Green Synthesis of Element-Doped Carbon Quantum Dots: Properties Tuning for Advanced Applications

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Abstract

Due to their unique optical properties, tunable surface chemistry, excellent biocompatibility and low toxicity, CQDs have emerged as a versatile class of zero-dimensional nanomaterials. Recently, the integration of green synthesis approaches with elemental doping strategies has created new research avenues for the sustainable development of high-performance CQDs. This review article gives an overview of recent advances in the green synthesis of element doped carbon quantum dots taking into account environmentally benign precursors such as plant extracts, biomass waste, and natural polymers together with energy-efficient routes of the synthesis including hydrothermal, microwave-assisted, and sonochemical methods. Special emphasis is placed on the effect of heteroatom doping (such as nitrogen, sulfur, phosphorus, and metals) on the electronic structure, surface functionality, quantum yield, and photoluminescence behavior of CQDs. The mechanisms for modulation of the properties induced by doping are critically discussed, with insights into structure-property relationships. Furthermore, the review also emphasizes the potential applications of green synthesized doped CQDs in different fields such as bioimaging, drug delivery, sensing, photocatalysis, energy conversion and environmental remediation. Despite the significant progress, issues associated with large-scale production, reproducibility and precise control of doping configurations are still persisting. Future perspectives are presented to overcome these limitations and promote the translation of sustainable CQD technologies into practical applications. This review is intended to be a useful resource for researchers working on the design of next-generation eco-friendly nanomaterials with enhanced functionality.

Keywords

Carbon quantum dots, Green synthesis, Elemental doping, Photoluminescence, Nanocomposites, Biomedical applications, Environmental remediation

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Introduction

Carbon Quantum Dots (CQDs) are a new class of zero-dimensional carbon-based nanomaterials with sizes usually smaller than 10 nm, showing good photoluminescence, large surface area, adjustable emission, and excellent biocompatibility (Baker & Baker, 2010; Li et al., 2012). Since their fortuitous discovery, CQDs have rapidly emerged as versatile platforms for applications ranging from bioimaging, sensing, catalysis, optoelectronics to energy conversion (Sun et al., 2006; Hola et al., 2017). CQDs are mostly composed of carbon, which are environmentally friendly and suitable for biomedical applications as compared with the traditional semiconductor quantum dots containing toxic heavy metals (Wang & Hu, 2014).

One of the most salient features of CQDs is the strong and tunable photoluminescence, which is attributed to the complex interplay of quantum confinement effects and surface/defect states (Zhu et al., 2015; Yuan et al., 2016). These functional groups (hydroxyl, carboxyl, and amino groups) are abundant, which render excellent aqueous dispersibility and provide reactive sites for further modification (Dong et al., 2012; Zhou et al., 2017). Together, these properties make CQDs excellent candidates for highly sensitive probes and effective charge mediators in different systems.

The synthesis of CQDs can be broadly divided into top-down and bottom-up approaches. Top-down approaches include arc discharge, laser ablation and electrochemical oxidation, while bottom-up routes refer to carbonization of molecular precursors by hydrothermal, solvothermal or microwave-assisted methods (Peng et al., 2012; Tang et al., 2012). Several classical routes are effective, but require harsh conditions or dangerous reagents. Thus, green synthesis has emerged as a sustainable option that uses renewable precursors and moderate conditions for the synthesis of CQDs with little environmental effect (Shen et al., 2012; Lim et al., 2015).

Green synthesis uses natural resources including plant extracts, fruit peels, biomass and agro-waste for CQDs synthesis. These precursors are rich in carbon and typically include heteroatoms such as nitrogen and sulfur that may be integrated into the CQD framework during synthesis (Sahu et al., 2012; Prasannan & Imae, 2013). Hydrothermal treatment of these materials gives CQDs with better surface functionality, enhanced fluorescence, and decreased cytotoxicity, making them especially suited to biological applications (Zhang et al., 2012; Sachdev & Gopinath, 2015).

Elemental-doping provides a strong way to modify electrical and optical characteristics of CQDs. Heteroatoms such as nitrogen, sulfur, phosphorus and boron may be used to modify the electronic structure, generate mid-gap states and improve the charge transfer capabilities (Qu et al., 2014; Wang et al., 2017). For example, N-doping improves the quantum yield and electron-donating capacity, while S-doping improves the surface reactivity and catalytic activity (Li et al., 2016; Ding et al., 2016).These effects are further enhanced when co-doping with multiple elements, providing for a fine tuning of the emission wavelength and functional performance.

Green synthesis and elemental doping are a synergistic strategy to prepare high-performance CQDs. The natural precursors containing heteroatoms may be used as self-doping sources, which naturally simplify the synthesis and reduce the demand of external dopants (Tyagi et al., 2016; Atchudan et al., 2017). This approach increases the optical characteristics and at the same time complies to the principles of green chemistry by producing less waste and using less energy.

Green synthesis and doping has aided in remarkable improvements in customizing CQDs for biological purposes. CQDs have minimal toxicity and are biocompatible, and have been employed for bioimaging, medication administration and diagnostics (Zhao et al., 2015; Miao et al., 2017). Their luminous properties allow real-time monitoring of biological processes and surface functionalization permits the targeted administration of therapeutic medicines (Liu et al., 2013; Chen et al., 2016).

Doped CQDs are efficient sensors for the detection of metal ions, organic pollutants and biomolecules in environmental applications. They exhibit good sensitivity and selectivity due to strong surface contacts and fluorescence modulation mechanisms (Qian et al., 2014; Lu et al., 2015). Moreover, CQDs have been widely employed in photocatalysis for pollutant degradation and energy conversion due to the improved charge separation and light absorption (Zhang et al., 2015; Yu et al., 2016).

Despite some progress, challenges remain in mass production and normalization of CQDs. Reckmeier et al. (2016) and Cayuela et al. (2016) proved that the variation of precursor composition, synthesis conditions and post-treatment might lead to the diversity in properties. The process of photoluminescence is also being studied and further research is needed to understand and control the emission properties.

Future prospects for CQD research include scalable green synthesis pathways, better doping strategies and integration with new domains like as artificial intelligence and nanomedicine

(Xu et al., 2020; Khan et al., 2021).Further development of sustainable and versatile CQDs is anticipated to enhance innovation across a broad spectrum of scientific and industrial areas.

Fundamentals of Carbon Quantum Dots

Carbon quantum dots (CQDs) is a class of quasi-spherical carbon-based nanomaterials with zero-dimensional structure, usually with sizes below 10 nm. Since their emergence as fluorescent nanostructures, CQDs have attracted much attention due to their unique combination of optical properties, chemical stability, aqueous dispersibility and low cytotoxicity. CQDs typically have a carbonaceous core containing a mixture of sp^{2} - and sp^{3} - hybridized domains, which is surrounded by a variety of surface functional groups, such as hydroxyl (−OH), carboxyl (−COOH), carbonyl (−C=O), and amino ($-NH_2$) moieties. This core–shell hybridized structure is important for their physicochemical and optical behaviour (Lim et al., 2015; Zhu et al., 2016).

The size-dependent photoluminescence (PL) is one of the characteristic features of CQDs, which is mainly attributed to the quantum confinement effects and surface-related emissive states. The bandgap is increased by decreasing the particle size to the nanoscale as a result of the spatial confinement of the charge carriers leading to the tunability of emission wavelength in the ultraviolet to near-infrared region. However, compared with the traditional semiconductor quantum dots, the PL behaviour of CQDs is often more complicated and more dependent on the surface defects, edge states and functional groups rather than only on the size effects (Jiang et al., 2018; Hola et al., 2017).

Surface states of CQDs are important to their fluorescence properties. Surface defects and functional groups with heteroatoms are responsible for localized energy levels in the bandgap and act as emissive centres. These states facilitate radiative recombination of electron–hole pairs, contributing to the excitation-dependent emission behaviour commonly observed in CQDs. Chemical modification or doping can passivate the surface, which can considerably improve the fluorescence intensity and quantum yield by inhibiting non-radiative recombination pathways (Dong et al., 2017; Li et al., 2016).

The electronic structure of CQDs is another important trait. It stems from the struggle between the π-conjugated carbon core and the surface functionalization. Graphitic (sp2) domains can efficiently delocalize electrons, whereas oxygen- and nitrogen-containing groups modify the electronic density and produce new energy levels. This adjustable property allows CQDs exhibit unique optical properties and hence makes them useful for different

applications, such as sensing, imaging, and catalysis (Zhao et al., 2020; Liu et al., 2018).Meanwhile, CQDs have outstanding photo stability and chemical stability, which are very different from the traditional fluorescent dyes and semiconductor quantum dots that are sensitive to light bleaching or toxicity concerns. Their high water solubility and simple surface modification in combination with their excellent resistance to UV degradation further boost their applicability for biological and environmental applications (Wang et al., 2019).

The mechanism of photoluminescence in CQDs is still a matter of current investigations with various variables contributing including intrinsic state emission (π–π* transitions), surface/defect state emission, and molecule fluorophore-related emission. Recent investigations show that the observed luminescence is often due to a synergistic mix of these processes, depending on the synthesis techniques and the precursor materials (Zhang et al., 2020; Miao et al., 2017).Generally, the unique properties of CQDs arising from their nanoscale size, hybrid carbon structure and rich surface chemistry offer a versatile platform for tuning functional nanomaterials. Understanding these aspects in depth is very important to maximize their performance, particularly when used in combination with green synthesis methods and elemental doping strategies.

Need for Green Synthesis

The rapid growth of research on carbon quantum dots (CQDs) has exposed the limitations of the conventional methods for the synthesis of CQDs such as chemical oxidation, laser ablation, and electrochemical methods. These techniques generally involve the use of strong acids (HNO_3, H_2SO_4), hazardous solvents and high temperature or high energy conditions which are of concern to the environment, pose safety risks and increase the production cost. Moreover, the production of toxic by-products and the need for complex purification steps further restrict their sustainability and large scale applicability (Lim et al., 2015; Dong et al., 2017).

Also, green synthesis has evolved as a sustainable and ecologically friendly alternative following the principles of green chemistry such waste reduction, utilization of renewable resources and energy efficiency. The carbon sources are natural and renewable such as plant extracts, fruit peels, agricultural residues and biopolymers which can reduce the environmental impact and add intrinsic functional groups to improve the physicochemical properties of CQDs (Zhang et al., 2021; Eftekhari et al., 2024).

One of the major advantages of green synthesis is the benign and energy efficient reaction conditions which commonly include hydrothermal, microwave assisted or sonochemical

processes .These approaches provide controlled synthesis with greater yield and repeatability minimizing the energy usage. In addition, the biocompatibility of CQDs is improved by the nonuse of hazardous chemicals, which makes CQDs more suitable for biomedical applications such as bioimaging and drug administration (Hola et al., 2017; Li et al., 2016).

Cost-effectiveness and scalability are some important benefits of green synthesis. The use of low-cost and well-available biomass waste resources not only decreases the manufacturing cost but also supports waste valorization and circular economy practices.Moreover, these approaches are more easily scalable up for industrial production as compared to conventional approaches which require stringent conditions and expensive equipments (Zhao et al., 2020; Wang et al., 2019).

Another important aspect is the improved surface functionality by green synthesis. Natural precursors contain heteroatoms such as nitrogen, sulfur, and oxygen, which can be introduced into the CQD structure during the synthesis without the need of additional doping agents . The doping is intrinsic and enhances the optical properties, quantum yield, and chemical reactivity, which broadens the application potential of CQDs (Zhu et al., 2016; Miao et al., 2017).

However, these benefits are still accompanied by problems such as variability of precursor composition, limited control over particle size distribution and reproducibility. But the limitations are being addressed by recent advances in process optimization, precursor standardization, and hybrid green synthesis methodologies, making green synthesis a promising route for the sustainable production of high-performance CQDs.

Green Precursors for Carbon Quantum Dots (CQDs)

The selection of appropriate precursors is a crucial factor for the green synthesis of carbon quantum dots, which has a direct impact on their structural, optical and functional properties. Biomass produced precursors have received significant research interests in the recent years (2020-2026) owing to their availability, renewability, cheap cost as well as environmental friendliness. These precursors include plant extracts, fruit peels, agricultural wastes, food waste and natural polymers as sustainable carbon sources for CQDs manufacturing.

Biomass materials are rich in organic compounds such as cellulose, hemicellulose, lignin, proteins and carbohydrates which provide not only high carbon content but also oxygen and nitrogen containing functional groups. These intrinsic parts facilitate the fabrication of the CQDs under moderate circumstances and give rise to good photoluminescence and surface functionality. Importantly, the natural heteroatoms (e.g., N, S, P) present in biomass enable

for in situ doping, eliminating the need of additional chemical dopants and enhancing quantum yield and electrical properties (Bioresource Technology Review, 2026).

Among the numerous biomass resources, fruit peels (orange, banana, lemon) and food waste are extensively used because of their higher polysaccharide contents which enable surface-state emission in CQDs. In contrast, the aromatic structure of lignin-rich materials, e.g. wood residues and nutshells, favors core-dominated emission. This highlights the important function of the chemical composition of the precursor in influencing the optical characteristics and performance of CQDs (Next Materials Review, 2026).

Agricultural and forestry waste, such as crop leftovers, husks and seed shells, have also been intensively researched as green predecessors. These materials provide a sustainable method for the CQD synthesis, thereby contributing to waste valorization and circular economy principles. CQDs synthesized from nutshells by hydrothermal techniques show outstanding optical characteristics and strong scaling potential, which suggests their use in industrial applications (Yu et al., 2025).

Another important class of green precursors is natural polymers like starch, chitosan, cellulose and proteins. These biopolymers enable controlled carbonization, homogeneous particle formation and improved biocompatibility, thus making them particularly attractive for biomedical applications. Moreover, bioactive molecules present in plant-based materials such as leaves, roots, and resins act as sources of carbon and surface passivating agents, which improve the stability and functionality of CQDs (Praseetha et al., 2024).

The great benefit of green precursors is the large number of surface functional groups (–OH, –COOH, $–NH_2$) which result in better water solubility, chemical reactivity and ease of functionalization. Such features are important for applications in sensing, catalysis, and bioimaging. Moreover, CQDs derived from biomass are low in toxicity and high in biocompatibility and can be used for environmentally and biologically sensitive applications (Biomass & Bioenergy Review, 2025).

Notwithstanding such benefits, there are still major challenges including variation in precursor composition, lack of standardization and batch-to-batch inconsistency. However, recent progress has focused on precursor characterization, controlled processing, and hybrid approaches to improve reproducibility and scalability .

Green precursors are of great importance for sustainable synthesis of CQDs as they provide green, cost-effective and functionally rich starting materials. The inherent chemical diversity

not only facilitates efficient CQD formation but also allows property tailoring for advanced applications.

Green Synthesis Techniques

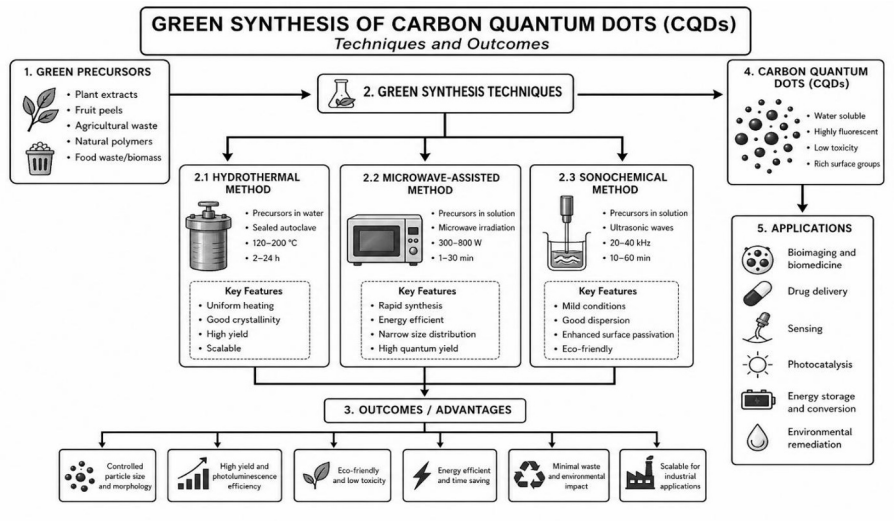


Figure 1: Green synthesis of carbon quantum dots

The green synthesis of carbon quantum dots (CQDs) saw significant developments between 2010 and 2026, with the hydrothermal, microwave-assisted and sonochemical processes being the most often used procedures. These technologies are recommended because to their eco-friendly nature, energy efficiency, and ability to produce CQDs with adjustable size, shape, and enhanced optical characteristics.

a. Hydrothermal Method

The hydrothermal method is one of the most popular green synthesis methods of CQDs. The carbonization, nucleation and growth of CQDs are promoted by thermally treating the carbon-rich precursors in a sealed autoclave under high temperature and pressure. This approach enables to regulate particle size, crystallinity and surface functionalization in a high degree by tuning parameters like temperature, time and precursor concentration. Furthermore, hydrothermal synthesis may allow high yield mass manufacturing and increased photoluminescence characteristics (Lim et al., 2015; Wang et al., 2019).

Recent research (2020-2026) show that CQDs derived from biomass using hydrothermal synthesis have improved fluorescence and scalability, making it a good approach for sustainable nanomaterial production (Yu et al., 2025; Bioresource Technology Review, 2026). The approach also enables the introduction of oxygen-rich functional groups that enhance the solubility and reactivity of CQDs.

b. Microwave-Assisted Synthesis

Microwave-assisted synthesis has gained considerable popularity as an alternative to traditional heating techniques because of its rapidity and energy economy. The technology relies on the direct interaction of microwave radiation with the precursor molecules leading to homogenous and immediate heating. However, the microwave synthesis may dramatically shorten the reaction time (from hours to minutes), while high quality products are still produced (Zhu et al., 2016; Dong et al., 2017).

Microwave heating efficiency increases the nucleation rates and leads to homogenous particle size distribution and better quantum yield. In addition, this technique may be used with green precursors such as glycerol, citric acid and plant extracts, which further promotes sustainable synthesis. Recent research (2024-2025) emphasize its employment in doped CQDs and nanocomposites for photocatalysis and energy applications. Microwave-assisted technologies are ideal for scale-up manufacturing owing to quick synthesis and less energy use.

c. Sonochemical (Ultrasonic) Method

The sonochemical method is based on the application of ultrasonic waves to generate acoustic cavitation in liquid media, leading to localized high (temperature) and pressure conditions. Such transient microenvironments allow the decomposition of precursors and the formation of CQDs without the need for high bulk temperatures or harsh chemicals. This technique is helpful to the synthesis of CQDs with narrow size distribution and high surface activity.

Sonochemical synthesis is regarded as a green and energy efficient approach due to mild operating conditions and reduced reaction time . This also permits the efficient dispersion and thus prevents aggregation of CQDs which is beneficial for their optical and catalytic properties. Recent studies have demonstrated that ultrasonic-assisted synthesis may increase surface passivation and functionalization, which can boost fluorescence and sensing performance (Jing et al., 2023).

d. Comparative Advantages of Green Techniques

The green synthesis methods of carbon quantum dots (CQDs) have many important benefits in comparison with traditional chemical synthesis methods in general. These methods provide better control over the particle size, morphology and surface properties by optimizing the reaction parameters such as reaction temperature, time, pH and concentration of precursor. Also, the green synthesis methods produce better product yield and photoluminescence efficiency due to better surface passivation and fewer structural defects. Furthermore, the use of natural, non-toxic and renewable precursors decreases the environmental pollution and hazardous waste generation and increases the biocompatibility. Most of the green approaches of synthesis are energy efficient, cost effective and suitable for large scale industrial production. Among the most common techniques, hydrothermal synthesis is advantageous for large-scale and uniform production due to its simplicity and high stability of the product. Microwave-assisted synthesis is favored for CQD formation because it is rapid and efficient with short reaction times and uniform heating. Sonochemical synthesis, on the other hand, offers fine control over surface functionalization and particle dispersion through acoustic cavitation effects. Thus, each green synthesis method has its own specific advantages, and can be selected according to the desired physicochemical properties and application of CQDs

Elemental Doping in Carbon Quantum Dots (CQDs)

Elemental doping is a very efficient approach to tailor the intrinsic properties of carbon quantum dots (CQDs) by embedding foreign atoms into their carbon skeleton or surface. This strategy has been extensively studied since the early studies (~2010) to recent developments (2026) to enable fine-tuning of the electronic structure, surface chemistry and optical properties. Doping is usually carried out with heteroatoms such as nitrogen (N), sulfur (S), phosphorus (P), boron (B) and different metals, alone or in combination, to improve the performance of CQDs in a wide range of applications.

Doping introduces new energy levels in the CQDs bandgap and modifies electronic band structure of the CQDs resulting in improved electron mobility and charge transfer. For example, nitrogen doping provides the extra electron density due to its similar atomic size and higher electronegativity, which contributes to the increased conductivity and fluorescence efficiency. Moreover, the bandgap and defect states of the material are tuned by doping with sulphur and phosphorus, which enhances the visible-light absorption and catalytic activity

(Zhu et al., 2016; Li et al., 2016). More recent studies confirm that heteroatom doping greatly improves quantum yield, photoluminescence tuning and sensing performance, thus making doped CQDs very versatile nanomaterials.

The doping mechanism is closely related to the formation of surface defects and functional groups. Dopant atoms may substitute carbon atoms in the graphitic core or be attached to the surface forming localized electronic states. These states act as emissive centres, affecting the fluorescence behaviour and allowing excitation dependent emission. Furthermore, doping can induce p- or n-type electronic features that are dopant-dependent and may have strong influence on charge-carrier dynamics and electronic conductivity.

Different types of doping strategies have been developed, including:

Non-metal doping (N, S, P, B): Improves photoluminescence, surface reactivity and chemical stability.Metal doping (Fe, Cu, Zn, Mn, Gd): Improves catalytic activity, magnetic properties and electron transfer efficiency.Co-doping (e.g. N,S or N,P) It results in synergistic effects, so that the optical and catalytic properties are better than those of single-element doping.

The co-doping tactics are especially significant in recent research (2020–2026), where the synergistic impact of numerous dopants results in an enhancement in charge separation, reactive oxygen species (ROS) generation and photocatalytic performance, notably in the environmental and energy fields.

Elemental doping also remarkably improves chemical reactivity and surface functioning of CQDs. Doping with heteroatoms boosts the density of active sites and their interaction with analytes, which makes doped CQDs very useful for sensing applications. Furthermore, doping enhances the stability and dispersibility of CQDs, which broadens their applicability in biological systems and severe environmental conditions (Miao et al., 2017; Zhao et al., 2020).

From the application point of view, doped CQDs shown better performance in the bio-imaging, sensing, photocatalysis, energy storage and environmental remediation.For example, nitrogen-doped CQDs have demonstrated high fluorescence and stability, which can be used for the sensitive detection of metal ions and biomolecules . Sulfur- and phosphorus-doped CQDs have exhibited enhanced catalytic activity for pollutant degradation and water purification .

However, challenges remain in achieving precise control of dopant concentration, distribution and bonding configuration, which directly affect reproducibility and performance

consistency. To overcome these restrictions, sophisticated synthesis methods and computational methods are being investigated for rational design of doped CQDs.

Types of Elemental Doping in Carbon Quantum Dots (CQDs)

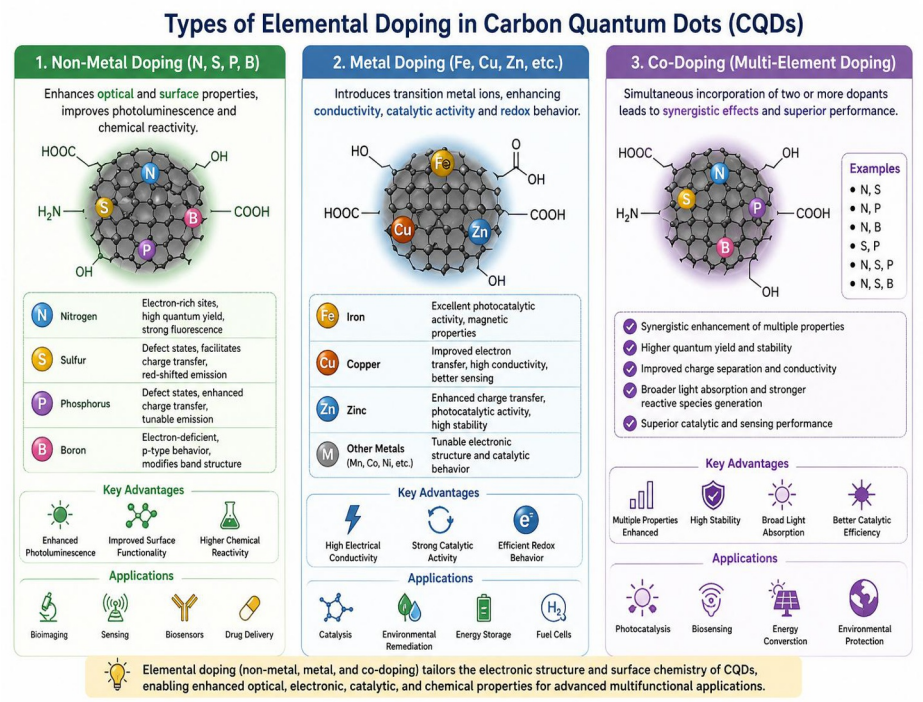


Figure 2: Carbon quantum dots doping types infographic

a. Doping with Non-Metals (N, S, P, B)

Non-metal doping is a common way to enhance the optical and surface characteristics of CQDs. The quantum yield and fluorescence intensity are enhanced with the introduction of electron-rich nitrogen (N) sites, while sulfur (S) and phosphorus (P) dopants create defect states that facilitate charge transfer and red-shifted emission. Boron (B) electron shortage causes P-type behavior and band structure changes. Generally, these dopants improve the photoluminescence, surface functionality and chemical reactivity of the CQDs, which are particularly beneficial for sensing and bioimaging applications (Zhu et al., 2016; Zhao et al., 2020; Saini et al., 2022).

b. Doping of metal (Fe, Cu, Zn etc.)

Metal doping, which is the introduction of transition metal ions into the CQD framework or on the surface, leads to a significant improvement in electrical conductivity, catalytic activity, and redox behavior of CQDs. For example, Fe-doped CQDs exhibit outstanding photo catalytic and magnetic capabilities, whereas Cu and Zn-doped CQDs enhance the efficiency of electron transfer and sensing performance. Such doped CQDs are especially useful in catalysis, environmental remediation, and energy-related applications where effective charge separation and transfer are critical (Li et al., 2016; Wang et al., 2019; Chemical Engineering Journal, 2025).

c. Co-doping (doping with several elements)

Co-doping is the simultaneous introduction of two or more dopants (e.g. N,S or N,P) resulting in synergistic effects better than those of single-element doping. This approach enhances at the same time numerous attributes such as quantum yield, stability, conductivity and catalytic efficiency. The co-doped CQDs show better charge separation, broader light absorption, and more reactive species formation, which are very promising for advanced applications such as photocatalysis, biosensing, and energy conversion (Zhang et al., 2020; Journal of Water Process Engineering, 2025).

Mechanism of Doping in Carbon Quantum Dots (CQDs)

Elemental doping is a crucial method to tailor the physicochemical and optical properties of carbon quantum dots (CQDs) by incorporating heteroatoms or metal ions into their carbon framework. Doping is a complex process that influences the electronic band structure, generates defect states and modifies surface chemistry, all of which are relevant to the charge transfer dynamics and photoluminescence behavior. The understanding of these mechanisms is important for the rational design of the CQDs with desired functionalities.

a. Band Structure Modulation

The electronic structure of pristine CQDs is mainly dominated by π-π^* transitions of sp^2 hybridized carbon domains and n-π^* transitions of surface functional groups. Doping adds

foreign atoms into the carbon lattice (substitutional doping) or attaches them to the surface (surface doping) to create new energy levels within the bandgap. These additional states effectively alter the bandgap energy thereby offering tunable optical absorption and emission properties.

For instance, nitrogen doping provides electron donating sites owing to its lone pair electrons, creating donor levels near the conduction band. This minimizes the band gap and enhances the density of electrons and improves the electrical conductivity and fluorescence intensity (Li et al., 2016). However, doping with boron is electron-deficient and creates acceptor states in the valence band, leading to p-type behavior and tuning the distribution of charge carriers (Zhu et al., 2016). Such a kind of band structure engineering is very important for applications requiring regulated electronic transitions, e.g. optoelectronics and photocatalysis.

b. Formation of Defect States

Doping also leads to the formation of structural defects and localized states in the CQD framework. These defects are attributed to lattice distortion, vacancies, and the incorporation of heteroatoms with different atomic radii and electro negativity as compared to carbon. These defect sites act as trapping centers for electrons and holes and promote radiative recombination and enhanced photoluminescence.

The defect states incorporated in sulfur and phosphorus doped CQDs enhance the density of the mid-gap energy levels and lead to excitation dependent emission behaviour. These localized states introduce multiple emission channels, and thus CQDs have tunable fluorescence emission in a broad spectral range (Miao et al., 2017). In addition, controlled defect engineering can be used to suppress non-radiative recombination and hence improve the quantum yield and stability.

c. Surface State Modification

CQDs are rich in functional groups on their surface such as –OH, –COOH, and $–NH_2$, which are important to determine their optical and chemical properties. Doping dramatically alters these surface states by introducing new functional groups or modifying existing ones. This results in changes in the surface energy levels and the electron distribution, which directly affect the fluorescence behaviour and the chemical reactivity.

Surface doping enhances surface passivation and reduces defects that serve as non-radiative recombination centres. For example, the nitrogen-containing groups might enhance the electron delocalization and stabilize the excited states, resulting in stronger and more stable emission (Zhao et al., 2020). Moreover, surface modified CQDs have higher solubility and interaction with the surrounding environment, which is of great importance for sensing and biological applications.

d. Charge Transfer Dynamics

Doping is an essential strategy to improve the efficiency of charge separation and transfer in CQDs. The dopant-induced energy levels help in the movement of electrons and holes, decreased recombination losses, and enhanced photocatalytic activity. The transition metal ions in the metal-doped CQDs may work as electron sinks or donors to promote the effective charge transfer in redox processes.

These effects may be further enhanced by co-doping tactics that induce synergistic effects among diverse dopants. For example, the N,S co-doping gives rise to dual electron donating and defect inducing sites, which leads to an increase in charge carrier mobility and light absorption. This improved charge transfer capability is especially helpful for applications such as photocatalysis, energy conversion, and environmental remediation (Zhang et al., 2020).

e. Influence on Photoluminescence Mechanism

The PL of CQDs is determined by a combination of intrinsic core states, surface states and molecular fluorophores. Doping affects all these factors resulting in improved and tunable emission properties. Introducing dopants alters the recombination pathways of electron-hole pairs, resulting in emission at different wavelengths.

PL emission in doped CQDs is usually associated with defect states and emissive sites on the surface and not solely with quantum confinement effects. This provides a rationale for the commonly observed excitation-dependent emission behaviour. Moreover, doping can lead to red or blue shift of emission spectra depending on the type and concentration of dopants. For instance, N doping may usually improve the blue or green emission, while the S and P dopants can tune the emission to red or near-infrared regions (Jiang et al., 2018).

f. Alignment of energy levels and catalytic activity

Doping modifies the alignment of energy levels in CQDs, which is significant for catalytic and energy applications. Good contact with the reactant molecules and redox reactions are possible due to the proper alignment of the conduction and valence band locations. Doped CQDs may serve as electron mediators in photocatalytic systems, transferring electrons to the catalytic sites and improving the kinetics of the process.

In particular, metal-doped CQDs have improved catalytic activity owing to the availability of active metal centers engaging directly in the chemical processes.These materials show improved activities in water splitting, CO2 reduction, and pollutant degradation processes.

g. Overall Structure-Property Correlation

The combination of band structure modification, defect engineering, and surface functionalization results in a strong structure–property relationship in doped CQDs. The degree of these modifications is determined by the type, concentration and distribution of dopants, which ultimately control the optical, electronic and chemical properties of the material. Advanced characterization techniques are needed to investigate these changes and to optimize doping strategies for specific applications.

Structure-Property Relationship in Carbon Quantum Dots (CQDs)

The performance of carbon quantum dots (CQDs) is fundamentally determined by the interaction between their structural features and resulting physicochemical properties. The particle size, surface functional groups and elemental doping are the key parameters that determine their optical behavior, electronic structure and chemical reactivity. A thorough understanding of this structure-property relationship is essential to rationally design CQDs with application-specific functions.

a. Size-Dependent Properties (Quantum Confinement Effect)

The size of CQDs, typically less than 10 nm, is a primary factor in determining their optical properties through the quantum confinement effect. As the size of the particles decreases, the bandgap increases leading to a shift in emission from long to short wavelengths (red to blue shift). In general, smaller CQDs emit at higher energies, while larger CQDs emit at longer wavelengths. The size-dependent tunability enables engineering of CQDs for multicolor emission and imaging applications. In addition, the uniformity of size results in consistent optical performance and better reproducibility.

b. Surface Functional Groups and Surface States

CQDs possess many surface functional groups such as hydroxyl (–OH), carboxyl (–COOH), carbonyl (–C=O) and amino ($–NH_2$) that greatly influence their solubility, stability and photoluminescence properties. These groups generate surface states in the bandgap that behave as emissive centers, controlling the fluorescence intensity and wavelength.

Functionalization increases dispersability and enables interaction with outer molecules . Surface passivation enhances luminescence by reducing non-radiative recombination . This is especially critical for sensing and biological applications where selective binding and signal production are desired. The type and density of surface groups also dictate the chemical reactivity and catalytic efficacy of CQDs.

d. Einfluss von Dotierungen mit Elementen

Elemental doping, i.e. the introduction of heteroatoms such as nitrogen (N), sulfur (S), phosphorus (P), boron (B) or metal ions into the structure of carbon quantum dots (CQDs), has a tremendous effect on their electrical, optical and chemical characteristics.The dopants introduce new energy levels in the band structure, change the charge distribution and enhance the electron mobility, thus improving the overall functionality of CQDs. The increased electron density and surface passivation by nitrogen doping resulted in an enhanced fluorescence intensity and quantum yield. The doping of sulfur and phosphorus creates defect states and surface traps to induce red-shifted emission, improve light absorption, and enhance the catalytic performance. Furthermore, the electrical conductivity is improved and efficient charge transfer is facilitated by metal doping, making doped CQDs promising for catalytic, sensing and energy storage applications. The type, concentration and spatial distribution of dopant atoms play a crucial role in determining the bandgap energy, emission characteristics, quantum yield and the overall performance of the doped CQDs in many sophisticated technological and biological applications.

d. Hybridization and Core Structure

CQDs have sp^2 (graphitic) and sp^3 (amorphous) internal structure and this determines their electrical activity. The increased sp2 domains allow better delocalization of pi electrons, which results in better conductivity and optical absorption. In contrast, sp^3 areas are involved in structural stability and surface functionalization. The interaction between these two domains is essential for maximizing electrical and optical performance.

e. Interdependence of Structural Factors

Importantly, these structural parameters are not independent, but are strongly interconnected. For instance, doping can change surface functional groups and synthesis conditions can change size, surface chemistry, and defect formation simultaneously. This mutual dependence leads to complex photoluminescence mechanisms, often resulting in excitation-dependent emission behaviour.

f. Implications for Tailored Design

Rational design of CQDs for specific applications is enabled by knowledge of the structure-property relationship. The emission wavelength, quantum yield, conductivity, and chemical reactivity of CQDs can be modified by controlling synthesis parameters, precursor selection, and doping strategies. This is particularly relevant for advanced applications in sensing, bioimaging, photocatalysis and energy conversion.

Optical Properties of Carbon Quantum Dots (CQDs)

Carbon Quantum Dots (CQDs) possess outstanding optical characteristics, which make them desirable for sensing, imaging, optoelectronics and photocatalysis. These features stem from their nanoscale size, quantum confinement effects and their rich surface functional groups.

a. Photoluminescence (PL) Behaviour

One of the most important optical properties of carbon quantum dots (CQDs) is strong photoluminescence behavior. CQDs can absorb suitable light sources and emit strong fluorescence in a wide spectral range, which makes them attractive for bioimaging, sensing, optoelectronics and photocatalysis. The fluorescence emission of CQDs can be adjusted from blue to red depending on particle size, surface functional groups, degree of oxidation and doping elements. Typically smaller CQDs show blue emission, while larger particles or surface-modified CQDs may exhibit green, yellow or red-shifted fluorescence. CQDs luminescence mechanism is attributed to a synergic effect of quantum confinement characteristics associated with the carbon core and surface defect states induced by functional groups or structural defects. In addition, surface passivation is also important for the enhancement of fluorescence efficiency by reducing the non-radiative electron-hole recombination channels and stabilizing the surface energy states. This results in higher quantum yield, better photostability and strong fluorescence intensity of well-passivated CQDs, which greatly improve their performance in a wide range of scientific and technological applications.

b. Excitation-Dependent Emission

Carbon quantum dots (CQDs) show a typical excitation-dependent fluorescence behavior, meaning that the emission wavelength can be tuned by varying the excitation wavelength. The unique optical property is attributed to the presence of multiple emissive centers, heterogeneous surface states, and a wide distribution of particle sizes in the CQD structure. Various energy levels are created by different surface functional groups, defect sites, and smaller particle domains, leading to different emission pathways. In this way, excitation at different wavelengths activates different emissive sites, hence enabling tunable fluorescence emission in a wide spectral range. The excitation-dependent PL of CQDs is highly advantageous for multicolour imaging, optical labelling and sensing applications as this allows simultaneous detection and visualization under different excitation conditions. In addition, this property could also improve the versatility of CQDs in biomedical imaging, environmental monitoring and optoelectronic devices with flexible and controllable fluorescence responses.

c. Quantum Confinement Effect

Carbon quantum dots (CQDs) belong to the class of zero-dimensional carbon nanomaterials with a size of a few nanometers or less. CQDs have attracted increasing attention due to their unique optical and electronic properties, as a consequence of the quantum confinement effects associated with their ultrasmall nanoscale dimensions, usually below 10 nm. In nano-sized CQDs, the motion of electrons and holes is spatially confined, such that the energy levels are discrete as opposed to the continuum of energy levels in bulk carbon materials. The band gap energy is increased with decreasing particle size and this causes modifications of the absorption and fluorescence behavior. Thus, smaller CQDs emit light at shorter wavelengths and hence blue-shifts the fluorescence, while larger CQDs with smaller band gaps emit light at longer wavelengths and hence red-shifts the emission. One of the most important features of CQDs is their size-dependent tunability of optical properties, which enables their application in bioimaging, light-emitting devices, sensors, photocatalysis, and optoelectronic systems.

d. Role of Surface Functional Groups

The optical and chemical behaviour of the carbon quantum dots (CQDs) are very important to be defined by the surface functional groups like hydroxyl (–OH), carboxyl (–COOH) and amino (–NH_2) groups. These functional groups induce surface energy states which are important emission centres and contribute significantly to the photoluminescence properties of the CQDs. Surface states affect the electron–hole recombination processes and can provide

tunable fluorescence emission over a range of wavelengths. Furthermore, the presence of these polar functional groups increases the hydrophilicity, solubility, and colloidal stability of CQDs in aqueous and biological media, making them highly attractive for biomedical and environmental applications. Surface modification or functionalization allows for the fine-tuning of the emission intensity, fluorescence wavelength, quantum yield, and chemical reactivity. Therefore, the tuning of surface chemistry of CQDs is a valid strategy to improve their performance for sensing, bioimaging, drug delivery, photocatalysis and optoelectronic applications.

e. Effect of Doping on Optical Properties

Heteroatom doping of carbon quantum dots (CQDs) with nitrogen, sulfur, phosphorus, and boron is a successful strategy to enhance their optical and electronic properties. The introduction of these dopant atoms alters the electronic structure of CQDs by introducing new energy levels and defect states in the band structure which has a pronounced effect on electronic transitions and fluorescence properties. Heteroatom doping generally enhances the fluorescence intensity and quantum yield by improving the surface passivation and reducing the non-radiative recombination processes . The emission wavelengths of CQDs shift to red or blue with the change of band gap energy and surface states depending on the types and concentrations of dopants. In addition, doped CQDs have higher charge transfer ability, electrical conductivity, and lower electron-hole recombination losses, which make them highly efficient for bioimaging, sensing, photocatalysis, solar energy conversion, and optoelectronic devices. Therefore heteroatom doping is a key strategy to tune the physicochemical properties and functional performance of CQDs for advanced technology applications.

f. Photostability

CQDs are widely recognized for their outstanding photostability in comparison with ordinary fluorescent dyes and semiconductor quantum dots, which is very useful for long term optical applications. CQDs are photobleaching resistant under continuous or lengthy light irradiation and retain their fluorescence capabilities for long periods of time. The constant fluorescence intensity and chemical degradation resistance enable dependable and predictable performance during multiple excitation cycles.The remarkable photostability is attributed to their strong carbon core structure and stable surface functional groups to reduce photochemical damage and fluorescence decay . Therefore, CQDs are particularly suitable for long-term bioimaging, fluorescence tracking, biosensing, and real-time monitoring applications where long-term and

stable optical signals are needed. The excellent photostability together with low toxicity and high fluorescence makes CQDs promising materials for advanced biomedical, environmental and optoelectronic technologies.

g. Absorption Characteristics

The strong optical absorption of carbon quantum dots (CQDs) in both ultraviolet (UV) and visible regions of the electromagnetic spectrum makes them a key factor for their versatile applications in optoelectronics, sensing and energy conversion. The strong UV absorption of CQDs is mainly due to the π–π* electronic transitions of the conjugated C=C bonds in the graphitic carbon core. Furthermore, the presence of heteroatom-containing surface functional groups, such as oxygen or nitrogen, can offer lone-pair electrons that promote n–π* transitions, extending the absorption behavior to the visible region. These surface-induced transitions have strong effect on the optical properties and enhance the light harvesting ability. The broad and tunable absorption spectra of CQDs allow them to efficiently use solar radiation, making them highly suitable for photocatalysis, solar energy conversion, photodetectors and light-harvesting systems. Furthermore, improved visible-light absorption results in faster charge formation and transfer processes, which leads to increased efficiency of catalytic and photoelectronic applications.

Surface Functionalization of Carbon Quantum Dots (CQDs)

Surface functionalization is an important factor that governs physicochemical and application-specific performance of Carbon Quantum Dots (CQDs). CQDs have a high versatility as nanomaterials because of the presence and modification of surface functional groups such as hydroxyl (–OH), carboxyl (–COOH) and amino (–NH_2) groups. These groups greatly enhance the solubility, stability and chemical reactivity of CQDs.

a. Role of Surface Functional Groups

CQDs are composed of organic precursors and thus have many surface functional groups. These groups are crucial in determining their behaviour:

Hydroxyl (–OH) and Carboxyl (–COOH) Groups Improve water solubility and dispersibility by hydrogen bonding with water molecules. Amino (–NH_2) Groups: Increase reactivity and offer sites for additional chemical modification. These functional groups also form surface energy states that affect the optical and electrical characteristics.

b. Better Solubility and Stability

Surface functionalization is very important to increase the dispersion and stability of carbon quantum dots (CQDs) in diverse solvent systems. Surface modification of CQDs with functional groups such as hydroxyl, carboxyl, amino or polymer coatings avoids the aggregation of nanoparticles by providing electrostatic repulsion and steric stability . Therefore, CQDs may remain well diffused in aqueous, organic and biological environments for a long period without significant sedimentation or clustering. Enhanced dispersion and colloidal stability guaranty repeatable optical characteristics, higher biocompatibility, and efficient interaction with target molecules or biological systems. Furthermore, stable and well-dispersed CQDs demonstrate enhanced fluorescence behavior, improved reactivity and superior transport characteristics in complicated situations. These features make surface-functionalized CQDs particularly desired for biological applications such as drug administration, bioimaging and biosensing, and for environmental applications such as pollution detection, water treatment and photocatalysis.

c. Increased Chemical Reactivity

Surface functional groups of carbon quantum dots (CQDs) are the essential active sites for a variety of chemical and biological interactions. Various functional groups such as hydroxyl, carboxyl, amino and carbonyl groups may improve the chemical reactivity of CQDs, and they may form strong binding contacts with metal ions, organic compounds, proteins, nucleic acids and other biomolecules. These interactions result in quantifiable changes in fluorescence intensity, emission wavelength or electrical characteristics upon engagement of the target and so provide excellent sensitivity and selectivity in sensing applications. Furthermore, these functional groups provide reactive surface surfaces which boost catalytic activity by promoting adsorption, electron transfer and charge separation during catalytic processes. Therefore, functionalized CQDs are widely used in biosensing, environmental monitoring, photocatalysis, drug administration, and biomedical diagnostics due to their superior surface reactivity, adjustable selectivity, and multifunctional performance.

d. Bioconjugation and Targeted Uses

One of the most important advantages of surface functionalization in CQDs is the possibility of conjugation with different types of biomolecules, resulting in enhanced biomedical and diagnostic applications. Surface functional groups such as carboxyl, amino and hydroxyl groups offer reactive sites for the attachment of proteins, enzymes, antibodies, nucleic acids and other physiologically active molecules. Conjugation with proteins and enzymes enhances the uses of CQDs in biosensing, bio-catalysis and real-time monitoring of biological events. Antibody attachment enables extremely selective and focused detection of particular

antigens, infections or disease biomarkers, enhancing the sensitivity and specificity of diagnostic systems.Similarly, functionalization with DNA or RNA allows applications in gene delivery, molecular diagnostics, and nucleic acid detection. These biomolecule-conjugated CQDs combine strong fluorescence, biocompatibility and selective targeting capability to support target-specific imaging, efficient drug delivery systems and precision diagnostics. Surface-functionalized CQDs are therefore highly promising nanomaterials for modern biomedical research, personalized medicine, and therapeutic applications.

e. Surface Passivation

Surface functionalization of carbon quantum dots (CQDs) is usually associated with surface passivation, which plays an important role in the improvement of their optical and physicochemical properties. Surface passivation is the coating or modification of the CQD surface with suitable molecules, polymers, or functional groups to minimize surface defects and trap states that normally promote non-radiative electron–hole recombination. Passivation minimizes these defect-related energy losses and results in a considerable improvement in fluorescence intensity and quantum yield of CQDs. In addition, passivated CQDs have higher photostability, chemical stability and resistance to environmental degradation, leading to better long-term performance. Surface passivation also plays a vital role for enhancing dispersibility and biocompatibility, which further extends the use of CQDs in bioimaging, sensing, photocatalysis, light-emitting devices and other advanced nanotechnology. Thus, surface passivation is an essential method to improve the efficiency and functional performance of CQDs.

f. Functionalization Methods

There are several successful ways for the surface modification of CQDs which may modify the optical, chemical and biological characteristics of CQDs for particular applications . A typical method is the in-situ functionalization, which consists in including precursors with suitable functional groups or heteroatoms during the synthesis. This technique allows simultaneous production and surface modification of CQDs, resulting to the improved stability, fluorescence and biocompatibility. Another major technique is post-synthetic modification, where the chemically generated CQDs are treated with other organic compounds, polymers or biomolecules after their synthesis to integrate new functional groups or targeting capabilities. This technique gives greater freedom to tune the surface chemistry for a given application.Moreover, doping and hybridization methods are widely used to

improve CQD performance by incorporating heteroatoms such as nitrogen, sulfur, phosphorus, or metals, or by combining CQDs with other nanomaterials, polymers, or semiconductors. These changes enhance the charge transfer, the optical absorption, the catalytic activity, the conductivity and the fluorescence behavior. These surface modification approaches in combination allow the design of highly versatile CQDs for applications in sensing, bioimaging, drug delivery, catalysis, energy storage and environmental remediation.

CQD-Based Nanocomposites

Carbon Quantum Dots (CQDs) can be efficiently incorporated into a variety of materials such as polymers, metals and semiconductors to form sophisticated nanocomposites. These hybrid systems combine the particular optical and electrical capabilities of CQDs with the structural, mechanical, and functional advantages of the host materials, resulting in an enhanced overall performance.

Types of CQD-Based Nanocomposites

a. Polymer-Based Nanocomposites

CQDs are commonly added to polymer matrices to improve the flexibility, processability, and multifunctional performance of the composite materials. The incorporation of CQDs into polymers improves the mechanical strength, toughness and durability of the resulting nanocomposites, due to the enhanced interfacial interactions and stress distribution in the polymer network. Besides mechanical reinforcement, CQDs can greatly enhance the optical properties of polymer composites by providing strong and tunable fluorescence, which is of great benefit for sensing, imaging and optoelectronic applications. The enhanced dispersibility and compatibility of CQDs in polymer systems are also beneficial to the stability and uniformity of the composite materials. Moreover, the CQD–polymer composites have demonstrated great potential for flexible electronics, smart coatings, wearable devices, light-emitting materials and biosensors due to their low weight, flexibility, conductivity and photoluminescence properties. These advantages make the CQD-based polymer nanocomposites very attractive materials for advanced technological and biomedical applications.

b. Metal-Based Nanocomposites

Hybrid nanocomposites based on carbon quantum dots (CQDs) and metal nanoparticles, such as gold, silver or platinum, are very efficient materials with extraordinary synergistic effects. The addition of metal NPs to CQDs enhances the conductivity of the composite system in

great extent by providing fast electron transport and high charge mobility. In addition, significant electron transfer interactions between CQDs and metal nanoparticles improve catalytic activity and make these nanocomposites particularly useful for photocatalysis, electrocatalysis, and energy conversion applications. Metal nanoparticles possess unique surface plasmon resonance capabilities, which may boost local electromagnetic fields and improve optical sensitivity. Such plasmonic interactions significantly improve the performance of the CQD-based sensing platforms for highly sensitive and selective detection of chemical and biological analytes. In addition, the combined optical, catalytic and electronic properties of CQD–metal nanoparticle composites make them promising materials for biosensors, imaging systems, solar cells, drug delivery and advanced optoelectronic devices.

c. Semiconductor-Based Nanocomposites

The integration of carbon quantum dots (CQDs) in a semiconductor material such as titanium dioxide (TiO2), zinc oxide (ZnO), or cadmium sulfide (CdS) leads to a significant enhancement of the optical, electronic, and photocatalytic properties of the resulting nanocomposites. CQDs are efficient electron acceptors and transport mediators and increase the charge separation and decrease the electron-hole recombination in the semiconductor system. This improved charge transfer method increases the synthesis and longevity of reactive charge carriers, which leads to the augmentation of photocatalytic efficiency for applications in pollutant degradation, hydrogen production and solar energy conversion. Besides, CQDs extend the absorption of semiconductor materials from ultraviolet region to visible region, which can expand the light absorption range and make better use of solar energy. Their excellent conductivity, fluorescence properties and surface functionalization further help to improve catalytic activity and stability. Therefore, CQD–semiconductor composites have been explored as very promising materials in photocatalysis, photovoltaic devices, environmental remediation, and optoelectronic applications.

Synthesis Strategies

Several versatile approaches are available for the synthesis of carbon quantum dot (CQD)-based nanocomposites as a function of structure, composition and application of the final material. In-situ synthesis is the direct synthesis of CQDs within a host matrix like polymers, metals, or semiconductor materials, leading to strong interface interactions, good dispersion, and enhanced stability of the composite system. In contrast, ex-situ blending is the embedding of pre-synthesized CQDs into other materials by physical mixing or by chemical interactions, which provides more flexibility to control the composition and properties of the

nanocomposite. The hydrothermal and solvothermal synthesis approaches are most frequently used for the synthesis of uniform and highly crystalline CQD-based composites due to the possibility of controlling nucleation, particle growth and strong integration of CQDs into the host material under conditions of high temperature and pressure. Moreover, electrochemical and microwave-assisted synthesis techniques provide fast, energy efficient and highly controllable fabrication processes. Uniform heating and fast reaction times are advantages of microwave-assisted synthesis, while electrochemical methods allow control of particle formation and surface properties. Together these synthetic techniques allow the production of CQD-based nanocomposites with increased optical, electrical, catalytic and mechanical capabilities for sensing, energy storage, photocatalysis, bioimaging and flexible electronics.

Improved Properties

The nanocomposites based on carbon quantum dots (CQDs) demonstrate a considerable increase in the physical, chemical, optical and functional characteristics of the materials owing to the synergic interactions between CQDs and the host matrix.These nanocomposites have improved mechanical properties such as strength, flexibility, toughness and structural stability due to the improved interfacial bonding and stress distribution by CQDs in the composite material. Incorporation of CQDs resulted in improved fluorescence intensity, photostability and tunable emission properties which are particularly helpful for imaging, sensing and optoelectronic applications.In electrical applications, CQDs improve conductivity, speed up electron transport, and boost charge mobility to enhance the performance of electronic and energy devices. Moreover, the CQD-based nanocomposites exhibit enhanced catalytic performance owing to the synergistic interactions that improve charge separation, electron transfer and increased active surface area. These improvements significantly improve the performance of photocatalytic, electrocatalytic and sensing systems. As a result, CQD nanocomposites have attracted much attention for advanced applications in flexible electronics, environmental remediation, energy storage, bioimaging, biosensing, and smart functional materials.

Applications

Composites based on carbon quantum dot (CQD) have attracted a lot of attention in a variety of advanced technological and biomedical applications owing to their enhanced optical, electrical, catalytic and biocompatible properties. CQD-based composites in photocatalysis improve light absorption and facilitate efficient charge transfer, which enhances the degradation of organic pollutants, water purification, hydrogen production, and solar energy conversion processes. Their ability to suppress the recombination of electron–hole pairs

greatly promotes the photo catalytic efficiency under visible-light irradiation. CQD hybrid materials have been extensively used in sensing applications due to the synergistic interactions between CQDs and host materials, enabling high sensitivity and selectivity for the accurate detection of metal ions, bio molecules, gases and environmental pollutants with optical or electrochemical responses. CQDs-based materials have been widely used in batteries, super capacitors, fuel cells and solar cells in the field of energy storage and conversion due to their excellent electron transport capability, high surface area, conductivity, and structural stability that improve device performance and energy efficiency. CQDs composites are also widely used in drug delivery, bioimaging, biosensing and therapeutic systems in biomedical applications owing to their low toxicity, biocompatibility, fluorescence properties and multifunctional behavior. These combined advantages make CQD-based composites very promising materials for next generation environmental, energy and healthcare technologies.

Advantages of CQD-Based Nanocomposites

Carbon quantum dot (CQD)-based nanocomposites have some important advantages including synergistic enhancement of optical, electrical, mechanical, and catalytic properties by interaction of CQDs with other materials. The design and composition versatility of these nanocomposites allows for tailored functionalities for specific applications. They also have better stability, durability and long-term performance in different environmental conditions. Due to their several functions, CQD-based nanocomposites have been extensively used in energy storage, photocatalysis, sensing, bioimaging, environmental remediation and biomedical engineering .

Future Scope and Challenges

There are still certain hurdles that restrict the large-scale and commercial uses of CQDs-based nanocomposites, while many benefits are available. The uniform dispersion of CQDs in host materials is still a difficulty, typically leading to aggregation and poor performance. Moreover, the interfacial compatibility between the CQDs and the composite matrices may influence the stability, charge transfer efficiency, and overall functioning.Another important challenge is the scale-up production for industrial applications due to the need for cost-effective, reproducible and controlled synthesis methods. Therefore, future research is directed towards the development of multifunctional nanocomposites with improved properties, controlled synthesis and surface engineering and the incorporation of CQD-based materials into sophisticated electronic, biomedical, environmental and energy-related devices for practical applications.

Biomedical Applications of Carbon Quantum Dots (CQDs)

Owing to their excellent biocompatibility, low toxicity, high fluorescence and eco-friendly synthesis routes, green synthesis routes of Carbon quantum dots (CQDs) have been widely explored in the biomedical field. Such properties make CQDs very promising candidates for applications in the fields of bioimaging, drug delivery and clinical diagnosis.

a. Bioimaging Applications

Carbon quantum dots (CQDs) are emerging as very promising nanomaterials in biomedical applications, due to their excellent fluorescence properties, low toxicity, biocompatibility and facile surface functionalization . CQDs are widely applied in bioimaging applications as fluorescent probes for imaging biological systems owing to their capability of efficiently penetrating cell membranes and generating bright and stable fluorescence that enables the detailed visualization of cellular structures and biological processes. Their excitation-dependent emission property allows for multicolor imaging at different wavelengths, which is very useful for tracking multiple biological targets simultaneously. Furthermore, the enhanced photostability of CQDs enables continuous and long-term imaging without considerable photobleaching. Due to the minimal cytotoxicity of CQDs, in vivo imaging in live species is also feasible.

CQDs also play an essential part in pharmaceutical delivery systems, where they are used as an efficient nanocarrier for targeted therapeutic delivery. Surface functional groups on CQDs may be conjugated with medications, biomolecules and targeting ligands for the targeted delivery of therapeutic agents to sick tissues with minimum negative effects on healthy cells.In addition, controlled drug release can be triggered by environmental factors such as pH, temperature or enzymatic activity. CQDs are also useful in theranostic applications where therapeutic delivery and diagnostic imaging functions are integrated into one nanoplatform.

CQDs exhibit highly sensitive fluorescence responses for rapid and accurate detection of biomolecules such as glucose, cholesterol, proteins, enzymes, and nucleic acids in biosensing and clinical diagnostics . CQD-based sensors are extensively investigated for early diagnosis of diseases such as cancer, bacterial infections and other pathological disorder. Functionalized CQDs can also be applied in immune sensing applications, where they are used to specifically bind to antigens or antibodies for highly selective and precise detection.

Besides the diagnostics, CQDs have high therapeutic potentials in antimicrobial and anticancer applications. CQDs show antibacterial activity by disrupting bacterial cell membranes and the generation of reactive oxygen species to repress the proliferation of

microorganisms. In cancer therapy, CQDs can also induce apoptosis in cancer cells . CQDs are also used in photodynamic and photothermal therapy . Moreover, functionalized CQDs can act as carriers for DNA and RNA delivery in gene therapy applications, thus providing the basis for advanced genetic and molecular therapies.

CQDs possess biomedical advantages such as low cytotoxicity, good biocompatibility, intense and tunable fluorescence, good water solubility, and easy surface modification for targeted purposes. In addition, green synthesis methods improve their environmental friendliness and suitability for biomedical applications. However, there are several obstacles that need to be overcome despite these promising features, such as the requirement for extensive long-term toxicity and biodistribution studies, the limited clinical translation due to regulatory and safety concerns, and the challenges in obtaining reproducible synthesis at a large scale. Future work will focus on the development of multifunctional CQDs with better targeting efficiency, better therapeutic performance and successful integration into advanced clinical and personalized medicine systems.

Sensing Applications of Carbon Quantum Dots (CQDs)

Carbon Quantum Dots (CQDs) are emerging as an efficient nanosensor due to their unique optical properties, strong fluorescence, high surface area and ease of functionalization. These properties enable CQDs to detect a wide variety of analytes with high sensitivity and selectivity, making them useful in environmental monitoring, biomedical diagnostics, and industrial analysis.

A. Mechanism of Sensing

The sensing performance of carbon quantum dots (CQDs) is mainly determined by the change of their fluorescence properties upon interaction with specific analytes. These fluorescence responses are accomplished through different mechanisms including fluorescence quenching (turn-off) where the fluorescence intensity is decreased due to electron transfer or energy transfer processes and fluorescence enhancement (turn-on) where the interaction with analyte reduces non-radiative recombination and increases the emission intensity. Besides, photoinduced electron transfer (PET) enables detection through electron exchange between CQDs and target molecules, while fluorescence resonance energy transfer (FRET) happens via energy transfer between CQDs and nearby molecules resulting in detectable fluorescence changes. These mechanisms endow CQDs with the ability to be sensitive and selective materials for sensing applications in environmental monitoring, biomedical diagnostics and chemical detection.

B. Detection of Metal Ions

The presence of reactive surface functional groups such as hydroxyl, carboxyl and amino groups make carbon quantum dots (CQDs) widely used for the detection of metal ions. These functional groups are capable of strong interactions with metal ions via coordination and electrostatic interactions, resulting in significant alteration of the fluorescence behavior of CQDs. Heavy metal ions, such as Hg^{2+} , Pb^{2+} and Fe^{3+} , can enhance or quench the CQD fluorescence greatly and can be used for highly sensitive detection at very low concentration. The sensing response is usually fast, selective and reliable because of the specific binding affinity between the target metal ions and the functional groups on the surface of CQDs. CQDs have been demonstrated to be very promising materials for environmental monitoring, water quality analysis and biomedical sensing applications.

C. Biosensing Applications

Carbon quantum dots (CQDs) are particularly ideal for biological sensing applications because of their low toxicity, great biocompatibility, intense fluorescence and simple surface functionalization. CQDs are widely employed with enzymes such as glucose oxidase for glucose sensing, where variations in fluorescence allow for precise detection of glucose.CQDs are also commonly used for nucleic acid detection because their interaction with DNA or RNA enables sensitive analysis for genetic studies, molecular diagnostics and disease detection . In protein sensing applications, the binding of proteins, enzymes or biomarkers on the surface of the CQDs leads to optical or fluorescence changes which are measurable and permit selective and rapid detection. Also, CQDs are good fluorescent probes for cell imaging, which makes it possible to visualize cellular structures, intracellular pathways and biological processes with high sensitivity and photostability. These multifunctional features make CQDs intriguing materials for biosensing, biomedical diagnostics and enhanced health care applications.

D. Environmental Monitoring

Carbon quantum dots (CQDs) are important nanoprobes for environmental pollution detection owing to their high sensitivity, adjustable fluorescence characteristics and robust surface reactivity. CQDs have been extensively employed for the detection of pesticides. Pesticide compounds interact with CQDs and induce visible changes in fluorescence via inhibition or electron transfer processes.They are also very effective for the detection of organic pollutants such as dyes, phenolic compounds and industrial contaminants, which alter the emission properties of the CQDs upon interaction. Moreover, the powerful electron acceptors can also be used to quench the fluorescence of toxic chemicals and explosive compounds, which is favorable for sensitive detection. The selectivity and low detection

limits of CQD-based sensing systems along with their fast responses make them useful for monitoring water quality, soil contamination and air pollution that benefits environmental protection and public health safety.

E. Advantages of CQDs in Sensing

CQDs have many significant advantages, which make them very promising for sensing, biomedical and environmental applications. Because of the tunable surface chemistry and fluorescence behavior, they exhibit high sensitivity and selectivity for a broad range of analytes. CQDs also possess strong and tunable fluorescence emission which allows efficient optical detection and imaging . Due to their good water solubility and stable dispersion in aqueous media, they are compatible with biological and environmental systems. Moreover, CQDs are low in toxicity and high in biocompatibility that are safe for biomedical applications such as bioimaging, drug delivery, and biosensing. Also, the synthesis of CQDs by easy, cost-effective and environmentally acceptable procedures from a range of natural and synthetic precursors favors their wide scale production and practical use.

F. CHALLENGES AND SCOPE FOR THE FUTURE

Despite the abundance of benefits of CQD-based sensors, there are still several limitations that restrict their practical and large-scale use. The main restriction is the influence from complicated sample settings. The sensing accuracy and fluorescence response might be affected by the presence of several compounds in the sample. In other circumstances, CQDs can have poor specificity to target analytes, leading to lower selectivity in complex biological or environmental samples. Furthermore, variances in synthesis techniques, precursor materials, and surface functionalization might result in discrepancies in particle size, optical characteristics, and sensing performance, influencing repeatability and uniformity. Thus, future investigations will be focused on improving selectivity and sensitivity through advanced surface engineering, the development of multifunctional and hybrid sensing platforms, and the integration of CQDs in smart, portable, and real-time sensing devices for healthcare, environmental monitoring, food safety, and industrial analysis.

Energy Applications of Carbon Quantum Dots (CQDs)

Carbon quantum dots (CQDs) have been extensively studied in the energy sector owing to their tunable bandgap, electron mobility and flexible surface chemistry . CQDs have features that allow for effective light absorption, charge separation and electron transport, thereby making them very appropriate for different energy conversion and storage technologies.

CQDs have an essential role in solar cells, as photosensitizers, electron transport materials or light collecting agents. Their wide absorption spectrum and variable photoluminescence are advantageous in solar energy collection and conversion efficiency.The charge transfer dynamics can be further improved and the recombination losses reduced by doped CQDs, which leads to better photovoltaic performance of devices such as quantum dot-sensitized and perovskite solar cells.

CQDs in supercapacitors have high surface area and excellent conductivity which improves the energy storage performance. Incorporation of CQDs into electrode materials results in enhanced charge accumulation, increased capacitance and improved cycling stability. Their capability of forming composites with graphene, polymers and metal oxides further enhances the electrochemical performance and makes them promising materials for next generation energy storage systems.

CQDs are also extensively studied for hydrogen production especially photocatalytic water splitting. Under light irradiation, CQDs stimulate the generation of electron-hole pairs to drive redox processes for producing hydrogen gas. Elemental doping improves light absorption and charge separation efficiencies, so considerably raises the hydrogen evolution rates. They are stable and ecofriendly, suitable candidates for the development of sustainable hydrogen energy technology. CQDs are also being introduced into fuel cells, batteries and electrocatalytic systems for enhanced conductivity, catalytic activity and overall device efficiency. They serve as electron mediators and conductive additives, improving the energy conversion processes and decreasing energy losses.

Environmental Applications of Carbon Quantum Dots (CQDs)

One of the best materials to tackle environmental concerns is carbon quantum dots (CQDs), particularly those produced by green techniques, due to its large surface area, adjustable surface chemistry and outstanding photoluminescence capabilities. These are also low toxic and eco-friendly that make them suited for sustainable environmental applications.

Water cleansing is one of the most essential uses of CQDs. CQDs have been shown to be effective photocatalysts for the breakdown of organic contaminants such as dyes, pesticides and pharmaceutical residues. Under light irradiation, CQDs release reactive oxygen species (ROS) including hydroxyl radicals and super oxide ions that may decompose complex contaminants into simpler and less toxic compounds. In particular, doped CQDs show higher photocatalytic efficiency owing to the greater charge separation and broadened light absorption.

CQDs are also commonly employed for detection of contaminants and environmental sensing.Their fluorescence properties enable highly sensitive and selective detection of heavy metal ions (e.g. Hg^{2+} , Pb^{2+} , Cd^{2+}), toxic chemicals and organic pollutants. Real-time monitoring of environmental contaminants is possible by changes of fluorescence intensity or wavelength upon interaction with analytes. Surface functional groups further improve their interaction with target molecules, thereby improving detection accuracy.

In waste treatment, CQDs are useful in removing and transforming toxic substances found in industrial and municipal waste streams. They can be added to filtration systems, membranes and nanocomposites to improve adsorption and catalytic degradation processes. In addition, the biomass waste-derived CQDs support the concept of waste valorization, converting low-value materials into high-performance nanomaterials.

Green-synthesized CQDs are in perfect agreement with sustainable environmental technologies, where the fabrication process minimizes the environmental impact, and at the same time it allows efficient remediation solutions. Their biodegradability, chemical stability and compatibility with aqueous systems make them ideal candidates for long-term environmental applications.

Moreover, CQDs are also investigated in air purification and greenhouse gas reduction, where they assist catalytic processes such as CO_2 reduction and pollutant oxidation . The efficiency of these materials is further enhanced and the range of their applications is extended through the use of hybrid systems of metal oxides and polymers.

Advantages of Green Doped Carbon Quantum Dots (CQDs)

Green-synthesized and element-doped carbon quantum dots (CQDs) possess the unique features of environmental sustainability and improved functional performance, which make them highly attractive for next-generation applications of nanomaterials.

A very important advantage is their low toxicity and good biocompatibility. CQDs are synthesized from natural precursors like plant extracts and biomass instead of toxic chemicals so that they are safe for biological systems. This makes them particularly useful in bioimaging, medication administration and diagnostics, among other biological uses.

Green doped CQDs are also environment friendly and sustainable. The synthesis process is in line with the green chemistry principles; it minimizes the hazardous waste, decreases the energy consumption and uses renewable resources. Furthermore, the utilization of agricultural and food waste favors waste valorization and promotion of circular economy practices.

Another major plus is how cost-effective they are. It is made from inexpensive and readily available raw materials and so production costs are low. The easy synthesis methods such as hydrothermal and microwave-assisted methods further reduce the operational costs that make the large-scale production economically feasible.

One of the major advantages is scalability, since green synthesis methods can be scaled up for bulk production using relatively simple equipment. In industrial applications we are developing continuous and optimized processes for further improving production efficiency and consistency, to provide our support.

Functionally, elemental doping along with natural functionalization significantly enhances the properties of CQDs. Doping generates novel electronic states and enhances quantum yield, conductivity and catalytic activity, while natural surface groups (–OH, –COOH, $–NH_2$) endow solubility, reactivity and facile modification. This double benefit enables precise control of CQD properties for particular applications.

Green doped CQDs also show improved optical properties such as strong and tunable photoluminescence, high photostability and excitation dependent emission behaviour. These features are important for sensing, imaging and optoelectronics applications.

Challenges and Limitations

Significant progress has been made in the development of green-synthesized, element-doped carbon quantum dots (CQDs); yet, numerous hurdles still impede their large-scale acceptance and practical deployment.

One of the major problems is reproducibility.The composition of the precursors, especially when using biomass or natural sources, is often different, resulting in inconsistencies in particle size, surface chemistry and optical properties. The batch-to-batch variability hampers the uniformity of the quality, which is important for the validation of research and industrial applications.

The other major drawback is the absence of scalable synthetic methods. Hydrothermal and microwave assisted methods are successful laboratory scale processes but scale-up to industrial production is not a straightforward process. Commercialization requires solving problems of energy efficiency, reaction uniformity and cost effectiveness.

Another important challenge is control of doping with elements. Current synthesis methods usually lead to the non-uniform distribution of dopants and vague bonding configurations that directly affect the electronic structure and performance of CQDs. Atomic level control and predictability for doping is essential in the design of materials with desired functionality.

Also, the stability is still a problem, particularly in case of long-term use. Over time, CQDs can experience photobleaching, oxidation, or aggregation, resulting in the degradation of their optical and chemical properties. Their long-term stability under different environmental conditions is important for their use in real world applications.

And the challenge of standardization makes progress in the field even harder. Currently, there are no universal consensus protocols for the synthesis, characterization and performance evaluation of CQDs. This hampers the comparability of results to other studies and the development of reliable, application-ready materials.

Recent Advances

In the last ten years, a lot of progress has been made in the development of carbon quantum dots (CQDs) in the areas of green synthesis techniques, elemental doping strategies, and advanced applications. Innovations in the processes of synthesis have led to improved control over particle size, shape and surface chemistry. Microwave-assisted and hydrothermal synthesis routes have been recently refined for the manufacturing of CQDs with high quantum yield, higher repeatability and reduced environmental effect (Wang et al., 2019; Zhang et al., 2021). More recently, hybrid and continuous-flow synthesis methodologies have been proposed (2022–2026) to increase scalability and to consistently produce CQDs.

Significant advances have also been achieved in elemental doping methods, including single-element doping, co-doping and gradient doping. These approaches allow tuning the electronic structure and surface states of the CQDs with high precision, resulting in increased photoluminescence, better charge transfer and greater catalytic activity. Recent research have demonstrated that co-doping (e.g., N,S and N,P systems) may synergistically enhance the optical and electrical characteristics, thereby widening their application possibilities in sensing, catalysis and energy systems (Zhao et al., 2020; Chemical Engineering Journal, 2025).

Another important breakthrough is the use of CQDs in nanocomposites and hybrid materials where they are integrated with polymers, metal oxides, graphene and other nanostructures. CQD based composites offer improved mechanical strength, electrical conductivity and multifunctionality. These materials have shown promising results in applications such as photocatalysis, supercapacitors, biosensors, and environmental remediation, where synergism between the components enhances the overall performance (Li et al., 2016; Journal of Cleaner Production, 2023).

One of the key growing trends is the use of artificial intelligence (AI) and machine learning (ML) in CQD research. Synthesis parameters are optimized, material characteristics are predicted, and CQDs with desired functions are designed by using data-driven methods. AI-assisted modeling shortens experimental time and expense, boosting repeatability and accuracy in material design. This combination is predicted to revolutionize the creation of next-generation CQDs, allowing rational and faster discovery (Materials Today, 2024).

Moreover, substantial advances have been achieved in the application-oriented engineering of CQDs, notably in the medicinal, environmental and energy fields. Functionalized and doped CQDs are being developed for targeted medication administration, real time biosensing, efficient degradation of contaminants and increased solar energy conversion. Furthermore, the increasing trend of sustainable and multifunctional nanomaterials has increased the relevance of CQDs in addressing global concerns in health, energy and environment.

However, there are still challenges in reproducibility, large scale production and precise doping control. However, these limitations are expected to be overcome with continuous research on green chemistry, design of advanced materials and computational tools. To sum up, recent progress suggests that CQDs are changing from nanomaterials at the laboratory scale to high-performance and application-oriented systems with high commercialization potential.

Future Perspectives

Going forward, the development of green-synthesized and element doped carbon quantum dots (CQDs) is likely to be heavily geared towards scalability, precision engineering and real-world implementation. Although promising results obtained by laboratory-scale synthesis are promising, the translation of these methods to industrial-scale production still remains a challenging task. Future research will be focused on the development of scalable, cost-effective and continuous synthesis systems incorporating flow reactors and automated microwave platforms to provide consistent quality and high production yield while ensuring environmental sustainability.

One major area of progress is the fine control on elemental doping. However, the current green synthesis approaches often lead to heterogeneous doping distributions and limited reproducibility. Therefore, developing controlled doping strategies including precursor engineering, template-assisted synthesis and in situ doping regulation will be essential to fine-tune the electronic structure and optimize functional performance. The exact role of

dopants at the atomic level will further allow a rational design of CQDs with targeted properties.

In addition, advanced characterization techniques will be essential for understanding the complex structure-property relationships of CQDs. More insights on surface states, defect structures and photoluminescence mechanisms are expected from high-resolution tools like transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy and ultrafast spectroscopy. These insights will help to close the gap between synthesis conditions and material performance.

Another promising area is the combination of computational modelling and artificial intelligence (AI). Machine learning algorithms can predict optimum synthesis parameters, precursor combinations and doping configurations, speeding up material discovery and reducing experimental effort. Data driven approaches will improve the reproducibility and allow the design of CQDs with specific functionalities for targeted applications.

From the application point of view, the future works should focus more on commercialization and device integration. This includes the integration of CQDs into functional systems, such as biosensors, optoelectronic devices, solar cells, and water purification systems. Challenges of long-term stability, toxicity assessment, and regulatory compliance will be critical for successful industrial adoption.

Also the concept of circular economy and waste valorisation will continue to drive innovation in this sector. The use of various biomass and industrial waste streams as precursors not only reduces the environmental burden but also adds economic value to the waste materials.

Conclusion

Green synthesis of element-doped carbon quantum dots (CQDs) is an emerging transforming approach in the field of sustainable nanotechnology offering an effective balance between environmental responsibility and advanced material performance. This strategy also minimizes the use of toxic chemicals and consumption of energy by using renewable biomass precursors and green synthesis methods. Therefore, it is highly compatible with the principles of green chemistry . On the other hand, elemental doping is a powerful strategy to finely modulate the electronic structure, surface chemistry and optical behaviors of CQDs, significantly enhancing their functional properties.

Green synthesis combined with the doping techniques has resulted in the production of CQDs with increased photoluminescence, greater quantum yield, better stability and superior catalytic and sensing capabilities . These improvements have increased their use in many fields including bioimaging, medication delivery, environmental monitoring, photocatalysis

and energy conversion. The ability to modify characteristics by precursor and synthesis conditions only further strengthens their potential as tunable nanomaterials for specialized applications.

However, hurdles still need to be overcome for the commercialization of these promising breakthroughs such as large scale manufacturing, repeatability, exact control of doping configurations and long-term stability. Future effort should be dedicated to the process standardization, sophisticated characterisation methods and integration of computational tools to further improve the understanding of structure-property connections. Furthermore, the development of scalable and industry-friendly synthesis techniques would be essential to transfer the laboratory-scale breakthroughs into practical applications.

In conclusion, the green-synthesized element-doped CQDs are extremely promising next-generation nanomaterials. Their sustainable origin, adjustable features and multipurpose uses render them significant participants in future developments in nanotechnology, environmental sustainability and biomedical innovations.

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