NONMETALLIC QUANTUM DOTS

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Nonmetallic Quantum Dots

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FOREWORD

Quantum dots (QDs) have emerged as a transformative class of nanomaterials, distinguished by their exceptional optical, electronic, and catalytic properties. Their versatility has opened new frontiers across various scientific domains, including catalysis, energy conversion, biomedical imaging, and environmental remediation. While conventional metallic QDs, such as cadmium and lead-based systems, have demonstrated remarkable efficacy, concerns about their toxicity and environmental impact have spurred the search for safer alternatives. This pursuit has led to the rise of nonmetallic quantum dots (NMQDs)—a class of materials that offer comparable or superior performance while minimizing ecological and health risks.

This book, *"Nonmetallic Quantum Dots"*, provides a comprehensive examination of the synthesis, properties, and diverse applications of NMQDs, positioning them as sustainable alternatives to traditional metallic counterparts. It addresses the critical need for sustainable and non-toxic materials in the field of water treatment, offering insights into the potential of non-metallic QDs to revolutionize water purification technologies. It offers an in-depth analysis of various types of NMQDs, including carbon, silicon, graphene, boron nitride, sulfur, and organic-based quantum dots. Each chapter not only explores their unique physicochemical characteristics but also delves into their practical utility across emerging fields—ranging from photocatalysis and energy storage to antimicrobial activity and advanced sensing technologies. A distinguishing feature of this book is its holistic approach to both the scientific fundamentals and real-world applications of NMQDs. It covers key topics such as the mechanisms underpinning their enhanced catalytic activity, innovations in surface functionalization, and their potential for addressing global challenges. The inclusion of case studies and comparative analyses further enriches the discussion, offering readers a practical understanding of how NMQDs are shaping next-generation technological solutions.

Beyond their functional capabilities, the book also addresses critical issues surrounding the environmental and health impacts of NMQDs. It emphasizes the importance of developing scalable, cost-effective, and environmentally responsible manufacturing processes while highlighting the need for regulatory frameworks to ensure safe implementation. By fostering a balanced perspective between innovation and sustainability, this work provides a roadmap for the responsible advancement of NMQD technologies. The breadth and depth of this book make it a valuable resource for researchers, industry professionals, and policymakers engaged in nanoscience, materials chemistry, and environmental technology. As the global scientific community strives to develop cutting-edge materials for a more sustainable future, "Nonmetallic Quantum Dots" serves as both a foundational text and a forward-looking guide, inspiring future research and real-world innovation.

It is with great enthusiasm that the authors introduce this timely and significant contribution to the expanding field of quantum dot research, offering a vision where scientific progress aligns seamlessly with environmental responsibility and human well-being.

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PREFACE

Water is an indispensable resource, critical to life and the health of our ecosystems. However, the challenges of water scarcity and pollution are escalating globally, driven by population growth, industrial activities, and climate change. Effective water treatment technologies are urgently needed to ensure access to clean and safe water. Quantum dots (QDs) have emerged as promising materials in the field of water treatment due to their unique optical and electronic properties. Yet, the widespread use of metallic quantum dots, such as those based on cadmium and lead, poses significant environmental and health risks.

This book, *"Nonmetallic Quantum Dots,"* aims to explore and present the potential of nonmetallic quantum dots as nontoxic and environmentally friendly alternatives. Nonmetallic QDs, including carbon, graphene, boron nitride, silicon, sulfur, and various organic-based quantum dots, offer a promising path forward. They provide comparable, if not superior, performance in water purification and pollutant detection, while significantly reducing the associated risks. The motivation for this book arises from the need to balance technological advancement with environmental sustainability. By focusing on nonmetallic quantum dots, we address the dual goals of improving water treatment efficiency and minimizing ecological and health impacts. This book provides a comprehensive review of the latest research, synthesis methods, properties, and applications of nonmetallic QDs in water treatment.

Throughout this book, readers will find detailed discussions on the mechanisms of pollutant removal, the advantages and challenges of nonmetallic QDs, and real-world case studies that highlight their practical applications. The aim is to equip researchers, engineers, policymakers, and environmental scientists with the knowledge needed to advance this important field. We hope this book will inspire further research and innovation in the development of safe and sustainable water treatment technologies, contributing to the global effort to secure clean water for all. The insights provided here are intended to pave the way for future breakthroughs and to foster a deeper understanding of the critical role that nonmetallic quantum dots can play in addressing one of the most pressing environmental challenges of our time.

I would like to extend my sincere gratitude to all the chapter contributors, whose expertise and dedication have enriched this book with valuable insights into the rapidly evolving field of nonmetallic quantum dots. I am also deeply appreciative of the broader community of academicians and researchers whose pioneering work continues to push the boundaries of this field, fostering innovation and sustainable advancements. A special thanks to Bentham Science Publications for their constant support and guidance throughout the publication process, making this collaborative effort possible.

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CHAPTER 1

Introduction to Quantum Dots

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Abstract: Quantum Dots (QDs) are nanoscale semiconductor structures, typically measuring between 2 and 10 nanometers, that possess distinctive optical and electronic properties resulting from their small size. These unique properties arise from quantum confinement, which takes place when the particle's size approaches the exciton Bohr radius, resulting in the formation of discrete energy levels. Quantum dots can be controlled by changing their shape, size, or composition. Due to their highly tunable emission wavelengths, they can be used in a variety of domains, including photovoltaics, biological imaging, light-emitting devices, and quantum computing. Quantum dots are also a subject of intense research in the field of quantum information science. Although quantum dots hold immense promise, their integration into real-world devices is not without challenges. Issues surrounding toxicity, long-term stability, and scalability of synthesis methods need to be addressed before they can fully transition from laboratory experiments to commercial applications. Nonetheless, with rapid progress, the ongoing advancements in nanotechnology and material science are likely to drive innovations in quantum dot-based technologies.

Keywords: Electroluminescence, Photoluminescence, Quantum confinement, Quantum Dots (QDs), Upconverted photoluminescence.

OVERVIEW OF QUANTUM DOTS

Quantum Dots (QDs) are semiconducting nanoparticles that are confined in all three dimensions within 2 to 10 nanometers. They have distinctive optical and electronic properties which depend on their shape and size, as well as the material composition, leading to quantum confinement effects [1, 2].

These properties can be owed to the unique quantum mechanical nature of the system, where the behaviour of charge carriers (such as electrons and holes) is influenced by the small size of the particles. The capability of changing the size of quantum dots allows specific control over energy levels and optical properties. This makes them highly beneficial for a variety of applications, including electro-

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nics, energy, medicine, *etc*. The bandgap of quantum dots is inversely proportional to their size. A reduction in the size of the quantum dots causes quantization of the energy levels of electrons and holes, thus resulting in an increased bandgap. Quantum dots can absorb photons of specific wavelengths and emit light of another wavelength through a process called photoluminescence. The quantum confinement effect is the reason behind narrow and tunable emission. Quantum dots are highly productive for light emission applications as they have a high photoluminescence quantum yield. Their size tunability alters the optical properties of the quantum dots. Having a shorter wavelength, smaller quantum dots emit higher-energy light, such as blue, while possessing a longer wavelength, larger quantum dots emit lower-energy light, such as red [3]. This tunability makes quantum dots ideal for various applications requiring specific emission colors, such as in LEDs and bioimaging [4]. A reduction in the size of quantum dots is found to enhance the surface area to volume ratio, which results in more surface states. This gives rise to surface-related phenomena such as increased reactivity and sensitivity to their environment, which is particularly useful in sensing applications. The properties of the surface of quantum dots also impact the activity of quantum dots. Ligands anchored onto the surface of QDs can passivate their surface, thus causing reduction of defects and improvement of the stability of quantum Dots [5]. The type of ligand and the surface treatment can be tailored to optimize properties like solubility, stability, and biocompatibility.

The recent years have witnessed a growing interest in research based on Photoluminescence (PL) properties of quantum dots, which is highly beneficial for photocatalysis. Their PL emission often obeys the Stokes shift, meaning the emission wavelength is longer than the excitation wavelength [6]. Some semiconducting materials, like cadmium telluride, cadmium selenide, lead sulfide, and indium phosphide, are used to compose quantum dots. The choice of material is found to affect both the electronic structure and the photoluminescence properties. Apart from these materials, some other materials also exhibit different Stokes shifts and quantum yields [7]. The composition of quantum dots also governs their extent of toxicity, which plays a crucial role in biological applications.

The optical spectra of QDs are very similar to those of organic fluorophores. It is observed that the organic dyes can be excited within a narrow wavelength range due to their narrow absorption spectra. This absorption is then followed by an asymmetric emission spectrum, which is broadened by a red tail. On the other hand, the broad absorption spectra of QDs enable excitation over a large range of wavelengths, followed by a symmetric and narrow emission spectrum. Furthermore, differently sized and different colored nanocrystals with a single wavelength of minimum overlap produce a short wavelength on excitation [8].

QDs are less prone to photobleaching than organic dye molecules as they are very stable light emitters [9]. The exceptional photostability of quantum dots makes them highly valuable as probes for visualizing thick cells and tissues over a long duration. This capability is crucial for imaging multiple optical sections without causing damage to the samples.

QDs have some photophysical properties that can be disadvantageous for blinking. Quantum Dots (QDs) can change from an emitting to a non-emitting state at random intervals. This universally observed intermittent behaviour of QDs results in some limitations in QD usage for the detection of single-molecule [10]. Also, upon excitation, an increase in QD fluorescence intensity is often observed, known as photobrightening. Although this property is beneficial in various cases, it limits the fluorescence quantization [11].

Quantum dots are used for high-performance displays. The size-tunable optical properties allow for precise color control, making QLEDs suitable for high-definition and energy-efficient displays (*e.g.*, TVs, monitors, and smartphones) [12]. Quantum dots have been used in photovoltaic cells to make solar energy conversions highly efficient. The coupling of their ability to absorb a broad spectrum of light with their tunable bandgap makes them ideal for third-generation solar cells. Quantum Dot Solar Cells (QDSCs) are an emerging technology that could outperform conventional silicon-based solar cells. Quantum dots are widely utilized as fluorescent probes in biological imaging owing to their narrow emission spectra, high brightness, and exceptional photostability. These properties make them ideal for tracking cells and tissues [13]. In addition to imaging, quantum dots are employed in diagnostic assays and biomarker detection. They are also widely used in biosensors for identifying biomolecules and pathogens [14]. The high fluorescence intensity and surface functionalization capabilities allow quantum dots to be incorporated into sensing platforms for early disease detection, environmental monitoring, and food safety testing.

TYPES OF QUANTUM DOTS

Quantum Dots (QDs) are divided into these categories: (a) on the basis of composition/structure: QDs are mainly classified due to structure as

1. Core QDs
2. Core and Shell QDs
3. Alloyed Quantum Dots.

(b) On the basis of their size, QDs are divided into two types, *i.e.*, larger QDs and smaller QDs.

CHAPTER 2

Introduction to Water Treatment: Blessings of Quantum Dots

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Abstract: This chapter, *"Introduction to Water Treatment: Blessings of Quantum Dots,"* discusses the significance of water treatment for health, economic growth, and environmental sustainability. While traditional methods, such as chlorination and filtration, have been widely utilized, they present certain limitations that necessitate the exploration of more advanced technologies. Recent advancements in nanotechnology, particularly the use of quantum dots, offer promising improvements in water treatment. Quantum dots, which are small semiconductor particles, exhibit unique properties such as quantum confinement, size-dependent emission, high luminescence, and a high surface area-to-volume ratio, making them highly effective in various applications. These applications include photocatalysis for degrading organic pollutants, sensing and detecting contaminants, antibacterial activity, heavy metal removal, and solar water splitting. Despite their advantages, challenges such as toxicity, cost, and environmental impact need to be addressed. This chapter provides a comprehensive overview of technological advancements in water treatment, the unique properties and applications of quantum dots, and future directions in this field. Quantum dots hold the potential to revolutionize water treatment processes, contributing to a cleaner and healthier world.

Keywords: Heavy metal and pollutant remediation, Nanotechnology in water, Photocatalysis and contaminant removal, Purification, Quantum dots, Sensing and detection in water treatment, Water treatment.

INTRODUCTION

Water treatment is crucial to provide clean and safe water for drinking, industrial use, and maintaining a healthy environment. Clean water is essential for our health, economic growth, and the well-being of ecosystems. Contaminants like bacteria, heavy metals, and chemicals in water can be harmful to humans and the environment. Thus, effective water treatment methods are necessary to remove these harmful substances and ensure a reliable supply of clean water.

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Kalyanjyoti Deori (Ed.)

IMPORTANCE OF WATER TREATMENT

The issue of access to clean water supplies has long existed. In recent decades, this concern has become increasingly severe and noticeable due to growing industrial activity and heightened awareness of health risks. The planet has a finite supply of freshwater, and pollution is becoming more diverse and widespread [1]. Contaminated water contains organic and inorganic pollutants that render it unfit for consumption and other uses. According to a recent World Health Organization (WHO) study, approximately 4 billion people experience health problems each year due to waterborne infections, and around 1.7 million people lose their lives as a result of drinking contaminated water [2]. Certain pollutants, such as heavy metals, have long-term adverse effects on human health. For instance, cadmium has a biological half-life of 10 to 35 years in the human body [3]. D-block elements, including lead, mercury, and cadmium, are pathologically bioaccumulative and can generate free radicals that damage DNA, lipids, and proteins [4]. Among organic pollutants, dyes are major contributors. Dyes are widely used in industries such as food, textiles, paper, rubber, plastics, cosmetics, leather, and pharmaceuticals. There are more than 100,000 commercially available dyes, with approximately 7×10^5 metric tonnes manufactured each year. The discharge of dye effluents from various industries poses significant environmental risks. Dyes in wastewater can be toxic, carcinogenic, mutagenic, and teratogenic, making their removal crucial [5]. To treat contaminated water, conventional physical, chemical, and biological methods have been used, including screening, sedimentation, skimming, aeration, coagulation, flocculation, precipitation, and electrochemical processes. However, these methods are often considered ineffective in fully meeting water quality standards. Furthermore, they have several drawbacks, such as the generation of sludge containing hazardous materials, inadequate pollutant removal, high energy consumption, process complexity, and operational costs. Given the various approaches available in water treatment technology, reliable and sustainable solutions should be developed for wastewater treatment [6].

GLOBAL WATER SCARCITY AND POLLUTION ISSUES

Water scarcity is defined as a lack of freshwater supplies to meet demand. Thomas S. Eliot (1888–1965) once said, “Drought is the death of the earth.” Water scarcity remains a serious problem in many regions of the world, despite advancements in infrastructure, management strategies, and technology aimed at enhancing Water Use Efficiency (WUE). It is ranked as one of the top global risks for the next decade. Throughout the world, millions of people continue to face water scarcity or lack access to sufficient and safe drinking water. Water shortages impose significant constraints on social stability and economic growth.

Agriculture accounts for nearly 80% of total water usage, while domestic water consumption has increased due to population growth, higher living standards, and rising temperatures. Inadequate water supply is driven by deforestation, pollution, climate change, and excessive water waste [7].

A wide range of industries, including alcohol production, tanneries, textiles, pulp and paper manufacturing, photography, oil refineries, automotive production, fertilizers, and pesticides, contribute to global water scarcity. These industries discharge wastewater into the environment, and because the effluent is often not adequately treated before being released into water bodies, it contains various mutagenic and carcinogenic organic and inorganic contaminants. The most common contaminants in industrial and household wastewater include organic (dyes, benzene derivatives, volatile carbon, *etc.*), non-heavy metals (CN, F, S, Se, *etc.*), heavy metals (Hg, Cd, As, Zn, *etc.*), inorganic compounds (Cl, N-containing compounds), and various microorganisms [8]. Reducing industrial discharges and agricultural runoff into water sources is a critical step in preventing pollution and addressing the issue of water scarcity (Fig. **1**) [9]. It is possible to safeguard our water supply and guarantee its availability for future generations by enacting more stringent laws and embracing sustainable practices.

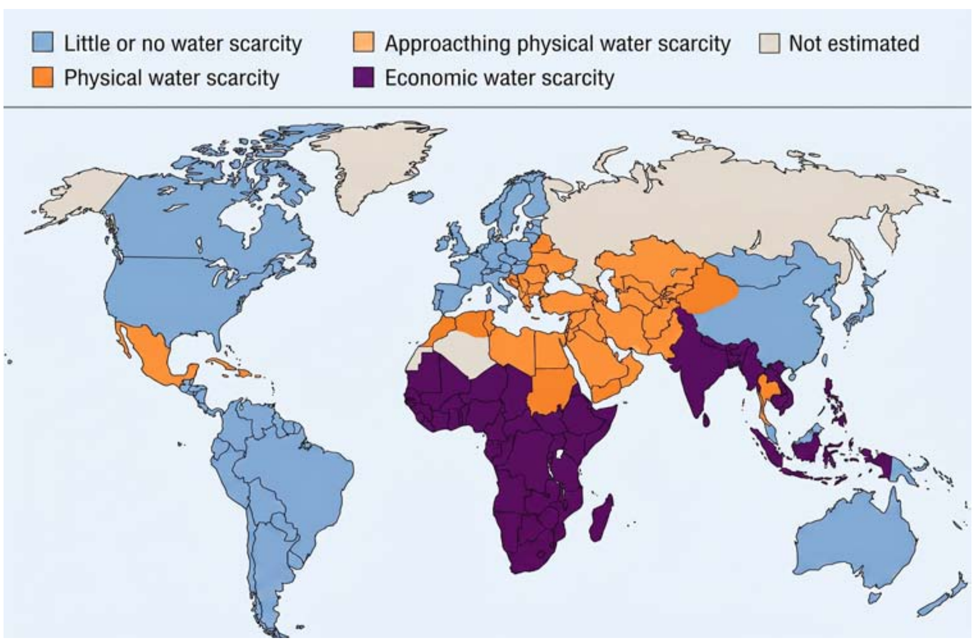

Fig. (1). Water scarcity map of the world [9].

CHAPTER 3

Metallic Quantum Dots

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Abstract: Metallic Quantum Dots (MQDs) have become rising stars in materials chemistry and engineering that signify a burgeoning ground of nanotechnology. Due to quantum confinement effects, MQDs have emerged in both industries and academia due to their shape- and size-dependent unique optical, electronic, magnetic, and structural properties. In recent years, research on MQDs led to immense commercial opportunities for chemists to harness their resourceful chemistries in a plethora of potential applications, including photocatalysis, optoelectronics, photovoltaics, energy production, environmental remediation, biological and biomedical applications to enable bioimaging, biosensing, drug delivery, diagnostics, single molecule probes, *etc.* Urbanization and industrialization have become a major threat to the world's aquatic system, causing serious health issues to humans and other living organisms. MQDs with superior properties, including sensing, could be a better choice for treating polluted water with potential pollutants like pharmaceuticals, pesticides, dyes, heavy metal ions, *etc.* With their rapid advancement in biomedical and commercial applications, MQDs may eventually enter the environment, and toxic metal ions can be released to the environment by residual MQDs throughout the weathering process, exhibiting toxicity to microorganisms, especially macroinvertebrates, bacteria, *Chlamydomonas reinhardtii,* and even human beings. This book chapter provides an overview of various types of MQDs, their unique properties, and applications in water treatment. Moreover, the environmental and health impacts of MQDs are also discussed in the chapter.

Keywords: Antimicrobial activities, Health impacts, Metal quantum dots, Quantum confinement effect, Sensing, Surface passivation, Toxicity, Wastewater treatment.

INTRODUCTION

Currently, nanoscience is one of the most active research areas, which is bringing researchers together from a variety of disciplines like physics, chemistry, electronics, materials science, biology, and medicine. Nanoscience is primarily focused on understanding the relationship between the structure of the material

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and its properties, including chemical, optical, and electronic properties, and the development of techniques for manufacturing nanomaterials for new applications. It is appreciated that nanomaterials have enormous industrial potential in various applications ranging from new electronic components to detectors, lasers, smart materials, and catalysts. A groundbreaking discovery in nanotechnology, comprising nano-sized metallic particles called "Metal Quantum Dots" (MQDs), which have gained a lot of interest among the scientific community over the last two decades, owing to their fascinating chemical and physical properties. MQDs are fluorescent types of semiconductor nanoparticles having a diameter of 2-10 nm. It is notable that MQDs possess size and shape-dependent unique optoelectronic properties and have been found to have potential in a plethora of applications, including solar cell technology, bioimaging, Light-Emitting Diode (LED) fabrication, photodetectors, pollution remediation, and computing over the past few years [1].

TYPES AND PROPERTIES

Types of MQDs

In general, Quantum Dots (QDs) are classified into three categories based on the composition/structure, size, and material used for preparation.

According to the structure, QDs can be mainly classified into Core-Type QDs, Core-Shell QDs, and Alloyed QDs. Whereas, according to size, QDs can be classified as:

a. Larger QDs with a diameter of 5–6 nm, which emit longer wavelengths with red or orange coloured emission. *e.g.*, Photovoltaic and LED.
b. Smaller QDs with a diameter of approximately 2–3 nm, which emit shorter wavelengths with green or blue coloured emission. The size can be increased by the addition of ligands, polymer coating, carrier molecules, *etc.* These QDs are used in biosensors, imaging, and other biological applications.

In terms of material used, QDs are divided into two broad categories:

a. Carbon-based QDs- they are made up of carbon-based material and possess a crystalline structure with sp-carbon of size less than 10 nanometres, which was discovered in 2004. Carbon QDs are hydrophilic and possess low toxicity.
b. Semiconductor QDs- these are three-dimensional nanoparticles consisting of inorganic elements, including heavy as well as non-heavy material (*e.g.*, zinc sulfide, cadmium, selenide, *etc.*), which were discovered in 1981. The particles are spherical, having a size of less than 6 nm. They exhibit size-dependent

photoluminescence, excitation-independent photoluminescence, and a long life expectancy.

By the elemental composition, MQDs are classified into nine types

1. I B-VI A (*e.g.*, Cu_2S)
2. I B-VII A (*e.g.*, AgBr)
3. II B-VI A (*e.g.*, ZnO, ZnS, CdS, ZnSe, CdSe, ZnTe, CdTe, HgS, HgSe, HgTe)
4. III A-V A (*e.g.*, AlP, AlAs, AlSb, GaAs, GaSb, InN, InP, InAs, InGaAs)
5. IV A-VI A (*e.g.*, PbS, PbSe, PbTe)
6. I B-III A-VI A (*e.g.*, $CuInS_2$, $CuInSe_2$, $AgInS_2$)
7. TMDCs (*e.g.*, TiS_2, $TiSe_2$, TaS_2, MoS_2, $MoSe_2$, WS_2, WSe_2, ReS_2)
8. MXene (*e.g.*, $Mn^{+1}XnTz$ where, M = transition metals; X = C and/or N; n = 1–3; Tz = F^-, O^{2-}, and OH^-)
9. Perovskite (*e.g.*, $MPbX_3$ where, M = Cs or CH_3NH_3; X = Cl, Br, or I)

Properties of MQDs

(i). Bulk Vs Quantum properties

In recent years, MQDs have gained enormous popularity owing to their striking optical and structural properties. In general, MQDs possess properties that predominantly depend upon the particle size and chemical composition of QDs. Minimization of the dimensions to a scale equivalent to the Fermi wavelength of an electron leads to some behaviors that are governed by the rules of quantum mechanics, and are likely to yield new properties that may be completely different from the bulk properties, and often totally unexpected. Quantum confinement is the characteristic that sets MQDs apart from their bulk materials (Fig. **1**). In many instances, MQDs comprise a semiconductor core and a shell made of a separate material that functions as a surface stabilizing layer. Designing MQDs with different shapes and sizes of the core and shell is possible, and their properties can be adjusted to meet specific applications. For example, rod-shaped MQDs differ from spherical MQDs in their electrical and optical characteristics. The core determines the optoelectrical properties of MQDs, while the shell is responsible for their interactions and stability. Semiconductor nanocrystals are distinguished by their band gap energy (The energy required to excite an electron from one electronic band at a lower energy level into another one at a higher energy level). This excitation generates an electron-hole pair, known as an exciton. On relaxation back to its ground state, the exciton releases energy in the form of a fluorescent photon. When the size of the semiconducting nanocrystal becomes equivalent to that of the bulk Bohr exciton radius, in the range of 2–10 nm, the particle acquires unique optical and electrical properties. In the case of MQDs

CHAPTER 4

Non-metallic Quantum Dots: An Introduction

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Abstract: Non-metallic Quantum Dots (NMQDs) are a unique class of Quantum Dots (QDs) that have dominated research in the field of zero-dimensional nanomaterials for decades. NMQDs exhibit superior properties and applications compared to Metallic Quantum Dots (MQDs). This chapter provides a comprehensive overview of NMQDs, highlighting their types, properties, current applications, challenges, and future prospects. The chapter also investigates major types of NMQDs, such as Carbon Quantum Dots (CQDs), Graphene Quantum Dots (GQDs), Boron Nitride Quantum Dots (BNQDs), Sulfur Quantum Dots (SQDs), Silicon Quantum Dots (Si-QDs), and Organic-based Quantum Dots (OQDs), all of which are promising candidates for next-generation applications in nanoscience, optoelectronics, bio-imaging, sensing, energy, water treatment, and other environmental applications. In addition to exploring their promising applications, the chapter also discusses the challenges faced during the commercial production of these types of NMQDs, like long-term stability under operational conditions and cost-effectiveness. By highlighting the key advancements and challenges of NMQDs in the field of quantum materials, this chapter sets a target for deeper exploration into the potential of NMQDs to drive innovation in nanotechnology and beyond.

Keywords: Bio-imaging, Boron nitride quantum dots, Carbon quantum dots, Challenges, Cost-effectiveness, Graphene quantum dots, Metallic quantum dots, Nanoscience, Nanotechnology, Operational conditions, optoelectronics, Organic-based quantum dots, sensing, water treatment, zero-dimensional.

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INTRODUCTION

Quantum Dots (QDs) have been a significant focus of nanoscience since their inception in 1980, shaping advancements in future science. Even today, nearly Five decades later, QDs hold a significant position in nanoscience and nanotechnology because of their unique optical and electronic properties. Over the years, QDs have mainly been synthesized using semiconductor materials such as Cadmium Telluride (CdTe), Cadmium Selenide (CdSe), and Lead Sulfide (PbS) [1]. These materials have contributed significantly to advancements in optoelectronics, photovoltaics, sensing, and biomedicine. However, their inherent toxicity and environmental impact have led researchers to search for sustainable alternatives. As a result, there has been a growing interest in Non-Metallic Quantum Dots (NMQDs). The NMQDs have unique structural, physico-chemical, and optical properties compared to traditional MQDs. NMQDs, which are typically composed of periodic table elements of groups III-V, or II-VI, offer several advantages over MQDs, including excellent dispersibility in water, biocompatibility, non-toxicity, high quantum yield, photostability, and quantum confinement effects with tunable optical properties [2]. The applications of NMQDs have garnered significant attention across various fields, including optoelectronics, electrochemistry, photocatalysis, sensing, bio-imaging, drug delivery, and environmental applications.

This chapter focuses on NMQDs, exploring their definition, types, importance, applications, and various fabrication methods with proper control over their size and shape. Also, the chapter examines the applications of NMQDs in fields such as environmental monitoring, optoelectronics, sensing, and water treatment. The chapter aims to comprehensively understand the current research on NMQDs, their advantages over MQDs, and the future directions in this rapidly evolving field.

DEFINITION AND TYPES

NMQDs are nanoparticles made from non-metallic elements such as carbon, sulfur, and silicon, boron-nitride, organic molecules, and various polymers. It is possible to precisely control the photophysical properties of NMQDs by adjusting their size, morphology, and surface properties. In addition to their versatility, NMQDs are also cost-efficient and scalable, making them ideal for various purposes. There are several types of NMQDs, as follows:

Carbon Quantum Dots (CQDs)

CQDs are a newly emerging type of zero-dimensional carbon nanomaterials with a size of ≤10 nm. They belong to the nanocarbon family of Carbon Dots (CDs) and were discovered during the purification of single-walled carbon nanotubes in 2004. CQDs are quasi-spherical carbon nanoparticles with a turbostratic or conjugated sp^2 carbon core structure surrounded by carbon nanostructures (amorphous or sp^2/sp^3 carbon) and oxygen-containing functional groups [3].

CQDs are synthesized using top-down and bottom-up approaches. Top-down methods involve disrupting bulk carbon resources through various methods (Fig. **1**). In contrast, bottom-up methods use molecular carbon precursors for preparation *via* methods like microwave and pyrolysis [4]. The top-down methods are more suitable for gram-scale production than the bottom-up methods. Various carbon resources, including natural sources like eggshells, coal, graphite, carbon nanotubes, and waste materials [5, 6], have been utilized for the fabrication of CQDs. Additionally, these CQDs can be modified with functional groups and heteroatom doping/co-doping to enhance the optical and electronic properties.

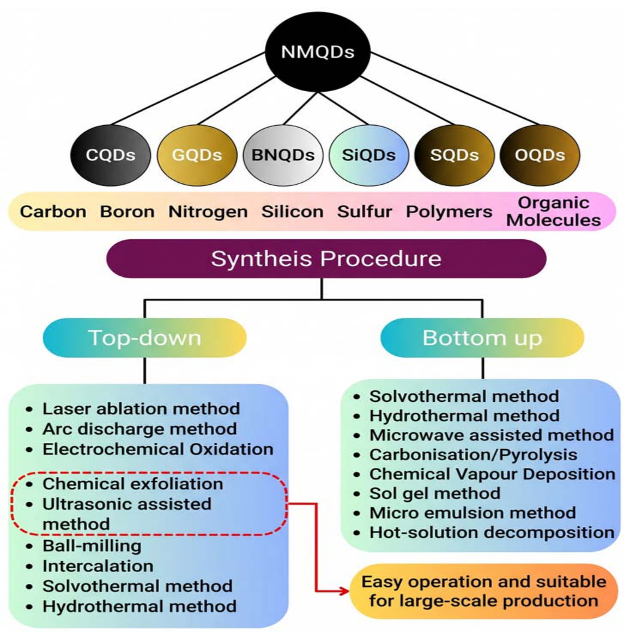

Fig. (1). Types and synthesis procedures of NMQDs.

CQDs have garnered significant interest among researchers due to their unique characteristics (Tables **1**-**4**). Compared to conventional organic fluorophores and semiconductor Quantum Dots (QDs), CQDs exhibit high emission Quantum Yield (QY), chemical stability, and similar fluorescence properties. (Fig. **2**) shows the Transmission Electron Microscopic (TEM) image and optical properties of CQDs [7].

CHAPTER 5

Full-colour Emitting Luminescent Carbon Quantum Dots (CQDS) Based on Natural Carbonaceous Precursor Materials

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Abstract: Carbon Quantum Dots (CQDs) are a unique class of zero-dimensional, quasi-spherical carbon nanodots, typically <10 nm in size. They consist of a sp^2 hybridized graphitic carbon core with various surface functional groups, including hydroxyl, carboxyl, and amino functionalities, which impart excellent photoluminescence, stability, water solubility, and negligible toxicity. They are often referred to as the rising star of the carbon family and a part of the Quantum Dots (QDs) family. These nanomaterials exhibit remarkable optical properties, negligible toxicity, eco-friendliness, and straightforward synthesis methods. Bottom-up and top-down approaches are employed to produce CQDs from natural or synthetic precursors. CQDs possess significant luminescent properties that enable them to emit various colours, leading to numerous novel applications. Factors such as quantum confinement effects, surface functionalities, and elemental composition contribute to the full-colour emission capabilities of CQDs. These features make them a focal point of extensive research due to their excellent photoluminescent properties, chemical reactivity, and solubility in aqueous media. CQDs are promising carbon nanomaterials with broad applicability in biomedicine (*e.g.*, bioimaging, cancer therapy, and drug delivery), sensing, photocatalysis, optoelectronics, and energy storage. CQDs are emerging as an environmentally friendly alternative to conventional Quantum Dots (QDs) due to their excellent properties. However, their large-scale industrial applications are still underdevelopment and require further optimization for practical commercialization. This chapter provides fundamental photophysical insights to guide future applications and delves into various synthesis methods of CQDs, with a particular emphasis on top-down approaches using naturally available precursor materials such as coal and petroleum coke. It also discusses advanced analytical characterization techniques, highlighting the optical properties of CQDs arising from their structural features and elemental composition. Furthermore, the chapter explores strategies for achieving full-

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colour emission, solid-state optical behaviors, and the application of CQDs as phosphors in optoelectronic devices, particularly Light-Emitting Devices (LEDs). Finally, the chapter provides an outlook on future perspectives of CQDs, emphasizing their potential for continued innovation and expanded applications acrossdiverse scientific and technological domains.

Keywords: Band-gap, Carbonaceous precursors, Carbon Quantum Dots (CQDs), Fluorescence, Full-colour emission, Functionalities, Luminescence, Optical properties, Photo-catalyst, Sensing, Solid state CQDs.

INTRODUCTION

Carbon Quantum Dots (CQDs) are zero-dimensional, quasi-spherical carbon-based nanomaterials with a typical diameter below 10 nm, consisting of a carbonaceous core ranging from amorphous to crystalline structures with mixed sp^2 and sp^3 hybridized carbon structures [1]. Their surfaces are rich in oxygen-containing functional groups such as hydroxyl, carboxyl, and carbonyl, *etc*., which impart excellent water solubility, chemical tenability, and unique size and surface-dependent photoluminescent properties arising from quantum confinement and surface state effects. Typically, the morphology is partially crystalline; however, it can range from amorphous to crystalline depending on the precursors and the synthetic route employed. The characteristics of precursors, including carbon content, carbon chain length, and embedded functional groups, also play a vital role in determining the propertiesof carbon nanoparticles. These nanostructures are among the youngest members of the carbon nanocrystal family. Notably, these unique carbon nanoparticles were discovered accidentally during the separation of single-walled carbon nanotubes (SWCNTs) by Xu *et al*. in 2004 [2]. Two years later, Sun and co-workers successfully demonstrated fluorescent carbon nanoparticles and, for the first time, introduced the term “quantum-sized carbon dots or Carbon Quantum Dots (CQDs)” [3]. CQDs possess graphitic layered core structures decorated with various functional groups distributed over their surface. Their luminescence originates primarily from intrinsic fluorescence and the quantum confinement size effect [4]. Owing to their exceptional photochemical properties, CQDs exhibit vast potential across a wide range of applications, including biomedicine, optoelectronic, catalysis, energy storage, drug delivery, water purification, gene therapy and, bioimaging These applications arise from their remarkable properties, such as high water solubility, stability, tuneable fluorescent properties, high fluorescent quantum yield, tenable electronic structure, electron conductivity, biocompatibility, facile synthesis, catalytic properties, negligible toxicity, and long-term chemical stability [5 - 9]. Structurally, CQDs consist of an ultra-small, partially crystalline core dominated by sp^2-conjugated carbon domain, and oxygen-containing functionalities such as ether, alcohol, carboxyl, epoxy, and aldehyde [4, 10]. The presence of these surface functionalities enables effective modulation of their optical and electronic properties through chemical treatments, making them suitable for tuning their structure easily. The quantum confinement effect in CQDs gives rise to discrete quantized energy levels and a size-dependent bandgap that resembles the molecular electronic structure [11]. Photoluminescence (PL) is the most prominent characteristic of CQDs, making them highly attractive for fundamental research and technological applications. Excellent Photoluminescence (PL) or Fluorescence (FL), high photostability, and low toxicity enable them as a potential competitor/ alternative to those of conventional semiconductor quantum dots, which contain toxic heavy metals. In this context, Quantum Yield (QY) is a major parameter governing the performance and applicability of CQDs in optoelectronics and bio-applications. The tuneable fluorescence property of CQDs is one of the properties used to address optical applications such as sensors for monitoring water treatment processes, phosphors in LEDs, sensing, and bioimaging due to the characteristic broad emission, high thermal stability, and low cytotoxicity. Distracting from other applications of CQDs, the subsequent sections also discuss full-colour emissive CQDs and CQDs in solid-state, LED applications, along with their applications in water treatment.

SYNTHESIS AND CHARACTERIZATION METHODS

Avariety of techniques were developed for the synthesis/ fabrication of CQDs and are broadly classified into two approaches, namely top-down and bottom-up approaches (Fig. **1**). The top-down approach mainly involves the decomposition or breakdown of large carbonaceous structures like graphite, fullerene, carbon nanotube, and activated carbon, smashed into ultra-small-sized CQDs through chemical, physical, or electrochemical methods. Although precise control over the particle size and morphological distribution is limited in this method, it offers the advantage of fabricating CQDs with diverse structural features and optical properties arising from the heterogeneous nature of the precursor carbon structure. Moreover, top-down techniques are considered advantageous due to the abundant availability and low cost of raw carbonaceous materials. In contrast, bottom-up approaches involve the construction or building up of CQDs from small molecular precursors, such as citric acid, glucose, sucrose, and other small organic molecules, through polymerization and carbonization processes. These methods allow better control over particle size, morphology, and surface chemistry by tailoring reaction conditions and precursor compositions, making bottom-up strategies particularly attractive for the synthesis of CQDs with tunable properties.

CHAPTER 6

Graphene Quantum Dots (GQDs)

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Abstract: Graphene Quantum Dots (GQDs), a nano-scaled synthesized graphene-based particle, offer unique chemical, physical, and biomedical applications. In addition, due to their exceptional electronic structure, biocompatibility, tunable band gap, excellent optical, electronic, and magnetic properties, these nanoparticles have been successfully exploited in cancer treatment, drug delivery, bioimaging, and biosensing fields of concern. Besides, due to the presence of oxygen-containing functional groups and water solubility, GQDs hold significant promise in a wide range of wastewater treatment applications, making them crucial for future technological advancements. In this regard, herein we have this chapter, which focuses on GQDs and their applications in pollutant degradation in wastewater treatment. The chapter outlines a brief introduction followed by a discussion of various features and properties of GQDs, their synthesis and functionalization, and the underlying mechanisms for eliminating pollutants like organic dyes, heavy metals, and microbial decontamination. Finally, other applicable areas, the current challenges, and future scopes of GQDs have also been explored.

Keywords: Band gap, Biomedical applications, Drug delivery, Functionalization, Graphene quantum dots, Heavy metals, Mechanism, Nanoparticles, Organic dyes, Pollutant degradation, Water treatment.

INTRODUCTION

Recently, numerous countries have grown increasingly alarmed by the escalating environmental degradation and energy crisis [1]. To raise global awareness and to promote environmental protection, research communities, including physicists, chemists, and biologists, are actively exploring novel sustainable energy resources and materials within their respective fields [2]. They are continuously seeking innovative materials with multifunctional properties, particularly for use in catalysis, photothermal applications, biomedical fields, bioimaging, drug delivery,

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antibacterial treatments, sensing technologies, energy storage, photodynamic therapy, and a wide range of other applications [3 - 7]. In the 19th century, the abundant and biologically essential element carbon, along with its allotropes, became the focus of extensive research, yielding innovative discoveries. These advancements have greatly contributed to addressing some of the world's most pressing health and energy challenges faced by the scientific community [8]. Most carbon-based nanomaterials are derived from naturally occurring graphite, which consists of stacked layers of graphene, few-layered graphene, graphene oxide, or reduced graphene oxide. The term "graphene" originates from "graphite" (with "graph" referring to graphite and "ene" indicating the presence of multiple double bonds). Graphene, however, has limitations such as a zero band gap and low absorptivity. These shortcomings have been addressed through structural modifications based on structure-activity relationships. To date, the discovery of various forms of graphite, including 0D fullerenes, 1D carbon nanotubes, 2D graphene, and 3D graphite, has significantly propelled research and development in this field [9]. Among these carbon-based materials, the properties and applications of graphene have been intensively studied and explored, and all of these can be engineered to form nanosized Graphene Quantum Dots (GQDs). Graphene consists of a single-atom-thick, single-layer of hexagonal arrays of sp^2 hybridized carbons. Photophysical and photochemical properties arise because of the nanoconfinement of the π electrons of GQDs. The properties of GQDs are highly sensitive to their size, structural defects such as sp^3 carbons, and the types of edge functional groups like hydroxyl, carboxyl, carbonyl, and epoxy groups. Their characteristics can be modified by introducing structural defects, such as carbon vacancies at the edges or by replacing 6-membered rings with 4- or 7-membered rings. Additionally, various molecules, including drugs, proteins, dyes, nucleic acids, antibodies, and enzymes, can easily bind to GQDs through these edge functional groups. These tunable structural properties play a key role in controlling their applications [10].

The synthesis of GQDs marked the beginning of a new era, driven by an in-depth investigation of their structural and electrical properties. Building on prior research on Carbon Dots (CDs), GQDs were developed, demonstrating a strength 200 times greater than steel. Additionally, their electrical conductivity surpassed that of copper, and they exhibited exceptional thermal conductivity due to their unique characteristics [11 - 13]. Experts predict that the future will be dominated by Graphene Quantum Dots (GQDs), often regarded as a "wonder material" due to their hexagonal lattice structure, which is only a single atom thick. GQDs' ultra-fine particle size and large surface area provide numerous active sites and edges for functional groups, dopants, and other modifications. Their non-zero bandgap and high dispersibility give them an amphiphilic nature and a strong edge effect. Additionally, GQDs hold immense potential due to their low toxicity, biomolecule-like size, photoluminescence, high surface grafting capacity, biocompatibility, outstanding mechanical strength, and chemical stability [14]. These special traits of GQDs permit the progress of photonic, high-performance electrical and energy-related devices, for example, Light-Emitting Diodes (LEDs), photodetectors, solar cells, rechargeable batteries, touch screen displays, flexible memory systems, in addition to supercapacitors. GQDs have also made significant strides in biomedical engineering, being utilized in areas such as bioimaging, drug delivery, and anticancer therapy, as well as in catalysis, nanofluids, sensors, and environmental clean-up [15]. As a result, GQDs are expected to see widespread applications in the future. The discovery of GQDs has turned scientists' dreams into reality, offering solutions to various challenges confronted by human civilization.

Due to their oxygen-containing functional groups and water solubility [11], GQDs show great potential for a wide range of wastewater treatment applications, making them vital for future technological advancements. This chapter focuses on GQDs and their role in pollutant degradation during wastewater treatment. It begins with a brief introduction, followed by a discussion of the key features and properties of GQDs, their synthesis and functionalization, and the mechanisms involved in removing pollutants such as organic dyes, heavy metals, and microbial contaminants. The chapter also explores other potential applications and future prospects of GQDs.

SYNTHESIS AND FUNCTIONALIZATION

Synthesis of GQDs

To date, the literature survey states that the synthetic method of GQDs can be categorized into two main classes, namely top-down and bottom-up synthetic approaches (Fig. **1**) [16]. The bottom-up process is difficult to optimize as it requires definite organic chemicals and complex reaction steps. Conversely, the top-down method benefits from the readily available and inexpensive carbon materials required as raw ingredients, making the synthesis of GQDs relatively simple and straightforward.

Top-Down Approach

The top-down approach is preferred, as it involves the direct cleavage of bulk carbon materials-such as graphene oxide, carbon fibers, carbon nanotubes, and carbon black-which contain a large volume of graphene structures. This method produces nanosized GQDs through various techniques, including the hydrothermal method, chemical peeling, electrochemical peeling, microwave- and ultrasound-assisted peeling, Chemical Vapor Deposition (CVD), electron beam

CHAPTER 7

Boron Nitride Quantum Dots: Revolutionizing Nanotechnology with Unique Properties and Applications

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Abstract: Boron Nitride Quantum Dots (BNQDs) are nanostructures composed of boron and nitrogen atoms arranged in a hexagonal lattice, resembling graphene. These have emerged as promising nanomaterials due to their unique properties, such as high thermal stability, exceptional mechanical strength, and excellent chemical resistance. Their exceptional properties have sparked significant research interest. Several methods have been developed to synthesize BNQDs, including chemical vapor deposition, hydrothermal processes, and liquid-phase exfoliation[1]. Each method offers different advantages in terms of scalability, cost, and quality of the produced BNQDs. BNQDs exhibit unique structural properties such as tunable band gaps, high surface area, and photoluminescence[2]. These properties are influenced by factors like size, shape, and surface functionalization, which can be controlled during synthesis. BNQDs show potential in applications like bioimaging, drug delivery, and optoelectronics[3]. However, there are challenges to overcome, such as achieving scalable production, modifying surfaces effectively, and understanding the toxicity of BNQDs. This chapter aims to throw light on the various synthetic methods involved in the production of BNQDs and their applications.

Keywords: Bioimaging and bosensing, Boron Nitride Quantum Dots (BNQDs), Hexagonal Boron Nitride (h-BN), Optoelectronics, Photocatalysis and water splitting, Photoluminescence (PL), Quantum confinement, Quantum information science, Thermoelectric applications, Top-Down and bottom-up synthesis.

INTRODUCTION

The structural diversity of Boron Nitride (BN) allotropes arises from the ionic nature of the B–N bond, which influences their electronic and mechanical properties. BN allotropes can adopt sp^2 or sp^3 hybridized structures. These

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allotropes range from bulk to nanoscale forms, including cubic BN, wurtzite BN, hexagonal BN (h-BN), rhombohedral BN, as well as boron nitride nanotubes in both single and multi-walled configurations. Other nanostructures include boron nitride nanoribbons with zigzag and armchair edges, boron nitride nanocages, and Boron Nitride Quantum Dots (BNQDs) [1]. Fig. (**1**) displays the structure of all forms of boron nitride [2].

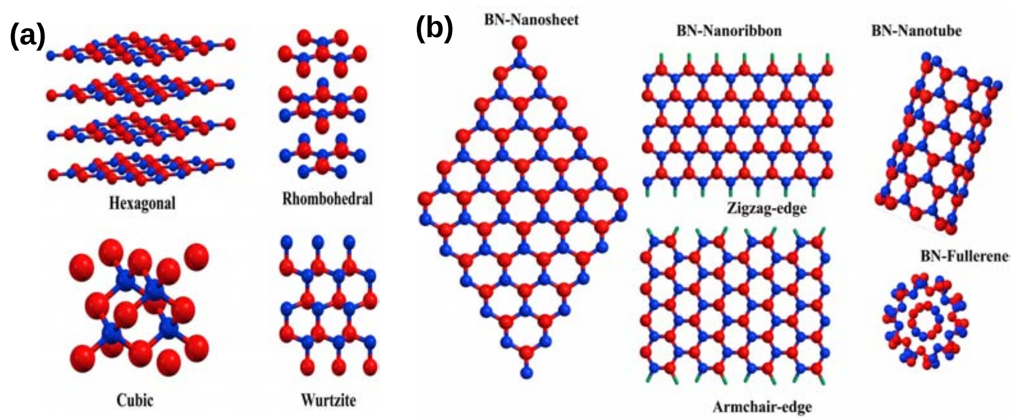

Fig. (1). Structural representations of boron nitride include: (a) Bulk BN, which exists in various crystal forms such as hexagonal, rhombohedral, cubic, and wurtzite, and (b) BN nanostructures, encompassing nanosheets, nanoribbons (with zigzag and armchair configurations), nanotubes, and zero-dimensional fullerenes. Reprinted with permission from [2].

Among these, h-BN, commonly referred to as "white graphene," is widely utilized in both industrial and scientific applications due to its outstanding chemical and thermal stability, along with its distinctive electronic and optical characteristics [3]. However, while these characteristics make h-BN valuable in many fields, they also pose limitations in thermoelectric applications, where materials require both high electrical conductivity and thermal resistance to be effective.

Recent research indicates that two-dimensional hexagonal Boron Nitride Nanosheets (h-BNNSs) exhibit superior performance compared to their bulk counterpart across various applications. h-BNNSs have shown significance due to their distinct and remarkable properties, setting them apart from graphene. These include a wide energy band gap, superior dielectric performance, excellent electrical insulation, high thermal conductivity, exceptional stability, strong resistance to oxidation, chemical inertness, and ultraviolet Photoluminescence (PL) [4 - 7].

BNQDs, the current material of interest, have gained significant interest due to their distinct quantum properties at the nanoscale (Fig. **2**). Their reduced dimensions introduce phenomena such as quantum confinement, macroscopic quantum tunnelling, surface effects, and size-dependent behaviours, which are not observed in bulk materials. As their three-dimensional structure shrinks to the nanometre scale, BNQDs exhibit unique physical and chemical characteristics, setting them apart from conventional macroscopic materials and making them promising for applications in optoelectronics, catalysis, and nanomedicine. The combination of low thermal conductivity and high-power factor makes BNQDs superior candidates for thermoelectric applications, outperforming graphene quantum dots in energy efficiency. Their ability to effectively convert thermal energy into electrical energy highlights their potential for next-generation thermoelectric devices.

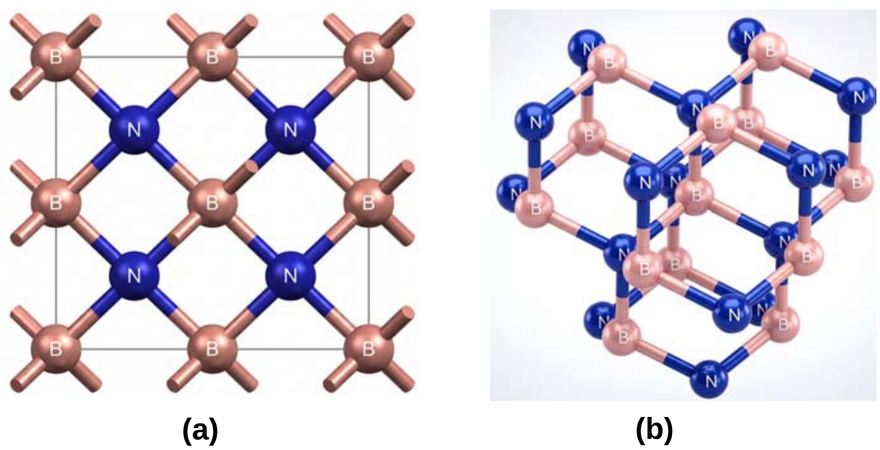

Fig. (2). (a) Bulk boron nitride (b) BN quantum dot of size 3 Å.

BNQDs are characterized by a hexagonal lattice structure composed of alternating boron and nitrogen atoms, resembling graphene but with distinct electronic properties. Their nanoscale dimensions introduce quantum confinement effects, arising from restricted electron movement within the quantum dot. Additionally, their high surface area-to-volume ratio enhances their reactivity and interaction with surrounding environments, making them highly suitable for applications in sensing, bioimaging, and optoelectronic devices. Their layered structure and tunable surface chemistry further contribute to their functional versatility in nanotechnology and material science.

SYNTHETIC METHODS FOR BNQDS

The unique characteristic properties make BNQDs highly promising for a range of advanced electronic, thermal, and optical applications. Consequently, there is an urgent need to develop efficient synthesis techniques capable of producing high-

CHAPTER 8

Silicon Quantum Dots (SiQDs)

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Abstract: Currently, QDs are gaining significant research attention due to their unique optoelectronic properties. To overcome the toxicity concerns of conventional QDs, researchers are inspired to develop new QD nanostructures with minimal toxicity and high quantum yield. Si QDs are an interesting topic of research because of their excellent biocompatibility and unique fluorescence properties. Various techniques are employed for synthesizing Si QD and modified Si QD structures that also play an important role in controlling environmental pollution and health-related issues of living beings. Their extensive applications in various optoelectronic devices are discussed in this chapter. We have highlighted the major fabrication techniques, including their applications in different sectors, and the advantageous factors that make it unique in QD chemistry.

Keywords: Applications, Chemicals, Devices, Efficiency, Emission, Environment, Excellent, Fabrication, Fluorescence, Health, Optical, Pollution, Semiconductor, Si QDs, Synthesis, Toxicity, Yield..

INTRODUCTION

Quantum Dots (QDs) act as ideal fluorophores having extensive applications from biological to solar cell applications. The unique electronic and optical properties of QDs come from their quantum confinement effect. Properties like high quantum yield, size-controlled fluorescence, and stable photobleaching inspire it to be used as an excellent optical probe. After the discovery of the emission spectra of silicon by Canham in 1991, silicon has gained attention in various optoelectronic applications. It is one of the most abundant and benign materials found in the Earth's crust. When the size of the Silicon (Si) crystal is reduced to less than the excitonic Bohr radius, *i.e.*, <5 nm, it results in an Si quantum dot nanostructure [1, 2]. The interesting observation is the abrupt change in properties with the decrease in crystallite size to the quantum level. Bulk silicon shows an indirect band gap, which results in slow e^--h^+ recombination and shows weak

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Photoluminescence (PL) spectra. Confinement in size to QD makes it more efficient for radiative recombination, which shows luminescence even at room temperature.

Thus, the reduction in the size of SiQDs results in a change in the bandgap of Si QDs from indirect to direct with excellent photoluminescence quantum yield [3]. It shows fluorescence spectra up to 60-75% yield. From the environmental point of view, Si QD and surface-modified Si QDs are found to have less toxicity than other conventional QDs. Si materials are highly biocompatible with blood, and a similarity in dimension is observed with macromolecules like proteins and nucleic acids, making them useful for different bio-related applications. Although various fluorophores are available commercially, such as organic dyes and fluorescent proteins, they possess a narrow range of absorption spectra. Compared to this, QDs allow excitation along a wide range of wavelengths. The range of spectra can be tuned by changing the compositions, surface coatings, or core sizes of the QDs. In this way, the emission spectra can be tailored. Thus, QDs are very useful in imaging processes due to their broad absorption spectra and narrow emission spectra.

FABRICATION TECHNIQUES

Numerous techniques are employed for the fabrication of Si QDs. This chapter discusses some chemical and physical routes for synthesizing SiQDs, namely plasma-based synthesis, laser ablation, electrochemical etching, solution phase oxidation/reduction method, and gas phase condensation. Among these, laser ablation, etching, *etc.*, can be categorized as top-down approaches that involve external control of large macroscopic objects to break into nanostructures. Another way is the bottom-up approach that involves the self-assembly process of the microcomponents to form the nanostructures. For example, the solution phase oxidation/reduction method, condensation, *etc.*

Plasma-based Synthesis

It is a single-step plasma process with a continuous flow of the argon-silane system. Si NCs of size 2-8 nm can be produced in a very short time, *i.e.*, milliseconds, with a yield of up to 14-52 mgh^{-1}. A novel strategy of fabricating H-terminated Si NCs grafted with organic molecules is demonstrated by Mangolini *et al*. [4]. Geisen and coworkers have carried out the preparation of Si NPs from silane in a microwave reactor that is further added in the environment of Ar/H_2 gases. The size of the NP formed as determined by a particle mass spectrometer is 5-8 nm [5]. A dry-etching process is reported by Pi *et al.* using CF_4-based plasma in the synthesis of Si NCs. When etching was done, the Si NCs PL spectrum showed a blue shift, indicating the reduction in size of the NCs. By tuning the CF_4

plasma power, the size of NCs can be changed. It is observed that etched Si NCs can be oxidized more readily than the unetched ones. The intensity of PL also gets lower after the etching is done [6]. For the synthesis of wavelength-tunable Si NCs, a microplasma reactor is developed. Here, a capillary glass tube generates nonequilibrium plasma gas and activates the mixture of H_2, Ar, and $SiCl_4$. Thus, the $SiCl_4$ decomposes into atomic Si in a very short time (100 microseconds). Then, gas phase nucleation takes place through a 3-body collision process followed by rapid crystal growth termination, for an H-concentration of approx.0.7-0.8% containing materials PL spectrum shows intense visible light emissions, while a shift in the blue region is observed with an increase in the H concentration [7]. Another method for synthesizing Si NCs from $SiCl_4$ has been developed by Gresback *et al.* The crystallinity of the NPs can be controlled by changing the H_2 gas concentration and plasma pressure. The residence time of the hydrogen in the plasma region controls the size and optical properties of the synthesized NPs [8]. A low-temperature SiH_4/Ar plasma is reported for synthesizing Si NPs in crystalline and amorphous forms with a 3-5 nm size range. An interesting transformation from amorphous to crystalline phase is observed on increasing the power of the plasma source. Along with it, the desorption rate of SiH_2 and SiH_3 increases. Finally, Si NPs are fabricated with no hydrogen species [9]. Das *et al.* reported a strategy for preparing QDs and thin films of Si. Herein, a CVD single-chamber reactor is used with a radio frequency plasma source (13.56 MHz). 150 W radio frequency power is employed to produce the plasma, helium as diluent, and SiH_4 as the feed gas. As a source of oxygen, a trace amount of CO_2 is introduced into the system. The system requires a temperature of about 300^{O}C and pressure of 1-4 torr for the fabrication of the nanostructures [10].

Laser Ablation

It is a fabrication technique for generating uniform and pure Si NPs that produces a very small amount of waste materials. Templates used for this method consist of monolayers of hexanethiol assembled on the Au (III) surface. The self-assembled monolayers by Si nanoparticles show interesting properties. These NPs are stable for a couple of months as they get attached to the surface firmly [11]. The first report of Si nanostructures was depicted by Okada and Iijima in 1991 [12]. They have reported almost spherical-type crystalline particles having a diameter of 20-500 nm and thin oxide layers covering about 1-2 nm of the surface of the particle. Herein, the ablation was performed in an Ar or O_2 environment with a wafer of Si. Werwa *et al.* reported the synthesis of Si QDs having luminescent properties in 1994. In this process, small QDs having a size of 2-3 nm are synthesized by ablating a wafer of Si at very low-pressure conditions (10-8 torr). These QDs show emission in the red region of the spectrum [13]. Makimura and co-workers reported Si QD synthesis in a helium gas atmosphere [14]. Color-tunable Si QDs

CHAPTER 9

Sulphur Quantum Dots: A Unique Class of Non-metallic Nanomaterials with Suitable Properties for Water Treatment

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Abstract: Sulphur Quantum Dots (SQDs) are zero-dimensional nanomaterials whose properties arise from quantum confinement and surface chemistry. This chapter summarises common SQD synthesis routes (hydrothermal/solvothermal, microwave-assisted, chemical oxidation, and electrochemical methods), key photophysical and chemical characteristics, and practical surface-modification strategies. We then focus on water-relevant applications, including sensing of metal ions and organic pollutants, and photocatalytic degradation pathways reported for aqueous systems. Current challenges and research directions are discussed with emphasis on improving synthetic control, stability, and application-specific performance.

Keywords: Ascorbic acid, Bioimaging, Bottom-up method, Chromium, Electrocatalyst, Energy storage devices, Fluorescent materials, Heavy metals, LEDs, Mercury ion, Nanoparticles, Nanosulphur, Non-metallic quantum dots, Photocatalyst, Quantum dots, Sulphur quantum dots, Sulphur, Top-down method, Tunable optical properties, Water treatment.

INTRODUCTION

Sulphur is one of the most abundant elements present in the Earth's crust, being 14^{th} among the list of abundant elements [1]. Sulphur is present in excess amounts in volcanic rocks and is a by-product of natural gas processing and petroleum refining. It is highly inflammable and is quite risky to store. Since the global sulphur production exceeds current demand, there arises a need to explore more options to make it worthwhile to avoid wastage and potential storage risks of sulphur. Over the years, sulphur has found applications in fields ranging from me-

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dicine and agriculture to the rubber industry and the production of sulphuric acid, lithium–sulphur batteries [2].

Nanomaterials have gained significant attention over the years owing to their diverse properties, leading to myriad applications. Metal-based nanomaterials, although in demand, are unstable and hazardous to humans and the environment due to their high metal concentrations [2]. Sulphur, being non-metallic, can overcome these challenges when prepared and used as nanoparticles. A new class of nanosulphur in the form of quantum dots called Sulphur Quantum Dots (SQDs) has been designed. Apart from being non-metallic, they are found to be sufficiently hydrophilic, small in size, cost-effective, and easy to synthesise, process, and modify [3]. Conversion of bulk sulphur to dots has improved their properties, enhancing their optical, photocatalytic, and sensing properties and enabling their diverse applications in chemical sensing, light-emitting diodes, catalysis, and bioimaging. Such a vast array of applications can be attributed to the presence of lone pairs on sulphur, which makes it prone to attach specific molecules and targets [2].

SQDs comprise a polymeric core made up of sulphur and various functionalities like sulphites, sulphates, passivation agents, *etc*. (Fig. **1**) [2]. Over the years, SQDs have attracted the scientific community owing to their stability, unique physicochemical and spectroscopic properties, tunable optical properties, and antibacterial properties.

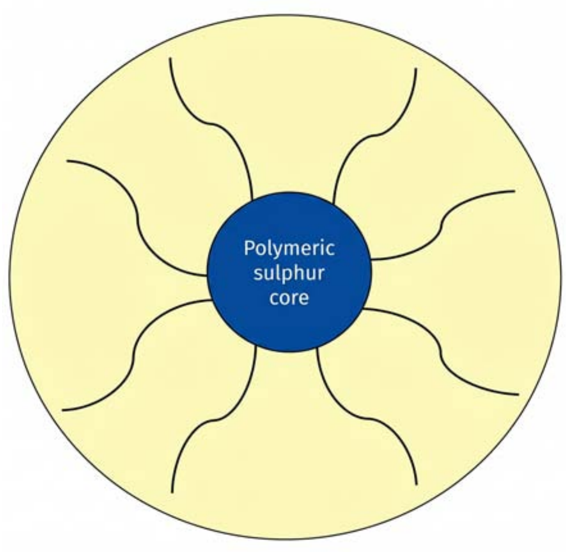

Fig. (1). Structure of SQDs (having a polymeric sulphur core and sulphates and sulphites group on the surface).

SQDs comprise quasi-spherical and discrete nanoparticles of size <10 nm [4, 5]. During the phase interfacial reaction of CdS Quantum Dots (QDs), a white suspension was obtained on the addition of nitric acid [3]. The resultant product was 1.6 nm in size and exhibited interesting characteristics, quite different from those of CdS QDs. Sulphur has already been used as a dopant in many carbon-based nanomaterials, such as carbon nanotubes and graphene QDs, to improve their optical properties [6, 7]. Keeping this in mind, nanosulphur was also prepared, and its properties were analysed. SQDs were found to be useful not only for their optical properties but also for their strong antimicrobial or antifungal properties owing to their high sulphur content. They have also been found to be suitable materials for energy storage devices, solar cells, heavy-metal recovery, and photo- and electrocatalysts [5].

SYNTHESIS OF SQDS

Two major approaches are used to prepare cost-effective, uniform-size SQDs with customizable optical properties, colloidal and thermal stability, and enhanced photostability. These are the top-down and bottom-up approaches, both of which are discussed in detail in this section.

In the top-down approach, SQDs are prepared directly from elemental sulphur in solution under different experimental conditions (Fig. **2a**). One example involves the use of readily available bulk sulphur powder, which is both abundant and cost-effective. This synthesis process involves dissolution of sulphur powder in an alkaline solution, followed by the oxidation of polysulphide ions to zero-valent sulphur. To reduce the synthesis time, ozone could be used for the oxidation step [8]. SQDs with enhanced electrochemical and optical properties can be synthesised *via* the assembly-fission process of sulphur. Sulphur precursors are dissolved in an alkaline solution (alkali etching), followed by surface passivation by Polyethylene Glycol (PEG) ligands. The oxygen-assisted oxidation of polysulphide S_x^{2-} ions of sulphur precursors led to the formation of SQDs *via* a hydrothermal process [9]. This process has been elaborated here to understand the importance of each step. An alkaline solution (generally NaOH) is used because sulphur powder is highly soluble in it. After keeping the solution for at least 30 hours, sodium polysulphide particles form from sulphur powder. This is followed by the assembling process and fission steps, which compete with each other. For up to 72 hours, assembly predominates, resulting in monodisperse sodium polysulphide particles that exhibit a new absorption band at 337 nm in Ultraviolet (UV) spectra. It is followed by the fission step, which results in clear, well-defined spherical particles. The fission step could be further improved by adding nitric acid, which etches sulphur particles, thereby resulting in monodispersed sulphur [9]. Apart from nitric acid, H_2O_2 has also been used for surface etching of

CHAPTER 10

Organic-Based Quantum Dots: Fascinating Nano-material for Water Treatment

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Abstract: Organic Quantum Dots (OQDs) have emerged as a fascinating nanomaterial providing advantages in terms of biocompatibility, tunability, and processability compared to traditional quantum dots. These promising nanomaterials are typically composed of small organic molecules or conjugated polymers. They show size-dependent optical properties as inorganic quantum dots, including size-tunable fluorescence and high quantum yields. One of the important features of organic-based quantum dots is that they have the flexibility to be designed to meet the necessity of organic synthesis. This allows precise control over the electronic and optical characteristics of OQDs by altering their chemical structure. This flexibility allows them to be useful in diverse fields, such as bioimaging, sensing, and light-emitting devices. Additionally, OQDs can also be used for detecting and removing contaminants from wastewater. The fluorescence properties of OQDs allow the detection of water pollutants even at low concentrations, enhancing monitoring capabilities. The tunable surfaces enable effective interactions and removal of harmful substances from water. This chapter highlights the synthesis, classification, and application of organic-based quantum dots, especially in water treatment, providing an in-depth overview of their current status and future scope.

Keywords: Biological imaging, Nanomaterial, Organic quantum dots, Photoluminescence, Sensing, Water treatment.

INTRODUCTION

Organic Quantum Dots (OQDs) lie at the fascinating intersection of organic chemistry, materials science, and nanotechnology.

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These OQDs are semiconductor nanomaterials with size-dependent optical and electronic properties, typically ranging between 4 and 10 nanometers in size [1 - 3]. They can exhibit quantum confinement effects. In OQDs, quantum confinement effects arise from the electronic structure of the organic semiconductors. These effects can be adjusted by altering the size and composition of the quantum dots [4, 5]. OQDs are typically constructed from small organic molecules and polymers and offer distinct benefits over their inorganic counterparts [6 - 8]. These nanomaterials are easier to synthesize, simpler to process, and exceptionally suitable for a wide range of applications in comparison to the traditional quantum dots [9, 10]. These fascinating nanomaterials are characterized by their unique π-conjugated systems, where the delocalized electrons are the cause of the electronic and optical properties of these OQDs. Unlike traditional inorganic quantum dots, which are derived from materials such as Cadmium Selenide (CdSe) or Lead Sulfide (PbS) [11, 12], OQDs are based on organic conjugated systems [13, 14]. These systems comprise small organic molecules, such as conjugated polymers or small molecules, like perylene diimide derivatives, with extended π-conjugation. These quantum dots can emit bright colors, which can be harnessed for various applications [15]. Notably, OQDs are non-toxic and metal-free, providing a safer alternative to their inorganic counterparts. Typically, OQDs are distinguished by their size-dependent electronic and optical properties, such as fluorescence and photoluminescence [16]. Although traditional inorganic quantum dots, such as CdSe and PbS, have been thoroughly explored, OQDs are emerging as a promising candidate with unique advantages.

One of the important features of OQDs is their size-tunability. By altering the size and shape of the quantum dots, one can tune their electronic and optical properties [17]. These size-dependent properties originate from the quantum confinement effect. As a result, OQDs can be engineered to emit light across a broad range of wavelengths, making them highly versatile for various applications, including biosensing and biological imaging.

One of the significant advantages of OQDs is their synthetic flexibility and processability. Organic materials can be synthesized through relatively simple chemical processes, enabling the production of quantum dots with precise manipulation of their surface properties, size, shape, *etc.* Moreover, OQDs can be incorporated with a variety of substrates.

Types of organic-based quantum dots

In 1941, the first reports published on nanocatalysis explored the potential of platinum and palladium nanoparticles, which are protected by poly(vinyl) alcohol.

These nanomaterials enable the synthesis of fluorescent OQD. The structure of OQD is primarily composed of a nanocrystalline core of size less than 10 nm. These nanocrystalline cores have sp^2 hybridised carbons, and the surface of the particles is covered with an amorphous shell having different functional groups. Organic quantum dots are divided into three main categories: polymer dots, carbon quantum dots, and graphene quantum dots [18, 19].

Polymer dots

Quantum dots that can be synthesized using both conjugated polymers and non-conjugated polymers are known as polymer dots [20, 21]. Conjugated polymers are suitable materials for synthesizing polymer dots. They possess photoelectric properties that arise from their unique π-conjugated backbones [22 - 25]. These quantum dots show excellent electronic conductivity due to their delocalized electronic backbone. Hence, they are applicable in optoelectronic devices, for example, photovoltaic cells and Light-Emitting Diodes (LEDs). As conjugated polymers can be easily modified to get desired properties, several conjugated polymers can be synthesized by altering the side chain as well as the main chain. These polymers can be folded or bent to produce desired conjugated polymer dots with unique properties. Also, these nanomolecules can be doped by biomolecules and small organic molecules to enhance their properties.

Polymer dots generally consist of conjugated polymers that are greater than 50% by weight. Consequently, the properties of conjugated polymer determine the properties of polymer dots. Polymer dots have features like optical properties, biocompatibility, easy surface modification, etc [26].

The synthetic procedures of polymer dots are mainly categorized into three types: (a) Hydrothermal method, (b) Nanoprecipitation method, and (c) Mini-emulsion method.

The properties of polymer dots can be enhanced by forming hybrids with inorganic nanomaterials. Additionally, improved interactions between polymer dots and hybrid nanostructures further enhance the properties of the nanomaterials. In their nanocomposite or hybrid structures, quantum dots show distinct morphological, conductive, and sensing behaviours [27, 28]. These nanomaterials integrating quantum dots find applications in various fields like fluorescence imaging, drug delivery, biological imaging, and biosensing [29, 30].

Hybrid polymer dots have attracted substantial attention due to their distinctive qualities and broad applicability. These hybrid polymer dots can be utilised to create cutting-edge quantum dots with special functionalities. Exploring the structure-property relationships of this type of quantum dots is expected to

CHAPTER 11

Chemical Stability and Photocatalytic Activity of Non-Metallic Quantum Dots

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Abstract: Photocatalysis is being highlighted as a promising technology that could help address environmental issues and energy shortages. Non-Metallic Quantum Dots (NMQDs) have garnered significant interest in this field because of their distinctive electronic and optical properties. Unlike metallic quantum dots, NMQDs are synthesized from earth-abundant carbon and sulfur sources, making them cost-effective, versatile, bio-compatible, and environmentally friendly. This chapter explores strategies to improve the photocatalytic performance and chemical stability of NMQDs, including surface functionalization, particle size control, and elemental doping. Various types of synthesis techniques are used to fabricate carbon and sulfur dots systematically, which pave the way for safer and greener alternatives to fluorescent toxic nanomaterials. Moreover, the chapter underscores the potential of NMQDs as effective photocatalysts for applications in pollutant degradation, hydrogen production, and energy and environmental remediation.

Keywords: Carbon dots, Chemical stability, Elemental doping, Environmental remediation, Hydrogen production, Non-Metallic Quantum Dots (NMQDs), Particle size control, Photocatalysis, Pollutant degradation, Sulfur dots, Surface functionalization.

INTRODUCTION

Over the past two decades, tiny particles called Quantum Dots (QDs) have gained significant attention among researchers because of their unique physical and chemical properties. Due to an effect known as quantum confinement, QDs

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display distinct optical, photochemical, and catalytic properties. This quantum confinement occurs when materials are reduced to a nanoscale size, typically between 1 and 10 nm [1]. When particles are so small, their properties change due to their reduced dimensions and high surface-to-volume ratio. This effect leads to several beneficial properties, such as increased luminescence efficiency, enhanced nonlinear optical behaviour, improved thermal stability, and distinctive electrical characteristics [2]. The chemical stability of non-metallic quantum dots is a topic of interest in the field of nanotechnology. Research has shown that heavy-metal-free quantum dots, such as InP and ZnE (E=S, Se, and Te), have similar optical properties to heavy-metal-containing quantum dots but with lower toxicity. However, InP quantum dots are sensitive to oxidation and require strict airless conditions during synthesis. Adding an appropriate shell layer to the core of InP quantum dots can improve stability and suppress surface defects [3].

NMQDs exhibit excellent chemical stability due to their unique properties. They are less prone to oxidation, which helps maintain their stability and optical properties. These materials tend to be less reactive, reducing the likelihood of chemical reactions that could alter their composition or structure. The strong bonds between atoms in NMQDs contribute to their stability and resistance to degradation. NMQDs can have an inert surface, reducing interactions with the environment and minimizing changes to their properties. They can also be designed to be soluble in various solvents, making them easier to process and use in different applications [4].

However, NMQDs can still be affected by several factors, such as photobleaching that occurs due to prolonged exposure to light, leading to a loss of optical properties. Extreme temperatures can also affect NMQD stability, potentially altering their structure or properties. High humidity can influence their stability, particularly for hygroscopic materials. NMQDs can interact with certain chemicals, potentially altering their properties or stability.

To enhance chemical stability, researchers use strategies like (1) Surface passivation: Coating NMQDs with a protective layer to reduce interactions with the environment; (2) Ligand exchange: Replacing surface ligands with more stable alternatives; (3) Core-shell structures: Creating a core-shell design to protect the core material; (4) Encapsulation: Encapsulating NMQDs in a stable matrix or polymer. By understanding and addressing these factors, researchers can develop NMQDs with improved chemical stability for various applications (Fig. **1**) [3, 4].

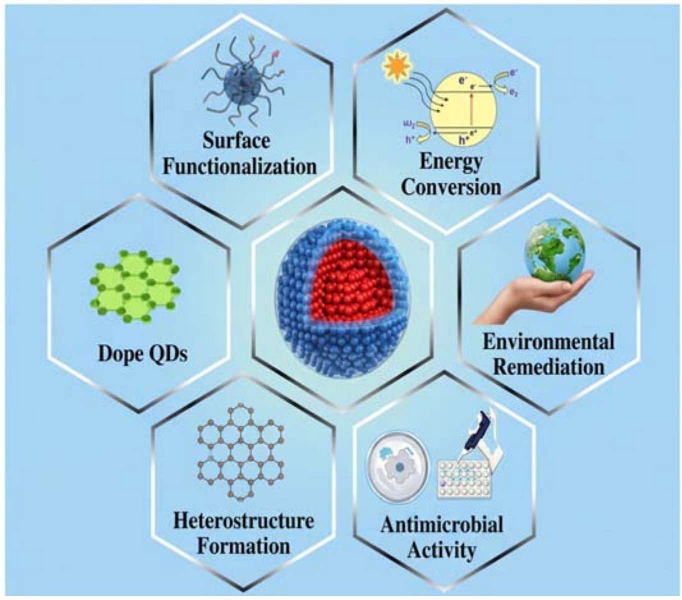

Fig. (1). Schematic illustration of chemical stability and photocatalytic activity of non-metallic quantum dots.

BASIC PRINCIPLES OF PHOTOCATALYSIS

Photocatalysis has been recognized as a light-driven redox process based on the energy band structure and charge-transporting abilities of semiconductor catalysts. Semiconductor photocatalysis consists of three main steps: (1) light absorption leading to the creation of electron (e^-)-hole (h^+) pairs; (2) separation and movement of charge carriers; and (3) oxidation and reduction reactions on the photocatalyst's surface. This process begins when the semiconductor (photocatalyst) absorbs photons with energy equal to or greater than its band gap (E_g). The photonic energy excites electrons in the semiconductor, pushing them from the Valence Band (VB) to the Conduction Band (CB) while simultaneously creating h^+ in the VB. These photoinduced electrons and holes move to the semiconductor’s surface. However, some e^- and h^+ recombine (volume recombination) as they generate electrostatic forces, producing either photons or heat. Surface recombination may also occur due to active states on the semiconductor's surface.

For creating effective photocatalysts, the band gap energy of the semiconductor is crucial. Sunlight is composed of about 6% Ultraviolet (UV) light, 42% visible light, and 52% Near-Infrared (NIR) light. The visible spectrum’s energy ranges from 2.43 eV to 3.2 eV, so a suitable photocatalyst should have a band gap within or below this range. In terms of energy levels, the VB should be more positive

CHAPTER 12

Antimicrobial Activity of Non-Metallic Quantum Dots

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Abstract: Non-Metallic Quantum Dots (NMQDs) have garnered significant attention in recent years as excellent alternative antimicrobial agents to traditional medicines. The NMQDs exhibit broad-spectrum antibacterial activity against Gram-negative and Gram-positive pathogenic bacteria, primarily attributed to their strong structural stability, unique physicochemical properties, biocompatibility, and distinctive electronic, catalytic, and photoluminescence characteristics. NMQDs exert their bactericidal effects primarily through the generation of Reactive Oxygen Species (ROS), such as hydroxyl radicals, loss of bacterial cell membrane integrity, interference with cellular metabolic activities, and gene expression arrest. Moreover, NMQDs hinder vital enzymatic processes and nutrient uptake, further impairing bacterial viability. The NMQDs exhibit strong pathogen elimination efficacy, dramatically lowering bacterial populations in various environments, highlighting their potential as powerful antibacterial agents for application in food safety, water treatment, and healthcare. NMQDs offer numerous advantages over conventional therapies, including improved specificity, less toxicity to animal cells, and environmental friendliness. Furthermore, unlike antibiotics, NMQDs have a versatile mechanism of action that lowers the chances of developing resistance. Moreover, their stability and ease of synthesis make NMQDs attractive for scalable production and practical applications. This chapter explores all aspects of NMQDs as a promising frontier in antibacterial approaches, including their mechanisms of action and pathogen removal efficacy. Furthermore, the article emphasizes the potential of NMQDs for early diagnosis of bacterial infections and future research prospects, paving the way for innovative solutions to combat bacterial infections.

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Keywords: Antimicrobial activity, Bactericidal, Bacterial imaging, Bacterial resistance, Biocompatibility, Biofilm inhibition, Carbon dots, Cell lysis, Multidrug-resistant bacteria, Nanomedicine, Non-metallic quantum dots, Oxidative stress, Pathogen removal efficacy, Photodynamic effect, Reactive Oxygen Species (ROS).

INTRODUCTION

The growing resistance to existing antimicrobial agents within the microbial communities is a severe threat to global public health [1, 2]. As a result, developing novel therapeutic alternatives with new mechanisms of action, particularly against pathogenic bacteria, is the most imperative need at present [3]. In order to defeat antibiotic-resistant bacteria, current research is increasingly focused on alternative strategies that can bypass existing resistance mechanisms, including phage therapy, antimicrobial peptides, microbiota-modulating therapies, combined therapies, antivirulence approaches, drug repurposing, the identification of small molecules, immunomodulators, and nanoparticles [4]. Nanoparticles (NPs) have emerged as promising therapeutics with broad-spectrum activity against Gram-positive and Gram-negative bacteria owing to their unique size-dependent physicochemical properties [5]. The introduction of nanoparticles has offered new avenues in the quest for novel antibiotic alternatives [6].

Quantum Dots (QDs), a class of nanoparticles, have received substantial interest since their discovery in the 1990s as quasi-zero-dimensional nanomaterials with promising biomedical applications [7]. QDs are unique, highly stable fluorescent semiconductor nanocrystals that range in size from 1-10 nm and possess excellent electrical and optical properties [6]. They are composed of transition metals and metalloid elements, including group II-IV and IV-VI elements of the periodic table [8]. QDs have high photoluminescence capabilities, a uniform nanocrystal structure, and quantized charge and energy levels [9]. They comprise a prolonged fluorescence lifetime, tunable emission, broad stroke shift, high quantum yield, and are resistant to photobleaching [10]. QDs are considered superior to conventional materials such as silica spheres and polymers owing to their environmental compatibility and low toxicity [11]. QDs, characterized by their small size, high surface-to-volume ratio, enhanced reactivity, and geometry-dependent electrical properties, have been extremely useful in photodynamic therapy, real-time tissue imaging, multicolour labelling and imaging, single-molecule probes, and drug delivery [8]. They additionally have applications in tissue engineering, cancer treatment, environmental contaminant detection, bioremediation, solar cells, and drug development as an alternative therapeutic approach [8]. QDs have also been used as Förster Resonance Energy Transfer (FRET) energy acceptors and donors due to their high quantum yield and long fluorescence lifetime. For example, FRET has been employed for identifying gene deletions that are linked to human breast cancer [7].

QDs are classified into three major categories based on their core material: metallic QDs, semiconductor QDs, and Non-Metallic QDs (NMQDs) [5, 7, 8]. They can also be categorized as hybrid and composite QDs, which combine multiple materials to maximize the advantages of each component [10]. Metallic QDs composed of Gold (Au), Silver (Ag), Iron (Fe), and Copper (Cu) are commonly used in antibacterial applications [6, 12]. Nevertheless, their clinical application is challenging due to their high potential cytotoxicity [8]. To address these toxicity concerns, the whole realm has shifted toward using NMQDs as promising, non-toxic therapeutic alternatives in antimicrobial research [10]. NMQDs offer broader biomedical applications compared to conventional drugs, exhibiting excellent antimicrobial properties, especially when functionalized with polymers like polyethyleneimine, polyethene glycol, and poly-L-lysine [10]. Among NMQDs, Carbon QDs (CQDs) are ideal candidates for biomedical applications owing to their strong luminescence, narrow emission spectra, and low toxicity [13]. Their advantageous properties include small size, photostability, high water dispersibility, good biocompatibility, cost-effective synthesis, and easily alterable surface charges through functionalization with groups such as carboxyl, hydroxyl, amino, epoxy, and amides [13, 14]. CQDs are widely applied in bioimaging, antibacterial, drug delivery, energy conversion, and sensing (Fig. **1**). CQDs, including carbon dots, nanodiamonds, carbon nanotube dots, graphene oxide, and polymer dots, are non-toxic and highly stable [11, 14]. Structurally, CQDs are quasi-spherical carbon nanoparticles composed of varying proportions of graphite and turbostratic carbon [8, 15]. They demonstrate good water solubility, biocompatibility, photostability, high singlet oxygen quantum yield, low toxicity, and chemical inertness [9, 12]. CDs are further categorized into graphene QDs and carbon nanodots [10]. Another category of NMQDs is biomolecule-derived QDs, or biodots, which originate from natural biomolecules [14]. The first biodots were synthesized from 20 natural amino acids using a green hydrothermal approach, exhibiting biocompatibility and outstanding intracellular uptake, which renders them perfect candidates for imaging applications [10]. Silicon Quantum Dots (SiQDs) are widely employed in light-emitting diodes, solar cells, and lasers because of their superior optical qualities. The green synthesis of NMQDs often utilizes plant extracts, microbes, or other bio-based materials as reducing and stabilizing agents [16]. This approach offers advantages in terms of sustainability, scalability, and reduced environmental impact, further enhancing the widespread use of NMQDs in various scientific and medical fields [11].

CHAPTER 13

Advances in Surface Modification and Functionalization

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Abstract: Non-metallic Quantum Dots (QDs) without any metallic equivalents are a sustainable substitute for regular QDs made from heavy metals. Numerous industries, such as water treatment, environmental cleanup, and healthcare, have adopted non-metallic QD technology owing to its optical tunability, sustainability, biocompatibility, cost-effectiveness, non-toxicity, high fluorescence stability, high fluorescence quantum yield, *etc*. In order to further improve their properties, such as morphology, facet, chemical composition, thermal stability, as well as conductivity, advanced surface modification and functionalization processes have been adopted in recent years. One of the significant approaches that alters the properties of materials is functionalization, leading towards the creation of high-performance component design and development. Other methods that are being used to modify the surface properties of non-metallic QDs include doping, polymer capping, core-shell formation, ligand exchange, and supramolecular click chemistry. This chapter primarily encapsulates the recent developments in surface modification and functionalization of non-metallic QDs, mainly towards water treatment, along with a few other applications. The chapter also discusses the techniques that were developed so far for the modification of surfaces and functionalization of non-metallic QDs.

Keywords: Bio imaging, Cancer treatment, LED, Nano composites, Non-metallic quantum dots, Surface functionalization, Waste water treatment.

IMPORTANCE OF SURFACE MODIFICATION

Surface functionalization is a helpful technique for making smart materials by altering their external environment. These changes in the properties of material make it possible to create and manufacture the responsive materials, which have a great impact on the rapid development of biomedicine and materials sciences.

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Smart materials have the ability to resist the changes in pH, temperature, moisture, light, and fluid composition in an external environment. This property of smart materials is primarily linked to its innovative features *via* which they activate their special functionalities. Some examples of smart nanomaterials are inorganic (metal, metal oxide, and metalloid nanoparticles), organic (mostly polymer-based), and hybrid materials including Quantum Dots (QDs) [1, 2]. The concept of artificial atoms, or QDs, was first introduced many years ago as a result of early studies on the reduced dimensionality of semiconductors. Today, every QD material system can typically produce core-shell structures, narrow emission, photochemical stability, and efficient Photoluminescence (PL), for which QDs have been used as active components in a large range of gadgets and applications [3, 4]. In addition, QDs are helpful in a variety of fields, including the conversion of light energy into electrical energy, the creation of coherent radiation sources, new generations of optoelectronic devices, biological object staining and contrast, medical diagnostics, directed drug transport, *etc* [5, 6]. The technological significance of surfaces and interfaces in the design and development of high-performance QDs has made them a very prominent issue in recent years. Advanced surface modification techniques can be used to change the mechanical, physicochemical, and aesthetic properties of QDs to a great extent [7].

The main goal of surface modification is to attach various organic, inorganic, and biological components to the surface of QDs by means of a sequence of chemical or physical processes. The surface-modified QDs can improve their light sensitivity, water solubility, and biocompatibility by minimizing or even eliminating surface flaws [8]. For instance, a family of carbon allotropes known as Carbon Quantum Dots (CQDs) is 0D nanoparticles with a diameter of less than 10 nm. It is anticipated that the chemical and physical changes made to CQDs will improve their photophysical characteristics and improve their performance across a range of applications. When heteroatoms are added to CQDs, their solubility is improved, and surface functionalization is made simpler. A variety of functional groups containing atoms like carbon, hydrogen, nitrogen, oxygen, and others improve dispersion in water and make it easier for diverse organic, inorganic, and biological moieties to further functionalize and passivate the surface [8, 9]. Depending on the source material, probable use, and the amount of time needed for the surface change, there are several methods for accomplishing surface modification. However, it may be said that the most popular methods are chemical, physical, and biological ones [7]. A brief synopsis and a more thorough explanation of the techniques of surface modifications are provided below.

TECHNIQUES FOR SURFACE MODIFICATION

Surface modification is the alteration of the surface properties of materials for better properties. This plays a key role in customizing a material for specific applications, as it significantly influences their electronic, optical, and chemical properties. In the case of Quantum Dots (QDs), surface functional groups strongly affect the properties of QDs. Recently, numerous research efforts have been devoted to developing different strategies for the functionalization and surface modification of CQDs using techniques like p–p interactions [10], sol–gel processes [11], coordination [12], and covalent bonding [13]. CQDs are abundant in oxygen-containing groups, which facilitate their covalent bonding with other functional groups. A common method for surface modification involves covalent bonds between the surface and chemical agents that possess amine functional groups, which has shown to enhance the PL properties of CQDs. For instance, three-nanometer CQDs emitting blue-green fluorescence were chemically modified using spiropyran compounds. This surface modification allowed the CQDs' emission at 510 nm to be quenched upon Ultraviolet (UV) light exposure, when excited at a wavelength of 650 nm, due to an energy transfer mechanism between the CQDs and the attached spiropyran groups [14]. This quenching could be reversed by irradiating with visible light. This method is highly stable and offers a promising route for the surface functionalization of CQDs. In another study, Zhang *et al.* demonstrated that using organosilane as a coordinating solvent could facilitate the ultrafast production of amorphous Carbon Quantum Dots (CQDs) with strong luminescence, completing the synthesis in only one minute [15]. This was achieved by pyrolyzing anhydrous citric acid with N-(--aminoethyl)-c-aminopropyl methyldimethoxy silane (AEAPMS) at 240°C for a duration of one minute. The resulting CQDs were enriched with methoxysilyl groups on their surface. These CQDs could also be easily converted into fluorescent films or monoliths composed of pure carbon dots by subjecting them to heating at 80°C for 24 hours. Additionally, CQDs, which are hydrophobic, can be modified into hydrophilic silica-encapsulated CQDs (CQDs/silica), which have been demonstrated to be non-toxic to specific cell lines and exhibit complete biocompatibility. In a comparable study, CQDs were integrated into a Molecularly Imprinted Polymer (MIP) composite, serving as a selective recognition component in a fluorescence-based Dopamine (DA) sensor. Luminescent CQDs were synthesized using AEAPMS through a one-step hydrothermal process and subsequently embedded within the MIP framework to create the CQDs@MIP composite. The resulting composite exhibited enhanced photostability and high selectivity toward the target molecule, emphasizing the synergistic interaction between the CQDs and the MIP [11].

CHAPTER 14

Metrology and Commercialization of Quantum Dots

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Abstract: Metrology is a highly essential aspect for the commercialization of high-quality Quantum Dots (QDs). Characterization techniques like Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), dynamic light scattering studies (DLS), Photoluminescence (PL), Electroluminescence (EL), Atomic Force Microscopy (AFM), *etc.*, ensure production of each batch of task-specific quantum dots, fulfilling specific requirements of shape, size, electronic and optical properties. Theoretical calculations like DFT and TDDFT help in understanding the underlying photophysical mechanisms of QD-based sensors. For large-scale production of quantum dots, easy processing, high reproducibility, cost-effectiveness, and the environmentally friendly nature of synthetic procedures are extremely crucial. Methods offering simultaneous crystal formation and growth are found to be excellent for size modulation of QDs. Keeping in view the potential toxicity of metallic QDs, current market demands large-scale production of non-metallic quantum dots like phosphides, dichalcogenides, carbon, and perovskite-based quantum dots. Carbon QDs are also becoming increasingly popular as biomedical carriers and probes. So, modulation of optoelectronic properties of carbon QDs to enhance their activity in the near IR and visible region is found to be extremely crucial and beneficial. So, this chapter will provide a discussion on the importance of metrology for the large-scale production of QDs, with special emphasis on non-metallic QDs. Moreover, this chapter also describes all the potential challenges associated with the commercialization of QDs, thus providing a better understanding of the difficulties and the current market for QD production and application.

Keywords: Commercialization, Current-market, Qualitycontrol, Quantum dots, Metrology, Scale-up.

INTRODUCTION

Recent years have marked a surge in the fabrication of Quantum Dots (QDs) as a next-generation semiconducting material with highly tunable properties. The less

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toxic, highly inert, and better functionalized non-metallic quantum dots are found to be a promising carrier for drug delivery and biomedical imaging [1, 2]. Metrology ensures the quality control and reproducibility for the large-scale production of these quantum dots. It makes sure that each batch results in the production of high-quality quantum dots that fulfill the specific requirements of size, composition, surface, and optical properties. The optical properties, like fluorescence emission of quantum dots, can be controlled by fine-tuning their sizes. The size tunability of quantum dots is extremely crucial for controlling the bandgap properties by influencing the quantum confinement effect. Characterization techniques like Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Dynamic Light Scattering Studies (DLS), *etc.*, are found to be extremely crucial for quality control of quantum dots to ensure their high reproducibility for commercial production. Thus, this chapter provides an insight into various characterization techniques important for maintaining the uniform quality of quantum dots in order to produce more task-specific quantum dots. Moreover, this chapter also discusses the scale-up challenges and current trends for the development of non-metallic quantum dots.

QUALITY CONTROL AND REPRODUCIBILITY

Characterization techniques like Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Dynamic Light Scattering Studies (DLS) are often used for ensuring uniform size distribution of quantum dots. For example, the absorbance of PbS quantum dots occurs in the near-IR region, due to which TEM imaging allows more accurate measurement of their shape and size distribution. HRTEM and FTIR can help with the study of crystal structure and variation in the surface properties with functionalization of the quantum dots [3, 4]. Recently, Atomic Force Microscopy (AFM) has been considered to be more advantageous over TEM for visualizing the morphology of quantum dots in 3D because of its ability to scan a large area in a short period of time in a vacuum-free condition [5]. The chemical composition of quantum dots can be determined by using EDX elemental mapping. However, accurate investigation of elemental composition with EDX is challenging as their measurements depend on a variety of factors ranging from the energy of the electron beam, the selected sample area, to the thickness of samples and the surrounding environment [6]. The size and composition of quantum dots can also be determined by using a combination of Photoluminescence (PL), Raman scattering spectroscopy, and field flow fractionation. Photoluminescence (PL) is one of the most attractive properties of quantum dots, which makes them a promising candidate for real-time monitoring of diseases by sensing and imaging. So, PL measurements provide accurate information about absorption peaks, emission spectra, and quantum yields, which are essential for sensing and imaging applications of quantum dots. The underlying photo-physical mechanisms of QD-based sensors can be characterized by using theoretical calculations like DFT and TDDFT. These theoretical studies help to guide the large-scale production of more task-specific quantum dots. The band gap and fluorescence energy of the quantum dots can be determined by using TDDFT studies, thus providing a wider possibility for tuning of quantum dot properties [7, 8]. The reproducibility of quantum dots for biomedical applications requires thorough examination of antimicrobial activity, antioxidant activity, DNA binding and cleavage studies, and cytotoxicity. UV-Vis spectra titrations are used for testing the binding affinity of DNA with quantum dots. Recording absorbance after incubation of quantum dots containing DPPH solutions gives information about the antioxidant behavior of quantum dots. Cell viability is another important factor that requires careful calorimetric studies for the prevention of possible harmful effects of quantum dots-based probes on health [6, 9]. Quantum dots also exhibit Electroluminescence (EL), which is beneficial for the production of QD-LEDs. The EL measurements give information about the spectral width of QD-emission, which is governed by the shape, size, and composition distribution within a QD-ensemble. A single dot measurement of about 20 nm is considered to be best for the fabrication of QD-LEDs [10 - 12]. The rapidly increasing advancement in synthetic strategies of quantum dots and their extremely small dimensions requires more high-resolution spectroscopic and microscopic techniques like Time-Resolved (TR) spectroscopy and Spatially-Resolved (SR) microscopy [13 - 15]. The shorter exciton lifetime of quantum dots requires ultrafast laser techniques like Time-Resolved Photoluminescence (TRPL) and Transient Absorption Spectroscopy (TAS) to monitor the exciton lifetime and possible relaxation pathways. TRPL provides information about the time-dependent photoemission rates by acting as a probe for recording emission decay curves. This technique also helps to determine Photoluminescence Quantum Yield (PLQY) and Photoluminescence (PL) lifetime. A high PLQY and long PL lifetime are considered to be great for quantum dots [6, 15]. TAS helps to understand the dynamics of excited carriers, which are probed for a shorter duration of about a femtosecond. In contrast to TRPL, it can also detect signals corresponding to non-emissive (dark) states [6, 16]. A combination of TR spectroscopy with SR microscopy made the study of blinking mechanisms possible by investigating the distribution and lifetime of energetic traps. It helps to understand various radiative as well as non-radiative mechanisms. Moreover, it also gives information about the Auger recombination rates [6, 17, 18]. TR microscopy and SR spectroscopy and microscopy techniques also help to study the fundamental properties of quantum dots, like size, morphology, work function, crystal structure, *etc.* The core-shell structure of quantum dots requires SP spectroscopy for the proper study of their structures and interface. With constantly evolving methodologies for the synthesis of quantum dots, TR

CHAPTER 15

Environmental and Health Impacts of Non-Metallic Quantum Dots

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Abstract: The realm of Non-Metallic Quantum Dots (NMQDs) includes carbon-based quantum dots, graphene QDs, boron nitride QDs, silicon QDs, sulphur-based QDs, and organic-based QDs. They are typically less than 10 nanometres in size and exhibit excellent biocompatibility, low toxicity, and chemical stability. Their tuneable photoluminescence, spanning from UV to near-infrared wavelengths, makes them promising for applications in bioimaging, sensing, drug delivery, and optoelectronics. They also show potential in environmental remediation and energy storage due to their high surface area and ability to catalyse reactions. These QDs generally exhibit lower toxicity than metallic QDs, making them attractive for biomedical applications. However, concerns regarding their health and environmental hazards primarily arise from the fact that they have the tendency to accumulate in biological tissues over time, leading to chronic exposure and unwanted bioaccumulation effects. Moreover, chemical modifications for specific applications may alter the QDs' toxicity profile, warranting careful consideration in biomedical and environmental contexts. Thus, proper disposal of QDs is critical to prevent environmental contamination. It is indeed a matter of serious concern that appropriate techniques for recycling or safe disposal of these widely used QDs, especially those containing hazardous materials, have not been investigated as much yet. Therefore, this chapter aims to elaborate on the less-understood detrimental effects of NMQDs on health and the environment, highlighting some of the recent reports on their toxicity studies and safety assessment for the benefit of the scientific community, who have been actively engaged in the production and commercialization of these tremendously promising NMQDs.

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Keywords: Bioaccumulation, Biocompatibility, Bioimaging sensing, Carbon-based Quantum Dots (CQDs), Cytotoxicity, DNA damage, Ecotoxicity, Fluorescence sensing, Nanomedicine, Nanotoxicology, Non-Metallic Quantum Dots (NMQDs), Photocatalysis, Photoluminescence, Photostability, Quantum computing, Quantum dot sensors, Wastewater treatment.

INTRODUCTION

Quantum Dots (QDs) are nanocrystals known for their bright, tunable fluorescence, making them highly desirable for applications in biomedical sciences and various industrial sectors. However, over the past decade, growing concerns have emerged regarding their potential toxicity to the environment and biological systems. Quantum Dots (QDs) have emerged as promising candidates for a wide range of applications due to their unique properties. In biomedical science, they show potential for biosensing, drug delivery, cell tracking, disease detection, and antimicrobial treatments [1]. However, as interest in QDs has grown, studies have indicated their potential toxicity to mammalian cells, fungal cells, plants, and other organisms [2, 3]. Despite ongoing advancements, the limited understanding of their impact on human health and the environment raises concerns about the safety of quantum dot-based products. The proven advantages of quantum dots, concerns about potential toxic effects have always accompanied them. QDs can be transported to different tissues and organs upon exposure, resulting in adverse effects in organisms.

Studies have shown that the intracellular uptake of Quantum Dots (QDs) increases Reactive Oxygen Species (ROS) levels, triggering a cascade of intracellular events that can damage DNA and proteins [4]. The inherently reactive nature of metallic and semiconductor QDs raises significant concerns in translational research, as they are often cytotoxic and non-biocompatible [5 - 7]. Furthermore, the human body lacks an efficient mechanism to eliminate these metallic ions, limiting their direct applications. To address these challenges, recent research has focused on developing non-metallic quantum dots, such as Carbon Quantum Dots (CQDs) and Black Phosphorus Quantum Dots (BP QDs), which demonstrate lower toxicity and immunogenicity, making them more suitable for real-world applications [8].

The non-metallic elements or compounds used to generate non-metallic quantum dots have benefits such as enhanced biocompatibility and less toxicity. They also exhibit high photostability, biocompatibility, and tunable optical characteristics, among other beneficial properties [9 - 11]. Several synthesis techniques, including Chemical Vapor Deposition (CVD), Molecular Beam Epitaxy (MBE), sol-gel processing, and hydrothermal treatment, have been employed in the literature to generate NMQDs. Non-metallic quantum dots have potential applications in biomedical imaging and diagnostics, optoelectronic devices, sensors and detectors, drug delivery and therapy [11 - 13].

They do, however, have several drawbacks. For instance, their quantum yield is lower than that of metallic quantum dots, and their large-scale manufacture may have potentially harmful effects on the environment. Hence, it is essential to dispose of QDs properly to avoid contaminating the environment. The fact that suitable methods for recycling or safe disposal of these commonly used QDs, especially those containing hazardous materials, have not received much attention up to this point is concerning. The lack of toxicology-based studies, the range of QD dosage/exposure concentrations reported in the literature, and the widely varying physicochemical properties of individual QDs are the main causes of the inconsistencies in the current literature regarding the toxicity of QDs. There are not many studies that are especially made for toxicologic logic assessment (*e.g.*, dose, duration, frequency of exposure, mechanisms of action). Rather than toxicologists or health scientists, nanotechnology researchers conducted many of the studies that have been mentioned in relation to QD toxicity, from which information about QD toxicity is generated [14].

In general, non-metallic quantum dots are regarded as less toxic compared to metallic QDs. Still, environmental buildup and prolonged exposure could be dangerous. Additional investigation is required to comprehend their influence on health and the environment. Therefore, this chapter tries to clarify the lesser-known harmful effects of non-metallic Quantum Dots (QDs) on the environment and human health while highlighting some recent reports on toxicity studies and safety assessments. Moreover, the regulatory guidelines imposed by the concerned authorities of various countries have also been discussed in one of the sections of this chapter for the benefit of the scientific community, which has been actively engaged in the development and commercialization of these greatly promising QDs.

EFFECT OF NON-METALLIC QUANTUM DOTS ON HEALTH: *IN-VITRO* AND *IN-VIVO* TOXICITY STUDIES

Non-metallic Quantum Dots (QDs), such as Silicon (Si), Sulphur, and carbon-based quantum dots, have attracted attention due to their lower toxicity compared to heavy metal-based QDs (*e.g.*, cadmium or lead). However, they can still exhibit cytotoxicity influenced by factors like surface functionalization, where the surface chemistry plays a crucial role in toxicity, as functional groups and reactive species (*e.g.*, fluorinated radicals) can interact with cellular components. Additionally, doped non-metallic QDs, such as silicon QDs doped with boron or phosphorus,

CHAPTER 16

Real-World Applications and Case Studies

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Abstract: Non-Metallic Quantum Dots (NMQDs) are highly versatile across diverse fields due to their excellent optical and electronic properties. The chapter examines the general applications of non-metallic QDs, like high-resolution and accurate bio-imaging, advanced solar cells for efficient energy conversion, and precise sensor technologies. The chapter also delves into the heavy metal remediation and photocatalytic degradation of organic pollutants by NMQDs from wastewater. An investigation of case studies was done to draw special attention to their practical utility in environmental remediation and sustainable water management practices. Challenges such as commercial production, potential toxicity concerns, and optimization of properties are discussed in the context of their practical applications. To optimize NMQD performances, robust characterization techniques, sustainable synthesis, and disposal practices are required. A comprehensive overview of how NMQDs are advancing technology and addressing critical challenges across biomedical, environmental, and energy sectors, offering insights into their transformative potential and the pathways for future developments, is provided.

Keywords: Advanced solar cells, Bio-imaging, Commercial production, Electronic, Energy conversion, Energy-efficient, Non-metallic Quantum Dots, Optical, Organic pollutant, Photocatalytic, Remediation, Toxicity.

INTRODUCTION

Non-Metallic Quantum Dots (NMQDs) are emerging as a versatile class of nanomaterials with diverse real-world applications due to their unique optical and

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electronic properties. NMQDs, including Carbon Quantum Dots (CQDs), Graphene Quantum Dots (GQDs), Silicon Quantum Dots (SiQDs), and Organic Quantum Dots (OQDs), offer distinct advantages over Metallic Quantum Dots (MQDs) such as improved biocompatibility, reduced toxicity, and tunable properties that can be tailored for specific applications. In real-world scenarios, NMQDs are being explored and utilized across Various fields, such as bioimaging, photovoltaic devices, optoelectronics, light-emitting devices, and sensors.

NMQDs offer improved fluorescence stability and reduced cytotoxicity compared to traditional MQDs, enabling more precise and safer bioimaging. NMQDs are utilized in advanced display technologies and light-emitting devices in optoelectronics due to their customizable emission properties. NMQDs are also used in energy applications to enhance solar cell efficiency and develop new energy storage devices, such as supercapacitors. Additionally, they have been incorporated into bioimaging probes to provide high resolution and low toxicity. Silicon QDs could also be used to develop next-generation solar cells and photodetectors.

This chapter explores NMQDs' real-world applications, especially in wastewater treatment, their commercial production challenges, potential toxicity, and the need for eco-friendly synthesis and disposal methods.

CASE STUDIES OF NONMETALLIC QDS (GENERAL APPLICATIONS)

Biomedical Applications

NMQDs excel in bio-imaging and biosensing due to their adjustable photoluminescence, low toxicity, and biocompatibility. They are also explored for drug delivery systems due to their small size and functionalization potential. These characteristics make them particularly advantageous for biomedical applications. Some of the examples of real-world applications of NMQDs in various biomedical fields are mentioned below:

Ali *et al.* developed nitrogen-doped CQDs conjugated with folic acid for treating breast cancer in mice [1]. Li's team created CQD-based nanocarriers for doxorubicin and enhanced drug delivery to HeLa cells and brain tumors [2]. Zavareh *et al.* used CQDs and 5-fluorouracil for targeted, regulated drug release, improving tumor cell eradication [3]. Duan *et al.* engineered a dual-responsive drug delivery system by modifying hyaluronic acid and heparin on the surface of Carbon Dots (CDs) while loading doxorubicin onto them [4]. The *in vitro* assessments of blood compatibility, drug targeting, drug release, and cell viability were conducted, accompanied by real-time imaging and monitoring of cellular behavior [5]. Choppadandi *et al.* synthesized both CQDs and Graphene Quantum Dots (GQDs), investigating photoluminescence-based bioimaging in MDA-M--231 and MCF-7 cell lines. The outcomes were corroborated through *in vivo* investigations and employing three-dimensional tumoroids [6]. Acar *et al.* prepared CQDs and GQDs from the flowers of *Hypericum perforatum L.* (St. John's Wort) utilizing a carbonization method, which exhibited blue photoluminescence, suggesting their application as drug delivery and bioimaging agents [7]. Edet *et al.* examined nitrogen, boron, and Sulfur-Doped Quantum Dots (SQDs) for their capacity to deliver the antitubercular drug isoniazid to the targeted site, aiming to mitigate its side effects. The research indicated that the heteroatom-doped QDs are capable of delivering isoniazid to the intended site of action [8]. Tehrani Fateh *et al.* developed hybrid Nanoparticles (NPs) composed of cetyl alcohol-modified GQDs and iron oxide magnetic nanoparticles, which demonstrated magnetic, photoluminescent, targeting, and drug-loading properties. Cell viability assessments were conducted with the hybrid NPs across two noncancerous types and one cancer cell line, alongside an investigation of *in vivo* toxicity in mouse liver and heart tissues [9]. Karami *et al.* employed a hydrogel nanocarrier incorporating chitosan, γ-Al_2O_3, and CQDs, developed *via* a double nanoemulsion technique, to selectively release curcumin as a therapeutic agent for the treatment of breast cancer tissues [10]. Lin *et al.* synthesized nitrogen-containing GQDs, subsequently coating them with branched Polyethyleneimine (b-PEI) and Polyethylene Glycol (PEG). These GQDs were then conjugated with anti-GD2 antibodies for application in *in vivo* imaging [11].

Xiao and his collaborators have engineered glycine-proline-glutamate conjugated Graphene Quantum Dots (GQDs) as a nanoscale drug delivery system aimed at the therapeutic management of Alzheimer's disease [12]. Shi *et al.* documented a colorimetric and fluorometric dual-mode nanosensor, specifically composed of Carbon Dots (CDs) and Gold Nanoparticles (AuNPs), aimed at discriminative detection of Glutathione (GSH) over Cysteine (Cys) and Homocysteine (Hcy). The selectivity of this method was evaluated using nineteen natural amino acids, inclusive of thiols such as Cys, Hcys, and glutathione disulfide, against GSH [13].

Photocatalysis

Researchers have devised an ecologically sustainable approach for the generation of energy and the mitigation of environmental pollutants utilizing NMQDs through photocatalytic processes, attributable to their capacity to absorb light and produce reactive oxygen species, thereby rendering them highly effective in facilitating chemical reactions upon exposure to light. Some of the recent developments in the field of photocatalysis are as follows:

CHAPTER 17

Future Perspectives and Concluding Remarks

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Abstract: This chapter discusses the current limitations and challenges associated with nonmetallic Quantum Dots (QDs) across various applications, including catalysis, sensing, bioimaging, and optoelectronics. Despite their promise as safer and more sustainable alternatives to metal-based QDs, issues such as material stability, controlled synthesis, and reproducibility hinder their widespread adoption. Nonmetallic QDs often exhibit lower quantum yield and face challenges in achieving precise functionalization for specialized applications. Additionally, concerns regarding environmental safety and regulatory compliance remain unresolved. Scalability and cost-effectiveness present further obstacles to industrial production. Overcoming these challenges through advanced synthesis methods, surface engineering, and interdisciplinary research is essential for unlocking the full potential of nonmetallic QDs in future technologies.

Keywords: Challenges, Commercialization, Degradation, Quality-control, Quantum dots, Recyclability, Stability.

CURRENT LIMITATIONS AND CHALLENGES

Despite the promising potential of nonmetallic Quantum Dots (QDs) as safe and sustainable alternatives for water treatment and various other applications, several limitations and challenges must be addressed before their large-scale adoption. These challenges span from fundamental material properties to regulatory and industrial barriers, which require comprehensive research and technological innovation.

One of the primary challenges is material stability and degradation [1]. Nonmetallic QDs, including Carbon Dots (CDs), Graphene Quantum Dots (GQDs), and polymer-based QDs, often exhibit instability under environmental conditions. Factors such as prolonged exposure to light, moisture, and varying pH levels can cause photobleaching, oxidation, and structural degradation [2, 3]. This instability affects their long-term performance, especially in water treatment

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processes where operational environments are often harsh and dynamic. Improving the stability of nonmetallic QDs through surface passivation, chemical modifications, and advanced synthesis methods is a critical area of ongoing research. Another significant limitation lies in controlled synthesis and reproducibility [4 - 6]. Achieving uniform particle size, shape, and surface functionalization is vital for consistent optical and catalytic performance [7]. However, current synthesis methods, such as hydrothermal, microwave-assisted, and solvothermal techniques, often lead to batch-to-batch variability. These inconsistencies impact the reproducibility of results and hinder the establishment of standardized protocols for industrial applications. Developing precise, scalable, and reproducible synthesis techniques is essential to ensure the reliability and effectiveness of nonmetallic QDs in large-scale water treatment systems.

Limited quantum yield is another challenge that affects the efficiency of nonmetallic QDs [8]. Compared to their metal-based counterparts, nonmetallic QDs generally exhibit lower photoluminescence efficiency due to non-radiative recombination pathways. This lower quantum yield reduces their effectiveness in photocatalytic and sensing applications. Enhancing quantum yield without incorporating toxic dopants remains a pressing challenge. Approaches such as heteroatom doping (with nitrogen, sulfur, or phosphorus), core-shell structures, and defect engineering are being explored to improve the optical properties of these materials [9, 10]. From a regulatory and environmental perspective, the safety profile of nonmetallic QDs requires further investigation. While these materials are considered less toxic than metal-based QDs, their long-term environmental fate and biocompatibility remain underexplored. Regulatory frameworks for nanomaterials are still evolving, and comprehensive safety assessments are needed to ensure that non-metallic QDs meet environmental and human health standards. Addressing these concerns through rigorous toxicity studies and lifecycle assessments will be crucial for their acceptance and commercialization.

Another challenge lies in functionalization for specific applications [11, 12]. Nonmetallic QDs must be carefully engineered to target specific pollutants in water treatment. Functionalizing their surface with chemical groups enhances selectivity and efficiency, but it may also reduce stability or introduce secondary contaminants. Optimizing functionalization strategies while maintaining structural integrity and performance is a complex task that requires a multidisciplinary approach. Additionally, understanding the interaction between functionalized QDs and various contaminants is essential to design more effective and adaptable water treatment solutions.

Finally, scalability and cost-efficiency present substantial challenges. While laboratory-scale synthesis of nonmetallic QDs is well-established, translating these methods to industrial-scale production remains difficult. Current manufacturing processes are often time-consuming, resource-intensive, and cost-prohibitive. Furthermore, large-scale synthesis methods must maintain the high purity and uniformity necessary for practical applications. Green synthesis techniques using biomass-derived precursors and continuous-flow reactors hold promise for addressing these scalability issues, but further optimization is required to make them economically viable.

SCALABILITY AND COST-EFFECTIVENESS

The successful commercialization of nonmetallic Quantum Dots (QDs) depends on the ability to scale up their production while maintaining cost-effectiveness. Although laboratory-scale synthesis methods, such as hydrothermal, solvothermal, and microwave-assisted techniques, produce high-quality QDs, these processes are often time-consuming, resource-intensive, and difficult to replicate on an industrial scale [13 - 16]. Large-scale production requires methods that can deliver consistent quality, uniform particle size, and reproducible properties while minimizing costs and environmental impact. One of the primary challenges in scaling up nonmetallic QDs lies in maintaining material consistency [17, 18]. Batch-to-batch variation in particle size, shape, and surface chemistry can significantly affect the optical, electronic, and catalytic properties of the final product. Continuous-flow synthesis techniques, which offer better control over reaction conditions, present a promising approach to overcome these inconsistencies. Additionally, green and sustainable synthesis methods, using biomass or waste materials as precursors, could reduce production costs while supporting environmentally friendly manufacturing processes.

Cost-efficiency is another crucial factor. While nonmetallic QDs are inherently less expensive than their metal-based counterparts due to the abundance and lower toxicity of their raw materials, the complexity of current synthesis techniques increases production costs. Optimizing reaction conditions, using renewable feedstocks, and developing energy-efficient manufacturing protocols can significantly reduce these expenses. Furthermore, improving post-synthesis purification methods is essential to enhance yield while maintaining the purity required for advanced applications. Integrating nonmetallic QDs into existing industrial systems poses additional challenges. For applications in catalysis, bioimaging, and electronics, these materials must be compatible with conventional manufacturing processes. This requires developing composite materials and hybrid systems that combine the unique properties of nonmetallic QDs with other functional materials while ensuring stability and ease of handling.

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Kalyanjyoti Deori

Dr. Kalyanjyoti Deori, currently working as an Assistant Professor at Dibrugarh University, Assam, holds his M.Sc. and Ph.D. degree in Chemistry from the University of Delhi, India and before joining this University in 2018, he was an Assistant Professor at Kirori Mal College, University of Delhi from 2015 to 2018. He has an extensive publication record in high-impact journals, book chapters and he is a co-inventor on multiple patent applications. His research focuses on the development of advanced functional nanomaterials for catalytic processes, including sustainable photocatalysis, electrocatalysis, and energy conversions. His research work has led to several funded projects supported by agencies like ANRF (formerly SERB, India), UGC and CSIR, contributing to the development of innovative, environmentally friendly nanostructured catalytic and energy materials. Dr. Deori has received numerous awards including research fellowships, Young Scientist award from University of Delhi in 2020, Dibrugarh University Teacher Award-2023, Chemical Research Society of India Young Scientist award in 2026 and multiple best poster and paper awards. He is a member of several professional bodies, including the American Chemical Society, the Royal Society of Chemistry, the Chemical Research Society of India, the Indian Society of Analytical Scientists and many more. He also serves as an editorial board member for multiple international journals. His work continues to advance the field of sustainable chemistry and environmental applications.