots emit fluorescence in the near-infrared (NIR) range. PbS, PbSe, and PbTe quantum dots are ideal materials that can be used as NIR fluorescent probes. They can take in photons from a wide range of wavelengths in the NIR region as well as in the visible light. All of them exhibit quantum confinement properties similar to those of CdS, CdSe and CdTe quantum dots. For PbS, PbSe, and PbTe quantum dots, the bandgap energies of them are notably different at 0.41 eV, 0.28 eV, and 0.31 eV respectively.

The optical qualities of quantum dots are characterized by a broadened absorption spectrum, a refined emission spectrum, considerable resistance to photobleaching, and superior stability. These make them exceptionally desirable for a broad spectrum of biological uses, especially in bio-imaging area [10]. At the same time, they still have some disadvantages, such as being harmful to the human body and not easily degradable in the human body. The unique optical and electronic properties exhibited by quantum dots stem fundamentally from the quantum confinement effects they experience. Fluorescent dyes, with their confined absorption bandwidth and wide emission spectra, face restrictions in multiplexed imaging applications. These constraints require the use of numerous excitation sources and may lead to overlap in the spectra of different dyes. Limited operational lifetimes and the propensity for photobleaching restrict the application of specific imaging tools in the prolonged visualization of cellular mechanisms. The effects on the band gap, absorption spectrum, and photoluminescence color are significantly determined by the exciton Bohr radius. That is the distance between

the excited electron and the hole that make up the exciton.

2.2 Surface Modification of Quantum Dots

Surface modification of quantum dots is also a very important aspect, which is usually used to improve their stability, dispersion, biocompatibility and optoelectronic properties. In medical imaging, quantum dots are often surface modified to make them easier to observe and track. However, carbon quantum dots (CQDs) and graphene quantum dots (GQDs) have gained substantial traction in medical applications. It is because of the easy-processing, high stability and superior biocompatibility within living organisms. The surfaces of CQDs can be customized with a multitude of functional groups. Typically, CQDs are characterized by the presence of oxygen-containing functional groups, such as hydroxyl and carboxyl, on their outer shell. An abundance of these oxygen-rich functional groups boosts the solubility in water. CQDs, due to their functional groups, can exist as stable colloids in aqueous or polar organic solvents. This stands in contrast to GQDs, which are characterized by low solubility in typical solvents. Fluorescent properties can be imparted to CQDs by their surface groups. The family of fluorescent carbon nanostructures is remarkably diverse. It comprises GQDs, carbon nanotube quantum dots (CNT QDs), nanodiamonds (NDs), and CQDs. There are currently two main luminescence modes in CQDs. One is from the band gap states based on conjugated π domains in the carbon core of CQDs. The other mechanism is from the surface-associated defective band states of CQDs. Usually, the colour modulation strategy of CQDs mainly includes selecting carbon sources of chemicals with different conjugation degrees, changing the polarity of solvents, adjusting the molar ratio of active pharmaceutical ingredients (APIs), and controlling the reaction temperature. The properties of CQDs are significantly impacted by surface groups, which can be incorporated through both covalent and non-covalent modifications.

3. Quantum Dots in Bioimaging

Bioimaging encompasses non-invasive imaging techniques that enable the visualization of biological processes with remarkable clarity. These methodologies are invaluable for monitoring cellular activities, assessing the concentrations of ions and metabolites, as well as quantifying molecular interactions. Through bioimaging, researchers gain profound insights into the complex mechanisms that govern life at the cellular and molecular levels. This can promote our understanding of biological phenomena and facilitating medical breakthroughs [11]. Bioimaging commonly utilized fluorescence or chemiluminescence techniques. However, these methods faced significant lim-

itations in animal models due to the poor penetration of visible light through tissues, a consequence of high light scattering and absorption by tissue.

Quantum dots have garnered considerable interest in the domain of bioimaging. The requirement for biocompatibility and hydrophilicity is very urgent in biological applications including bioimaging.

Due to their exceptional water solubility and the capacity to evenly distribute in biological media, quantum dots exhibit hydrophilic properties that make them reliable candidates for use in biomarker identification and bio-imaging studies [12]. Quantum dots possess a remarkable feature of size adjustability, enabling precise regulation of their physical and optical attributes. By fine-tuning the synthesis conditions, such as reaction duration or precursor concentration, the size of these quantum dots can be customized, optimizing their luminescent qualities for targeted bio-imaging uses. Quantum dots, particularly those carbon-based QDs, demonstrate low cytotoxicity and excellent compatibility with biological systems. This makes them well-suited for in vivo imaging applications and long-term tracking studies.

In order to improve the gathering of detailed data during specific cellular occurrences in real-time, QDs must be linked with target-specific molecules. This linkage is crucial for enhancing the precision of information acquired during critical cellular activities [13]. Such surface modifications are instrumental in preventing aggregation. Besides, they can minimize non-specific binding. The surface modifications are pivotal for achieving targeted imaging precision in biological research contexts.

Quantum dots are used in cell and tissue imaging, because they exhibit high brightness and narrow spectral width. They maintain stable luminescence even under weak light conditions, which is important for improving imaging quality and reducing background noise [14]. The emission peaks of quantum dots exhibit greater sharpness compared to those of organic fluorescent dyes, enabling the production of more precise and detailed images. Meanwhile adjusting the size and composition of quantum dots allow for the creation of a palette of fluorescent colors. They can be used to track cell migration, detect intracellular dynamics and observe cell-cell interactions. Furthermore, quantum dots can be integrated with alternative imaging techniques, such as magnetic resonance imaging and computed tomography, to enhance diagnostic capabilities. This facilitates improved diagnostic accuracy and sensitivity [15]. In addition, the development of new near-infrared quantum dots overcomes limitations in conventional fluorescence imaging, such as self-absorption, background fluorescence interference, improves imaging depth and contrast. This feature makes them particularly well-suited

for conducting imaging in deep tissue regions and within live subjects.

A lot of laboratories have committed themselves to the development of quantum dots with outstanding properties and good compatibility with biological systems. It is reported that electrochemical method is employed to electrolyze graphite rods under alkaline conditions. Afterwards, they are reduced with hydrazine hydrate at room temperature to obtain GQDs. The GQDs have low toxicity, good water solubility, fluorescence stability and biocompatibility. These enable the dots to enter the cells smoothly [16]. GQDs have become a hotspot in analytical chemistry and biological research. The adjustable intrinsic attributes of graphene nano-sheets, encompassing dimensions, layering, edge condition, and morphology, provide a platform for the engineering of GQDs with customizable photoluminescent properties. The pronounced cytotoxic impacts associated with quantum dots significantly constrain their applicability in in vivo scenarios, thus prompting ongoing quests for safer alternatives.

Moreover, the development of biocompatible luminescent substances for the detection of cancer in its early stages remains a formidable challenge [17]. Carbon nanotubes, distinguished by their singular optical attributes and compatibility with biological systems, present themselves as promising candidates for contrast enhancement in bio-imaging applications. It is essential to overcome the challenges related to the biocompatibility and toxicity of quantum dots to ensure their successful deployment in biological environments [18]. Given their large surface area-to-volume ratio, nanomaterials have an active surface that requires addressing issues of solubility and potential contaminants. The foundational elements that influence the toxicity and biocompatibility of quantum dots encompass dimensions, electrostatic charge, concentration, properties of the capping material, bioactivity, presence of functional groups, photolytic stability, and mechanical robustness. With the evolution of innovative quantum dot materials and enhanced compatibility in biological systems, it is anticipated that QDs will assume a more critical function in clinical diagnostics and therapies in the future.

4. Conclusion

The singular optical features of QDs have placed them at the epicenter of bio-imaging techniques. This paper elaborates on these properties, including their high fluorescence, the capability to finely adjust emission wavelengths, and their extensive excitation spectrum. Surface engineering of these quantum dots allows for targeted localization, which can greatly enhancing the accuracy and sensitivity of imaging. Meanwhile, it also offers a robust

tool for advancing biomedical research. However, the application of quantum dots in biomedicine still faces many challenges. Biocompatibility and safety of QDs need to be further investigated. The technological breakthrough of quantum dots in bio-imaging would also foretells its broad prospect in biomedical field.

Authors Contribution

All the authors contributed equally and their names were listed in alphabetical order.

References

- [1] Mohammad Jafar Molaei. The optical properties and solar energy conversion applications of carbon quantum dots. A review *Solar Energy*, 2020, 196: 549-566.
- [2] Vinod Kumar, Munesh Bansal, Priyanka Ritu, et al. Optical properties of spherical quantum dot using screened kratzer potential. *Physica B: Condensed Matter*, 2024, 683: 415920-415931.
- [3] Biswajeet Acharya, Amulyaratna Behera, Suchismeeta Behera, et al. Carbon quantum dots: A systematic overview of recent developments in synthesis, properties, and novel therapeutic applications. *Inorganic Chemistry Communications*, 2024, 165: 112492-112513.
- [4] Angela M. Wagner, Jennifer M. Knipe, Gorka Orive, et al. Quantum dots in biomedical applications. *Acta Biomaterialia*, 2019, 94: 44-63.
- [5] Mkabu-Assy, Juhaina Mtaha, Zael-Wahab, et al. Quantum size effects in nanostructures: Engineering the optical properties of quantum dots, *Physica B: Condensed Matter*. 2024, 690: 416128-416134.
- [6] Canan Baslak, Meltem Demirel Kars, Mustafa Karaman, et al. Biocompatible multi-walled carbon nanotube-CdTe quantum dot-polymer hybrids for medical applications. *Journal of Luminescence*, 2015, 160: 9-15.
- [7] Parisa Gouran Oorimi, Aliakbar Tarlani, Reza Zadnabad, et al. Synthesis of photoluminescent composite based on graphene quantum dot@ZIF-11: a novel sensor for extremely efficient nano-molar detection of CN. *Microchemical Journal*, 2023, 189: 108494-108501.
- [8] Akhtar Rasool, Tasneem Zahra Rizvi, Nayab Sana, et al. Raman spectroscopy, thermal stability and dielectric properties of CdS quantum dots polyaniline nanocomposites. *Physica B: Condensed Matter*, 2022, 646: 414291-414295.
- [9] Ramadurai M, Silambarasan TS, Raghunandhakumar S, et al. Sustainable carbon quantum dots enhanced photoluminescence for bioimaging applications: an in vitro and in silico analysis. *Journal of Photochemistry and Photobiology A: Chemistry*, 2024, 453: 115669-115696.
- [10] Wu J, Li J, Cheng M, et al. Water-soluble near-infrared AgInS₂ quantum dots for Ca²⁺ detection and bioimaging. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2024, 322: 124859-124971.
- [11] Sulaxna Pandey, Dhananjay Bodas. High-quality quantum dots for multiplexed bioimaging. a critical review. *Advances in Colloid and Interface Science*, 2020, 278:102137-102153.
- [12] Xing Liu, Yang Luo. Surface modifications technology of quantum dots based biosensors and their medical applications. *Chinese Journal of Analytical Chemistry*, 2014, 42: 1061-1069.
- [13] Hai X, Feng J, Chen X, Wang J. Tuning the optical properties of graphene quantum dots for biosensing and bioimaging. *Journal of Materials Chemistry B*, 2018, 6(20): 3219-3234.
- [14] Fan Z, Li S, Yuan F, et al. Fluorescent graphene quantum dots for biosensing and bioimaging. *Rsc Advances*, 2015, 525: 19773-19789
- [15] Yao J, Li P, Li L, et al. Biochemistry and biomedicine of quantum dots: from biodetection to bioimaging, drug discovery, diagnostics, and therapy. *Acta Biomaterialia*, 2018, 74: 36-55.
- [16] Hussein Riyadh Abdul Kareem Al-Hetty, Abduladheem Turki Jalil, Jabbar Hassoon Zamil Al-Tamimi, et al. Engineering and surface modification of carbon quantum dots for cancer bioimaging. *Inorganic Chemistry Communications*, 2023, 149: 110433-110444.
- [17] Huang S, Huang G. The utilization of quantum dot labeling as a burgeoning technique in the field of biological imaging. *RSC advances*, 2024, 14(29): 20884-20897.
- [18] Wagner AM, Knipe JM, Orive G. Quantum dots in biomedical applications. *Acta biomaterialia*, 2019, 94: 44-63.