



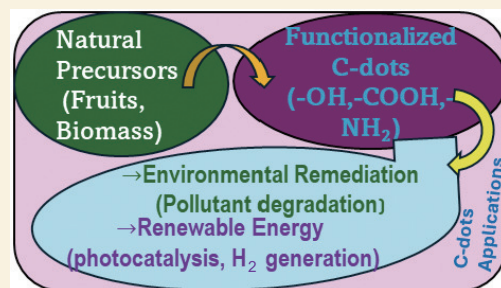
# Functionalized carbon dots from natural precursors for environmental remediation and renewable energy technologies

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**Abstract:** The green synthesis of functionalized carbon dots (C-dots) from natural precursors is reviewed, providing a sustainable and versatile platform for environmental remediation and renewable energy technologies. The focus is on methods such as hydrothermal, microwave-assisted, pyrolytic, solvent-based, and ultrasonic routes, with an emphasis on biomass-derived precursors and green solvents. Strategies are given for surface passivation, hybridization, and composite formation to tailor their optical properties and their applications in sustainable technologies are examined. In environmental remediation, they act as efficient photocatalysts for degrading organic pollutants and reducing carbon dioxide (CO<sub>2</sub>). For renewable energy, they improve light-harvesting in solar cells and dye-sensitized solar cells. Their notable stability and efficiency are highlighted, alongside persistent challenges in controlling their size, uniformity, and scalability of quantum yield. Future work must clarify the structure-activity relationships for multifunctional compounds, facilitating commercial deployment.

**Key words:** Carbon dots; Renewable energy; Energy conversion; Natural resource



## 1 Introduction

Global environmental crises<sup>[1]</sup>, including polluting, green house gas accumulation, and the pressing need for clean energy<sup>[2]</sup>, have catalyzed the search for sustainable and high-performance nanomaterials<sup>[3]</sup>. In this context, carbon dots (C-dots) have risen as a prime candidate<sup>[4]</sup>, distinguished by their excellent photoluminescence, high aqueous solubility, tunable electronic properties, and facility surface functionalization<sup>[5]</sup>. The synthesis of C-dots from biomass such as agricultural waste<sup>[6–7]</sup>, lignocellulosic residues, and other natural precursors embodies green chemistry principles<sup>[8]</sup>, transforming abundant, low-value resources into functional nanostructures with a minimal environmental footprint<sup>[9–10]</sup>. This approach not only addresses waste valorization but also offers a sustainable pathway for nanomaterial production, as highly lighted in recent reviews on circular economy-driven synthesis<sup>[11]</sup>.

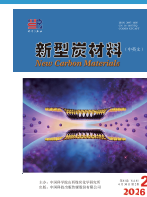
Functionalization of biomass-derived C-dots<sup>[12–13]</sup> opens a gateway to modify their characteristics and develop target-specific applications<sup>[6,14–15]</sup>, which is

important. This contribution highlights the latest developments in green synthesis and modification of C-dots with a particular focus on their environmental applications regarding the mechanism of action and efficiency for environmental cleaning by means of photocatalytic dye degradation<sup>[16]</sup> and heavy-metal sensing<sup>[17–18]</sup>. Furthermore, it delves into their burgeoning potential in the renewable energy sector, in including applications in hydrogen evolution reaction (HER), CO<sub>2</sub> reduction<sup>[19]</sup>, and as components in supercapacitors and dye-sensitized solar cells (DSSCs)<sup>[20–21]</sup>. By critically assessing current synthesis bottlenecks, performance limitations, and scalability challenges, this work aims to provide a forward-looking perspective on bridging laboratory-scale innovation with industrial-scale application<sup>[19,21–22]</sup>.

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## 2 Green synthesis of biomass-derived carbon dots: experimental and theoretical advances

Biomass-derived carbon dots (B-CDs, also called carbon quantum dots, CQDs) are now a mature and fast-growing subfield of luminescent nanocarbon research<sup>[23]</sup>. Over the last 3 years the literature has moved from demonstrations of proof-of concept syntheses (fruit peels, agro-waste) to systematic studies of process, structure and property that connect stock feed chemistry, green processing (hydrothermal microwave, pyrolysis, ultrasonic and solvent-based) and purposeful heteroatom functionalization with optical performance, photocatalytic activity and device integration<sup>[2]</sup>.

### 2.1 Plant-based sources

#### 2.1.1 Experimental outputs: fruits, peels and leaves

Plant juices, fruit pericarps and peel powders are converted to water-dispersible CDs commonly by (1) hydrothermal/solvothermal carbonization (sealed autoclave, 140–220 °C, 2–12 h), (2) microwave-assisted one-pot carbonization (minutes to tens of minutes at 600–1200 W), and (3) simple pyrolysis followed by acid/water extraction and dialysis<sup>[24–25]</sup>. Hydrothermal and microwave methods dominate because they are solvent efficient, low energy and easily scalable. These protocols produce quasi-spherical nan-

oparticles (1–10 nm) with abundant oxygen and nitrogen-containing surface groups<sup>[26]</sup>. Black mulberry (*Morus nigra*) recent literature reports that the hydrothermal synthesis from black mulberry extract (fruit juice) at ~ 180–200 °C for 6–8 h; resulting C-dots show blue/green emission, good aqueous stabilization and measurable photocatalytic activity for dye degradation under visible light<sup>[27]</sup>. Reported studies emphasize surface rich functional groups (–OH, –COOH, C=O) as active centers for photogenerated charge separation<sup>[28]</sup>. Orange peel/orange pomace. Microwave or hydrothermal treatment of orange peel produces CQDs with reported fluorescence quantum yields (QYs) ranging from ~ 10% to over 50%, depending on the solvent, passivation, and removal of larger graphitic fragments. For example, an orange-pomace CQD study reported a QY ≈ 54.3% and excellent photostability when purified and surface-passivated; other orange peel syntheses report QYs in the 10%–30% range using simpler treatments. Applications demonstrated include metal-ion sensing, bioimaging and food-safety sensing (Fig. 1)<sup>[29]</sup>.

Natural precursors of C-dots offer sustainable, cost-effective, and eco-friendly alternatives to synthetic chemicals. Here we discuss major synthesis methods with detailed comparisons.

In Table 1, it is clear that hydrothermal methods are the most common for achieving balanced proper-

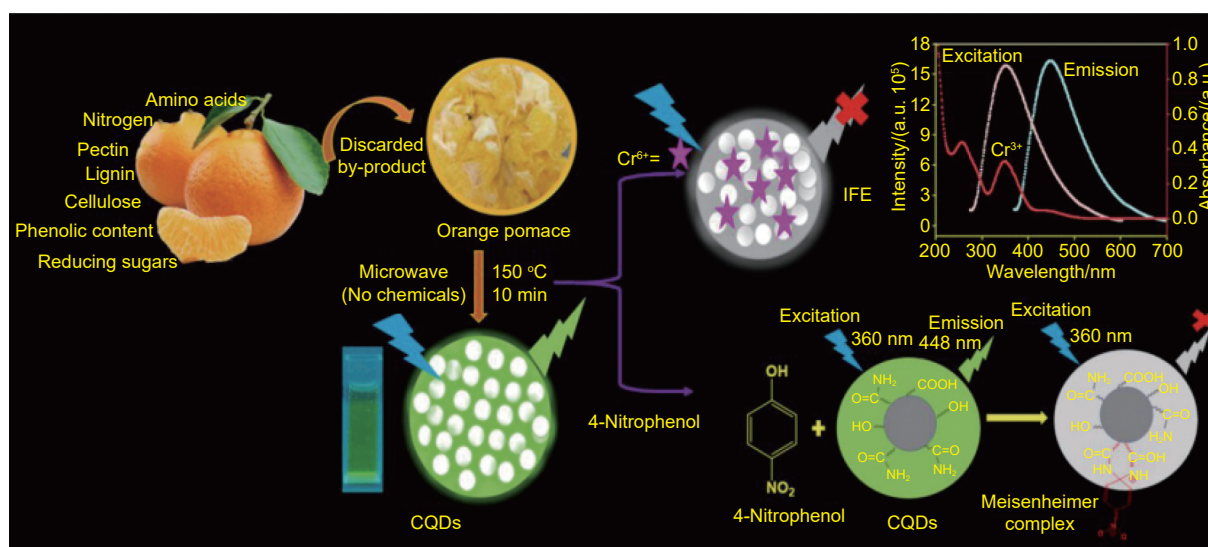


Fig. 1 Orange peel extracted<sup>[29]</sup>. Copyright 2023, American Chemical Society

**Table 1 Bioderived precursor synthesis of carbon dots**

Hydrothermal synthesis from natural precursors								
Precursor	Temperature/°C	Time/h	Size/nm	Shape	Surface area/(m <sup>2</sup> /g)	Yield/%	Application	Ref.
Orange juice	180	12	2–6	Spherical	~ 45	18–22	Fe <sup>3+</sup> sensing, bioimaging	[30]
Banana peel	200	5	3–8	Quasi-spherical	~ 52	15–20	Antibacterial, photocatalysis	[31]
Egg shell membrane	200	10	2–5	Spherical	~ 60	12–15	Cr(VI) detection, cell imaging	[32]
Aloe vera	180	8	3–7	Spherical	~ 48	20–25	Drug delivery, bioimaging	[33]
Coffee grounds	220	6	4–9	Spherical	~ 55	10–14	LED fabrication, sensing	[34]
Microwave synthesis from natural precursors								
Garlic	160	10	2–5	Spherical	~ 40	25–30	Antioxidant, bioimaging	[35]
Honey	140	20	2–4	Spherical	~ 38	30–35	Biocompatible imaging probes	[36]
Sugarcane juice	170	12	2–5	Spherical	~ 41	22–28	Anticancer drug carrier	[37]
Carrot juice	180	8	3–7	Quasi-spherical	~ 45	20–25	Metal ion sensing	[38]
Pyrolysis from natural precursors								
Soybean	300	2	4–10	Irregular	~ 65	35–40	Bioimaging, sensor	[39]
Grass	350	1.5	5–12	Spherical	~ 70	30–35	Photocatalysis	[40]
Egg	280	2.5	4–9	Spherical	~ 62	28–33	Fluorescent ink, sensor	[41]
Solvent-based synthesis from natural precursors								
Cinnamon	Water/Ethanol	120	6	2–6	Spherical	15–20	Antioxidant, anti-inflammatory	[42]
Tulsi leaves	Water	100	8	3–7	Quasi-spherical	12–18	Anticancer, bioimaging	[37]
Potato peels	Ethanol	110	5	4–9	Spherical	10–15	Heavy metal detection	[43]
Turmeric	Ethanol	90	10	2–5	Spherical	18–22	Cellular imaging, drug delivery	[44]
Ultrasonic synthesis from natural precursors								
Lemon peel	30	45	2–5	Spherical	8–12	pH sensing, bioimaging	Lemon peel	[45]
Papaya	40	60	3–6	Spherical	10–15	Antioxidant, metal ion sensing	Papaya	[46]
Tea leaves	50	30	3–7	Quasi-spherical	12–16	Fe <sup>3+</sup> detection	Tea leaves	[47]

ties. Microwave synthesis offers speed, whereas pyrolysis yields large yield. Solvent-based methods typically allow for greater control over chemical tuning. Ultrasonic methods are energy-efficient.

As revealed in Table 2, solvent usage is strongly protocol dependent. Hydrothermal syntheses are typically aqueous but use large water dilutions. Microwave methods are often run at higher concentration, and for shorter times, so the effective L per kg final product tends to be lower. (See Crista 2020 LCA and supporting tables for per-kg inventory)<sup>[48]</sup>. The ranges above combine direct experimental energy measurements and published LCA conclusions.

Where authors gave per-kg LCA inputs (e.g., inputs for producing 1 kg of CDs), those were used to derive per-kg energy/solvent estimates; where only small-batch energy was reported I scaled to kg using the reported yields. See the cited LCA / experimental papers for protocol-level details and the supplementary inventory (e.g., inputs for 1 kg production in Crista et al. 2020)<sup>[48]</sup>.

This comparative Table 2 quantitatively substantiates that microwave-assisted synthesis is a significantly more environmentally efficient green synthesis route for carbon dots (C-dots) than the hydrothermal method across all measured metrics. The microwave

**Table 2 Comparison table: hydrothermal vs microwave-assisted method**

Method	Measured energy consumption/(kWh·kg <sup>-1</sup> , CDs)	Solvent usage (typical, L·kg <sup>-1</sup> , CDs)	Estimated carbon footprint (kg CO <sub>2</sub> -eq · kg <sup>-1</sup> CDs)
Hydrothermal	Reported / reviewed values: ~ 10 – 35 kWh/kg (literature reports up to ~ 35 kWh per 1 kg CDs for some protocols; values vary widely because of low yields and long heating times) <sup>[49]</sup>	Mostly water (but large dilution): tens → hundreds of L per kg (depends on precursor concentration; hydrothermal studies commonly use mL per g precursor — scales to large L per kg of final product) <sup>[50]</sup>	~ 8.6 – 30.3 kg CO <sub>2</sub> e/kg using SA grid factor 0.8665 kg CO <sub>2</sub> e/kWh (0.8665 × 10 → 0.8665 × 35). (Replace factor for other) <sup>[51]</sup>
Microwave assisted	Reported / measured values: reported single studies ~ 1–5 kWh/kg (example: 4.33 kWh/kg reported for a microwave N-doped CD study; LCAs and comparative studies consistently show microwave to be much lower energy per kg than hydrothermal) <sup>[52]</sup>	Usually water or small solvent amounts; overall much lower solvent volumes per kg than hydrothermal because of small reaction volumes and short times (typical lab reports use mL scale but higher yield reduces per-kg solvent) <sup>[48]</sup>	~ 0.9 – 4.0 kg CO <sub>2</sub> e/kg using SA grid factor 0.8665 kgCO <sub>2</sub> e/kWh (0.8665 × 1 → 0.8665 × 4.33) <sup>[53]</sup>

process consumes an order of magnitude less energy (1–5 vs. 10–35 kWh kg<sup>-1</sup> of C-dots), directly resulting in a proportionally lower carbon footprint (0.9–4.0 vs. 8.6–30.3 kg CO<sub>2</sub>-equivalent per kg). Furthermore, due to higher reaction efficiency and yields, microwave synthesis requires substantially less solvent per kilogram of final product, minimizing water usage and waste. Therefore, while both methods utilize green precursors, the microwave route's drastic reduction in process time and energy intensity provides a far superior environmental profile, validating stronger sustainability claims.

### 2.1.2 Theoretical/mechanistic outputs

The generally accepted multi-step formation mechanism for plant-derived CDs is (1) dehydration and polymerization of soluble biomolecules (sugars, pectins and amino acids), (2) nucleation of conjugated aromatic clusters by aromatization/carbonization, and (3) surface functionalization/passivation by residual bio-molecules or added dopants. The relative abundance of carbohydrates, polyphenols and proteins in the precursor controls the chemical pathways and the degree of graphitization. Recent experimental-theoretical studies provide kinetic/engineering in-

sights into how hemicellulose/cellulose fractions versus polyphenols steer nucleus formation and surface chemistry<sup>[54]</sup>.

As shown in Fig. 2, the schematic illustrates the green conversion of rice husk waste into carbon dots (CDs) by optimised hydrothermal synthesis<sup>[55]</sup>. Rice husk, produced in massive quantities worldwide (157.5 million tons in 2021), is rich in cellulose, hemicellulose, lignin, extractives, proteins, and ashes, all of which serve as carbon sources. During hydrothermal treatment (149–220 °C, solid load 2.93–17.07 m/v), these biopolymers undergo dehydration, polymerization, and aromatization reactions to generate small conjugated carbonaceous nuclei, which subsequently evolve into nanoscale carbon dots<sup>[56–57]</sup>. The process converts the molecular building blocks such as glucose units from cellulose, xylose/arabinose from hemicellulose, phenylpropanoids from lignin, amino acids from proteins, and various extractives into fluorescent sp<sup>2</sup>/sp<sup>3</sup>-hybridized carbon structures with surface functional groups that provide water solubility and tunable photoluminescence. The resulting CDs exhibit strong blue emission under UV light and can be tailored by adjusting synthesis parameters, making

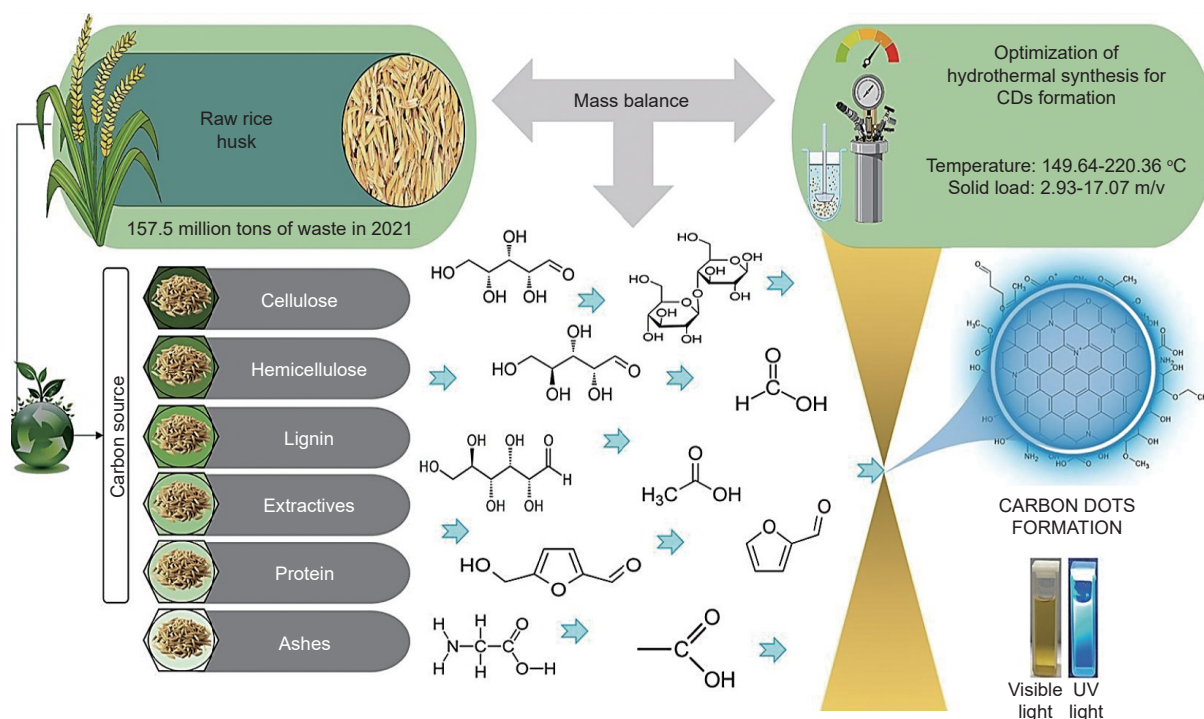


Fig. 2 Mechanism for plant-derived CDs<sup>[54]</sup>. Copyright 2025, Elsevier

this approach an environmentally friendly valorization route for agricultural waste<sup>[57]</sup>.

## 2.2 Synthesis methods

Since their discovery, the methods for producing carbon quantum dots (CQDs) have evolved into convenient, low-cost and scalable processes (Fig. 3). These synthesis strategies fall into two main categories: top-down and bottom-up. Despite the relative ease of production, challenges remain in preventing nano-material aggregation, controlling size and uniformity, and fine-tuning surface properties. To enhance performance, post-treatment methods can modify surface functional groups. For instance, surface passivation boosts quantum yields by removing emissive traps, while doping with heteroatoms (N, P) or metals (Au, Mg) improves solubility and conductivity. Although both synthetic approaches are used, the bottom-up method is generally favored for its cost-effectiveness and environmental benefits<sup>[58]</sup>.

### 2.2.1 Hydrothermal/solvothermal carbonization: controlled, tunable, widely used

Mix a carbonaceous precursor (sugars, fruit peels, proteins, citric acid, lignin, etc.) in a solvent (water is most common), seal in an autoclave and heat at elevated temperature and autogenous pressure. Un-

der those conditions the precursor molecules dehydrate, polymerize and aromatize. Nucleation and carbonization produce nano-sized  $sp^2/sp^3$  carbon cores while the solvent and reaction chemistry leave oxygen- and nitrogen-containing surface groups ( $-COOH$ ,  $-OH$ ,  $-NH_2$ ) that dominate solubility and surface chemistry<sup>[60-61]</sup>. Typical condition ranges & tunable knobs: 120–240 °C (many reports use 160–220 °C), reaction times from tens of minutes up to 12–48 h; precursor concentration, pH (strong effect on surface groups and emission), solvent (water vs alcohols), and added dopants (urea, ammonia, thiourea) strongly change size, surface functionality and quantum yield<sup>[61]</sup>. Higher temp/longer time  $\rightarrow$  more carbonization (smaller, more graphitic cores) and often bathochromic shifts; pH controls protonation/deprotonation of surface moieties and hence PL and surface charge<sup>[62-63]</sup>.

This method is green (water solvent possible), easy to implement, good control over surface chemistry (important for adsorption/photocatalysis), and adaptable to many biomass wastes. It also scales reasonably (batch scale-up and microreactor/continuous hydrothermal reactors have been demonstrated)<sup>[64]</sup>. Relatively slow (hours), product often contains a mix-

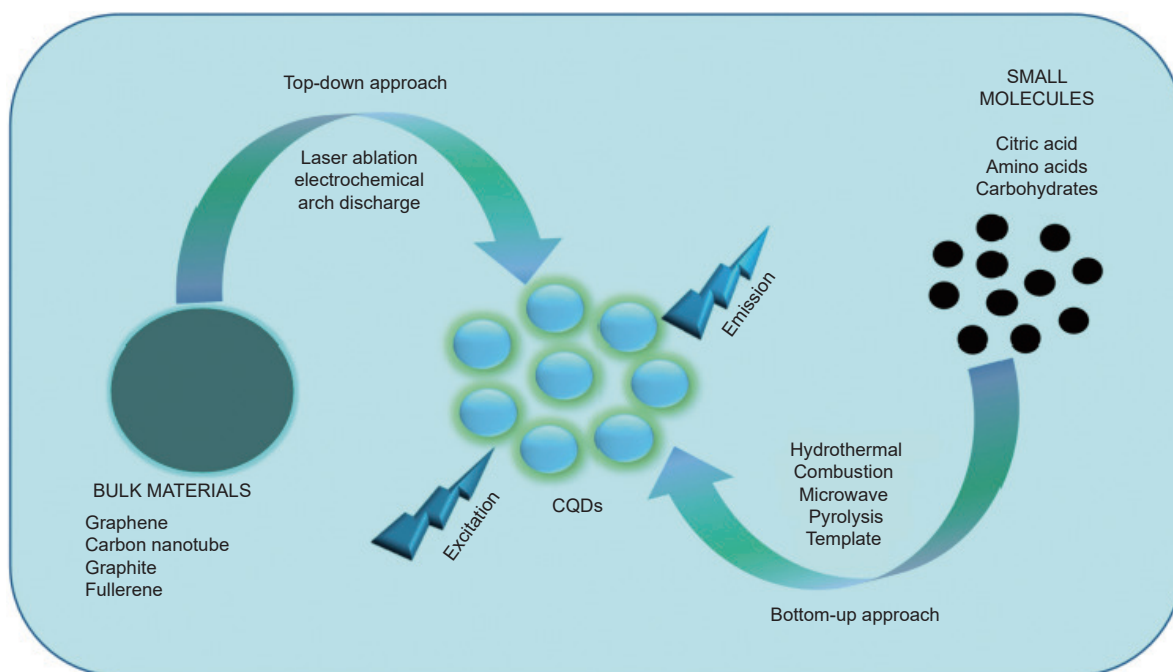


Fig. 3 The typical approaches for the synthesis of CQDs<sup>[59]</sup>. Copyright 2023, MDPI

ture of small molecules, oligomers, and true nanodots so purification (centrifugation, ultrafiltration, dialysis, column chromatography) is commonly required to isolate narrow size fractions and remove small fluorescent byproducts. Reproducibility between labs can be an issue unless conditions and precursor composition are tightly controlled<sup>[65]</sup>. Applications where well-defined surface groups matter, e.g., photocatalyst modifiers, pollutant adsorption/photodegradation (surface carboxyls and hydroxyls help binding and charge transfer), biosensing and biological applications where water-compatibility and gentle processing are needed<sup>[66]</sup>.

### 2.2.2 Microwave-assisted synthesis: ultrafast, energy-efficient, great for doping

Use microwave irradiation (household or lab microwave reactors) to heat the precursor mixture volumetrically<sup>[67]</sup>. Microwave heating accelerates the dehydration/carbonization/polymerization steps by very fast heating rates (tens to hundreds °C/min); local “hot spots” and rapid kinetics favor quick nucleation and carbon core formation<sup>[68]</sup>. Heteroatom dopants (N, S, P, B, metals) can be introduced simply by adding small molecules (urea, thiourea, ammonium salts, metal salts) to the precursor mix<sup>[69]</sup>. Typical condition ranges & outcomes: reaction times of seconds-to-minutes (commonly 1–10 min) at modest bulk temperatures; reported quantum yields can be high when appropriate passivation/doping is used<sup>[70]</sup>. Because the process is so fast, reaction power, microwave absorption properties of the precursor, and precursor ratios are the critical knobs<sup>[71]</sup>. Advantages: extremely fast, energy-efficient, often single-step, easy doping for improved electronic/photocatalytic properties, and promising for rapid prototyping or small-scale production. Many studies report good PL and high QY using microwave routes<sup>[72–73]</sup>. Limitations & cautions: microwave chemistry is sensitive to the exact apparatus (field distribution, cavity, vessel geometry) so reproducibility and scale-up are non-trivial<sup>[74]</sup>. “Hot-spot” effects can produce broader size distributions unless carefully optimized. Safety note: some precursor/solvent combinations (closed metal vessels, flam-

mable solvents) require proper microwave reactors<sup>[75]</sup>. Best for: rapid generation of doped CDs for sensor strips, fluorescence-based pollutant detectors, or applications where fast screening of dopants/conditions is valuable<sup>[76–77]</sup>. With optimization it also yields photoactive doped CDs useful as electron-mediating additives in photocatalysis or as conductive additives in electrodes.

### 2.2.3 Pyrolysis/combustion/ thermal decomposition: solvent-free, highly scalable, but less uniform

Dry (solid-state) heating of biomass or organic precursors in air-limited or inert atmosphere (pyrolysis) to thermally decompose polymers into carbonaceous residues; at controlled temperatures organic fragments aromatize and nanoscale carbon domains form<sup>[78–79]</sup>. Combustion/combustion-assisted methods (flame, spontaneous combustion) and solvent-free thermal carbonization are also used for fast, large-scale production. Reported thermal treatments for CDs vary widely: some solvent-free thermal degradations run at ~200–300 °C, while conventional pyrolysis for more graphitic chars spans 300–1000 °C depending on desired product<sup>[80]</sup>. Advantages: simple (often no solvent), low-cost, easily applied to large volumes of waste biomass, and can yield high mass conversion (some reports show high carbon yield at optimized calcination conditions)<sup>[81]</sup>. Pyrolytic CDs tend to have more conjugated (sp<sup>2</sup>) cores useful where conductivity and graphitic domains are needed (e.g., electrode additives, some photocatalytic supports)<sup>[2]</sup>. Limitations: broader size distributions, more structural heterogeneity, surface functional groups are less abundant (so surface activation/passivation often required), and the product contains large particulates and ash that must be removed. Purification is often more involved; control over PL color and bright QY is harder than with wet bottom-up routes without extra passivation<sup>[4]</sup>. Best for: large-scale, low-cost production where absolute nanoscale monodispersity is less critical e.g., bulk adsorbents, composite fillers, electrode materials, or when the CD is used as a conductive/photoactive additive rather than as a discrete fluorescent probe.

### 3 Optical properties of carbon dots

CDs, due to their carbon-based structure, typically absorb ultraviolet (UV) light strongly, with this absorption often extending into the visible range. Their optical profile is generally characterized by a primary absorption peak around 250 nm, resulting from the  $\pi-\pi^*$  transitions of C=C bonds, and a secondary peak between 300–400 nm caused by  $n-\pi^*$  transitions of C=O or C=N bonds (Fig. 4a). Some CDs can absorb light across a wider spectrum, even into the visible and near-infrared (vis-NIR) range. For instance, fluorine-doped CDs show specific peaks at 556 and 624 nm, which are linked to C=N bonds in specific nitrogen structures (Fig. 4b). Additional NIR

peaks have been attributed to large  $sp^2$  carbon domains connected by strong hydrogen bonds.

A defining and attractive feature of CDs observed, in early studies, is their bright, multi-color fluorescence, which is both stable and easily adjustable. This photoluminescence (PL) occurs when the dots absorb energy and then re-emit it as light. For graphene quantum dots (GQDs) and CQDs, the emission color is heavily dependent on their size due to the quantum confinement effect; larger dots emit redder light, while smaller ones emit bluer light (Fig. 4c).

Furthermore, post-synthesis modifications like surface passivation or functionalization profoundly impact their light-emitting properties. For example, Sun and colleagues used a polymer to passivate CDs,

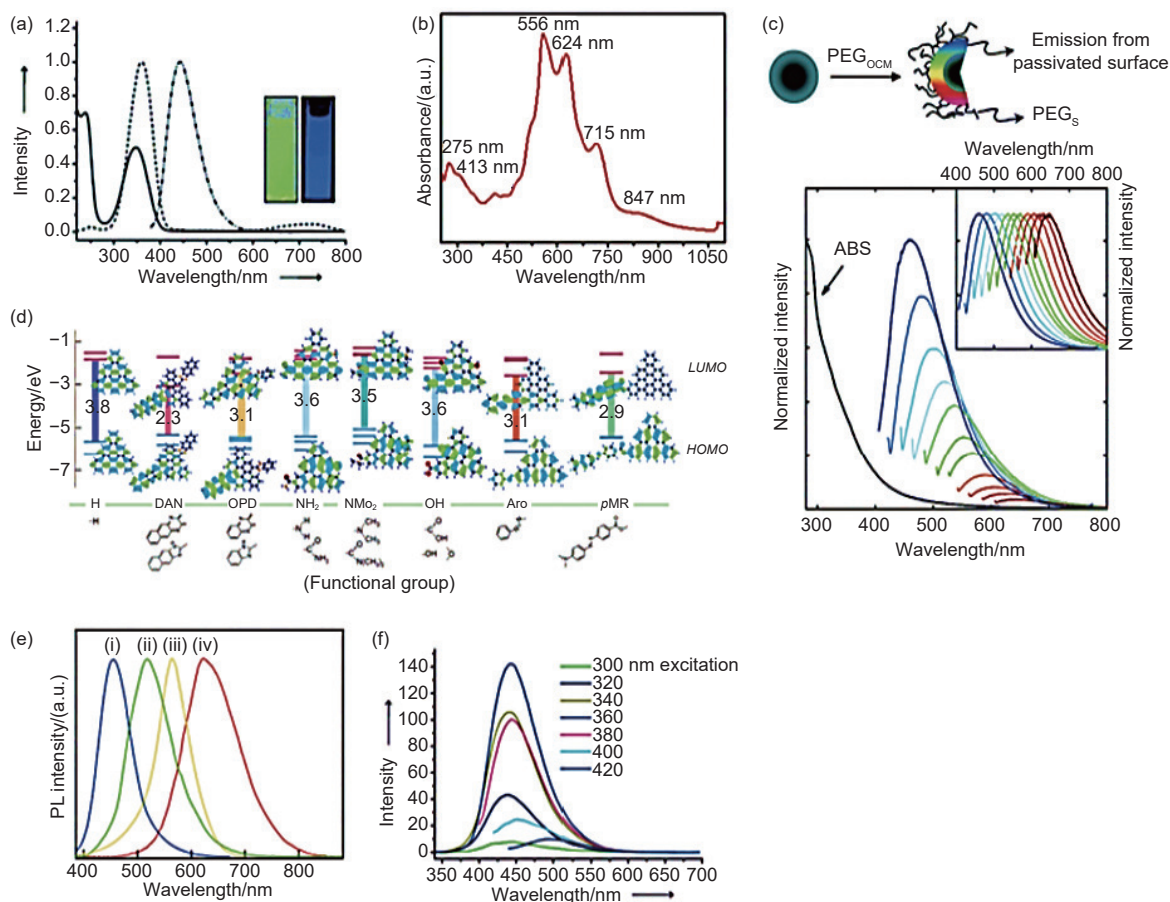


Fig. 4 (a) UV-vis absorption spectra (solid line) of CDs in aqueous solution hydrothermally synthesized from CA and EDA. Reproduced with permission<sup>[82]</sup>. Copyright 2013, Wiley-VCH. (b) UV-vis absorption spectra of F-doped CDs prepared by solvothermal method. Reproduced with permission<sup>[83]</sup>. Copyright 2020, Wiley-VCH. (c) Schematic illustration of surface passivation and PL emission spectra of PPEI-EI passivated CDs in an aqueous solution. Reproduced with permission<sup>[84]</sup>. Copyright 2006, American Chemical Society. (d) Predicted energy level diagrams for GQDs with different nitrogen functional groups. (e) Normalized PL spectra of (i) Azo-GQDs, (ii) NH<sub>2</sub>-GQDs, (iii) OPD-GQDs, and (iv) DAN-GQDs from blue to red. Reproduced with permission<sup>[85]</sup>. Copyright 2016, Wiley-VCH. (f) Excitation dependence of CDs in aqueous solution hydrothermally synthesized from CA and EDA. Reproduced with permission<sup>[85]</sup>. Copyright 2016, Wiley-VCH

resulting in intensely bright, multi-colored emissions. The researchers explained this was due to the stabilization of surface energy traps. In another case, Tetsuka's team created amino-functionalized GQDs (Fig. 4d). They found that modifying the dots with different amine compounds could raise or lower their energy levels, enabling the production of CDs that emit light across the entire visible spectrum, from blue to red. One of the most intriguing features of CDs lies in their stable, easily tunable, and multicolored fluorescence, which attracted great attention during the early stages of research. PL typically arises from radiative transitions following photon energy absorption. The emission wavelength of GQDs and CQDs is strongly size-dependent due to the quantum confinement effect (QCE), where an increase in particle size leads to a red shift in PL emission, and a decrease results in a blue shift. Furthermore, surface modifications such as passivation or functionalization have a substantial impact on the PL properties. For example, Sun et al. enhanced the bright multicolor fluorescence of CDs synthesized via laser ablation by passivating them with poly(propionylethyleneimine-co-ethyleneimine) (Fig. 4e). This enhancement was attributed to surface energy traps that became emissive after polymer stabilization. Similarly, Tetsuka et al. prepared amino-functionalized GQDs through nucleophilic substitution reactions between amine groups and oxygen-containing functional groups on the GQDs (Fig. 4d). They observed that GQDs modified with primary or dimethyl amine groups exhibited elevated energy levels due to degraded HOMO orbitals, whereas modifications with o-phenylenediamine, diaminonaphthalene, or azo groups resulted in lower energy levels, thereby yielding multicolored luminescent CDs with emissions ranging from blue to red (Fig. 4e). The PLs behavior of carbonized polymer dots (CPDs) differs somewhat from that of CQDs and GQDs. Typically, CPDs exhibit a broad full width at half maximum (FWHM) in their PL spectra, with emissions primarily in the blue or green regions, and they often display strong excitation-dependent fluorescence (Fig. 4f). This distinct behavior arises from

the complex polymer/carbon hybrid structure of CPDs, which allows the coexistence of multiple fluorescent centers within a single nanoparticle, leading to varied emission energy levels.

Table 3 summarizes the synthesis of CDs derived from various renewable feedstocks using green solvents. The quantum yield (QY) and particle size of CDs depend strongly on the nature of the precursor and synthesis route. For instance, o-phenylenediamine and wild raw neem bark yield notably high QYs of 98.5% and 36.25%, respectively, while natural precursors such as kiwifruit juice, soybeans, and citric acid produce moderate yields ranging from 2.4% to 16.7%. The particle sizes of CDs vary between 0.66 and 20 nm, reflecting the influence of carbon source composition and processing conditions. These findings highlight that biomass-derived precursors not only serve as sustainable and cost-effective carbon sources but also enable tunable control over the optical and structural properties of CDs through eco-friendly synthesis pathways.

**Table 3** Carbon dots synthesis using green solvents

Renewable feedstock	QY of CDs/%	CDs particle size/nm	Ref.
Kiwifruit juice	2.4–10.0	4.8–6.9	[86]
Urea	16.2	3.9	[87]
Soybeans	16.7	1.0–3.0	[88]
Glycine	14.0	4.0–20.0	[89]
Crab shells	14.5	8.0	[90]
Dextrose	-	3.2	[91]
o-phenylenediamine	98.5	0.7–2.7	[92]
Wild raw neem bark	36.3	2.0–10.0	[93]
Vine tea	20.4	2.7	[94]
Sophora flavescens aiton	31.6	2.8	[95]
Citric acid	2.4	3.1	[96]

## 4 Functionalization strategies of carbon dots

In a study by Chen et al. [97], a fluorescent probe for copper and sulfide ions was created. The team synthesized carbon dots (CDs-5) from citric acid and ethylenediamine (Fig. 5), followed by surface modification with cyclam a molecule known for its strong binding with  $\text{Cu}^{2+}$ . The mechanism relies on FRET:  $\text{Cu}^{2+}$  binding quenches the CDs' fluorescence, while

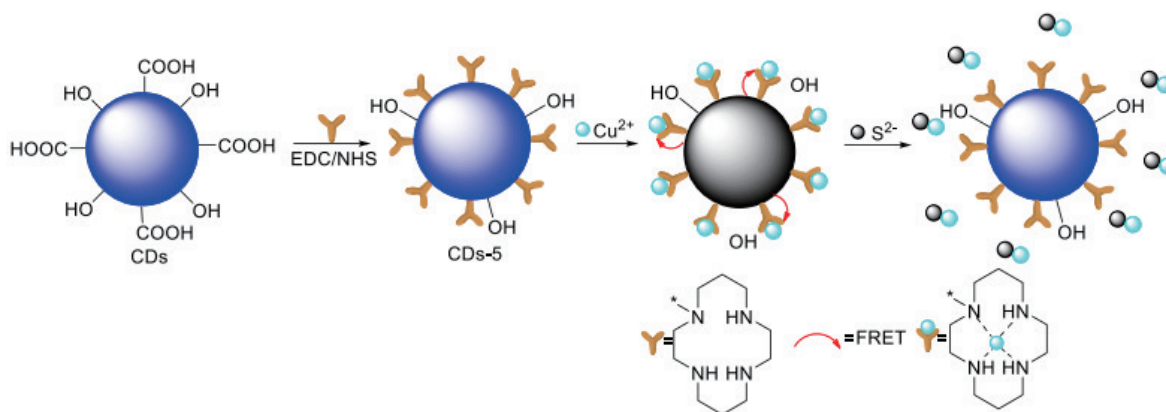


Fig. 5 The synthesis process of CDs-5 via amide coupling reaction and the detection mechanism for  $\text{Cu}^{2+}$  and  $\text{S}^{2-}$  [98].

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subsequent addition of  $\text{S}^{2-}$  displaces the copper, restoring the signal due to the higher stability of the formed CuS. This highly sensitive assay (LOD:  $0.1 \mu\text{mol L}^{-1}$  for  $\text{Cu}^{2+}$ ,  $0.13 \mu\text{mol L}^{-1}\text{M}$  for  $\text{S}^{2-}$ ) was also non-toxic and effective for monitoring these ions within biological systems, specifically HeLa cells. Fig. 5 illustrates a two-part process centered on specially functionalized CDs-5. First, the CDs are synthesized through an amide coupling reaction, which introduces specific surface groups that act as binding sites. These engineered CDs then serve as a fluorescent sensor for the sequential detection of  $\text{Cu}^{2+}$  and  $\text{S}^{2-}$ . The mechanism is based on a fluorescence “on-off-on” response: the initial fluorescence is quenched when  $\text{Cu}^{2+}$  binds to the CD surface, and the signal is subsequently restored when  $\text{S}^{2-}$  is introduced, as the sulfide ions selectively remove the bound copper due to their stronger affinity, forming CuS. This design enables a highly specific and reversible detection method for both ions.

#### 4.1 Heteroatom doping

Heteroatom doping is a cornerstone strategy in the engineering of CDs, fundamentally aimed at tailoring their intrinsic electronic structure, surface chemical properties, and ultimately, their functional performance. The incorporation of atoms with different electronegativities and atomic sizes into the carbon lattice (lattice doping) or attached to the surface (surface doping) disrupts the uniform electron density distribution of the  $\text{sp}^2$  carbon framework. This perturbation introduces defect states, modulates the bandgap,

enhances charge separation/transfer, and creates active sites, leading to significant improvements in properties such as fluorescence quantum yield, catalytic activity, and electrochemical performance.

The efficacy of doping is governed by the dopant's electronegativity ( $\chi$ ) relative to carbon ( $\chi = 2.55$ ). Nitrogen ( $\chi = 3.04$ ), being more electronegative, acts as an electron acceptor, while sulfur ( $\chi = 2.58$ ) and phosphorus ( $\chi = 2.19$ ) can act as electron donors, each creating unique local electronic environments.

#### 4.2 Nitrogen doping

Nitrogen doping (N doping) is the most prevalent and extensively studied doping method for CDs due to its comparable atomic size and the strong valence bonds it can form with carbon (C–N, C=N). The enhancement in properties is primarily attributed to the increase in electron density and the creation of new energy levels within the carbon matrix. The coexistence of N-types creates a heterogeneous electronic environment that facilitates electron-hole pair separation and narrows the bandgap, leading to a red-shift in fluorescence and enhanced photoluminescence quantum yield (PLQY). The electron-rich sites created by N-doping are highly effective for catalytic processes, particularly the oxygen reduction reaction (ORR). The lone pairs of electrons on pyridinic N can chemisorb  $\text{O}_2$  molecules and facilitate their reduction. Bandgap Engineering: The larger covalent radius of S ( $1.04 \text{ \AA}$ ) compared to C ( $0.77 \text{ \AA}$ ) induces significant structural distortion and strain in the carbon lattice

when it substitutes a carbon atom (thiophene-S). This lattice strain leads to a narrowing of the bandgap, often resulting in longer-wavelength (red) emission, which is highly desirable for biomedical applications to reduce background autofluorescence and increase tissue penetration.

**Enhanced redox activity:** Sulfur-containing functional groups like sulfoxide ( $-S=O$ ), sulfonic acid ( $-SO_3H$ ), and thiol ( $-SH$ ) on the CD surface can participate in reversible redox reactions. This makes S-doped CDs excellent for electrochemical sensing and as catalysts for oxidation reactions. The electron-donating capability of thiol/sulfide groups can also improve charge transfer.

### 4.3 Phosphorus doping

Phosphorus (P), which has a lower electronegativity, donates electrons and modifies carbon formation by creating Lewis basic sites on carbon, driven by changes in electronic energies. It introduces electron density into the carbon network by phosphonate/phosphate groups or lattice dopants (as C-P bonds) and creates electron-rich centers that function as adduct sites for Lewis acid species such as metal ions or electron-accepting gases. These features can improve the charge storage performance and ion-transport capability for supercapacitors and batteries. Phosphorus atom also creates defects promoting electrochemistry.

### 4.4 Boron doping

To achieve p-type semiconductor C-dots, boron (B) served as an electron acceptor owing to a lower electronegativity. Replacing a tetravalent carbon with a trivalent boron will form a “hole” structure in the valence band and endow B-doped C-dots as p-type materials which are necessary for p-n heterojunctions in optoelectronic devices. Boron species could be active sites for oxidants ( $H_2O_2$  or molecular oxygen) activation and B-doped C-dot acted as efficient catalyst in the oxidation reaction. Heteroatom doping is a powerful approach for the functionalization of carbon dots (with different heteroatoms providing specific electronic features), more precisely, N increases electron density, S creates strain in the lattice and red-shifted emission, P induces Lewis basicity and improves

electrochemical storage capacity, B introduces p-type character useful for optoelectronics and oxidative catalysis.

Furthermore, co-doping (e.g., N,S, N,P, B,N) has emerged as a superior strategy, where the synergistic effect between dopants can create even more pronounced modifications. For instance, N,S-co-doping can create a charge-polarized surface with N as the electron-accepting site and S as the electron-donating site, leading to unprecedented catalytic activity, as highlighted in works like Sun et al.,<sup>[99]</sup>. This level of control positions heteroatom doping as an indispensable methodology in the rational design of carbon dots for advanced technological applications.

## 5 Surface passivation of carbon dots

Boron surfactant passivation alleviates the surface defects introduced non-radiative recombination, leading to the enhanced PLQY and stability of C-dots<sup>[100]</sup>. Passivants are polymers, small molecules, and inorganic shells. Polymer films, such as polyacrylamide, increase emission by reducing vibrational energy loss. Low-molecular-weight passivating molecules, such as polyethyleneimine (PEI), endow optoelectronic controllability. Silica acts as shield for the core C-dots against quenchers, which leads to higher photostability and chemical stability. Advanced surface passivation of C-dots can open up its complete photophysics.

### 5.1 Hybridization and composite formation

CDs are ultrasmall, surface-functionalized carbon nanoparticles whose optical/electronic properties (strong, tunable photoluminescence, surface states, and facile surface chemistry) make them excellent photosensitizers, charge-transfer mediators, and surface-active co-catalysts when coupled to wide-bandgap semiconductors. Hybrid CD/semiconductor composites ( $TiO_2$ , ZnO, g- $C_3N_4$ ) typically show extended visible-light absorption, suppressed electron-hole recombination, and enhanced surface redox chemistry (higher ROS formation or  $H_2$  evolution), provided the energy-level alignment and interfacial contact are optimized<sup>[101]</sup>.

Fig. 6a(i) illustrates the dual functionality of CD/TiO<sub>2</sub> nanocomposites under solar light. In processes like water splitting and pollutant degradation, sunlight excites TiO<sub>2</sub>, generating electrons and holes. The electrons reduce water to produce hydrogen gas (H<sub>2</sub>), while the holes oxidize and break down pollutants into harmless CO<sub>2</sub> and water. The incorporated CDs play a crucial role by extending the composite's light absorption into the visible spectrum and acting as electron conduits, which enhances the overall efficiency. Fig. 6a(ii) illustrates an advanced application in organic synthesis. Here, the light-driven electron transfer between the CDs and TiO<sub>2</sub> is harnessed to activate a nickel-based catalyst. This activation enables cross-coupling reactions, where aryl halides (Ar–X) bond with various nucleophiles (Nu–H) to form new carbon-carbon (C–C) or carbon-heteroatom (C–X) bonds, yielding valuable coupled products (Ar–Nu).

Fig. 6b details the mechanism by which CQDs-modified ZnO degrades Rhodamine B (RhB) dye. Upon light exposure, ZnO absorbs energy, exciting electrons to its conduction band and leaving holes in its valence band. The CQDs, bonded to ZnO, act as efficient electron acceptors. This rapid electron transfer to the CQDs prevents the charges from recombining. The separated charges then drive the formation of reactive oxygen species: the electrons on the CQDs convert oxygen (O<sub>2</sub>) into superoxide radicals ( $\cdot\text{O}_2^-$ ), while the holes in ZnO oxidize water to generate hydroxyl radicals ( $\cdot\text{OH}$ ). These powerful radicals collaboratively attack and mineralize the RhB dye molecules. The CQDs thus boost performance by improving visible-light capture and sustaining charge separation.

Fig. 6c shows the wide application of a combination between g-C<sub>3</sub>N<sub>4</sub> and CDs using composite. The synergy effects from g-C<sub>3</sub>N<sub>4</sub> and CDs bring relatively unique light-adsorption, more effective charge separation, and greater surface activity. Overall, these data collectively demonstrate that the combination of the carbon dots with semiconductor photocatalysts (TiO<sub>2</sub>, ZnO, g-C<sub>3</sub>N<sub>4</sub>) leads to versatile composites with enhanced efficiency and potential extensive applications

in not only environmental remediation but also solar fuel production and organic synthesis.

In CD/TiO<sub>2</sub> composites, the wide bandgap of TiO<sub>2</sub> (3.2 eV), suffers from photocorrosion and electron hole recombination<sup>[105]</sup>. The addition of CDs sensitizes ZnO to visible light and protects it from photocorrosion by rapidly extracting photogenerated electrons and passivating the surface. Heteroatom-doped CDs (such as N- or S-doped) can also modulate the electronic structure of ZnO, inducing midgap states that broaden absorption and improve redox activity. Consequently, CDs/ZnO systems often exhibit superior degradation efficiency for organic pollutants and higher photocurrent density compared to pristine ZnO. CD/g-C<sub>3</sub>N<sub>4</sub> composites are notable for their metal-free composition, narrow bandgap (~ 2.7 eV), and layered structure, making g-C<sub>3</sub>N<sub>4</sub> an attractive photocatalyst for solar energy conversion<sup>[106–107]</sup>. However, pristine g-C<sub>3</sub>N<sub>4</sub> suffers from low quantum efficiency and rapid carrier recombination. When hybridized with CDs, visible-light absorption increases, and overall charge separation efficiency improves. CDs can function as electron mediators in a direct Z-scheme system or participate in a Type-II heterojunction mechanism, depending on their energy-level alignment. Reports indicate that the photocatalytic activity of g-C<sub>3</sub>N<sub>4</sub> can increase by more than tenfold with optimal incorporation of CDs, especially for hydrogen evolution and pollutant degradation. The formation of CD/semiconductor composites is a promising approach for efficient and stable environmental remediation and energy conversion applications. Key factors influencing photocatalytic performance include interfacial contact between CDs and semiconductor particles, optimal loading content, and controlled synthesis routes (hydrothermal, solvothermal, or in-situ growth). Although significant progress has been made, challenges remain in standardizing synthesis protocols, understanding charge-transfer pathways (Type-II vs. Z-scheme), and ensuring long-term stability for practical applications. Future research should incorporate time-resolved spectroscopy,

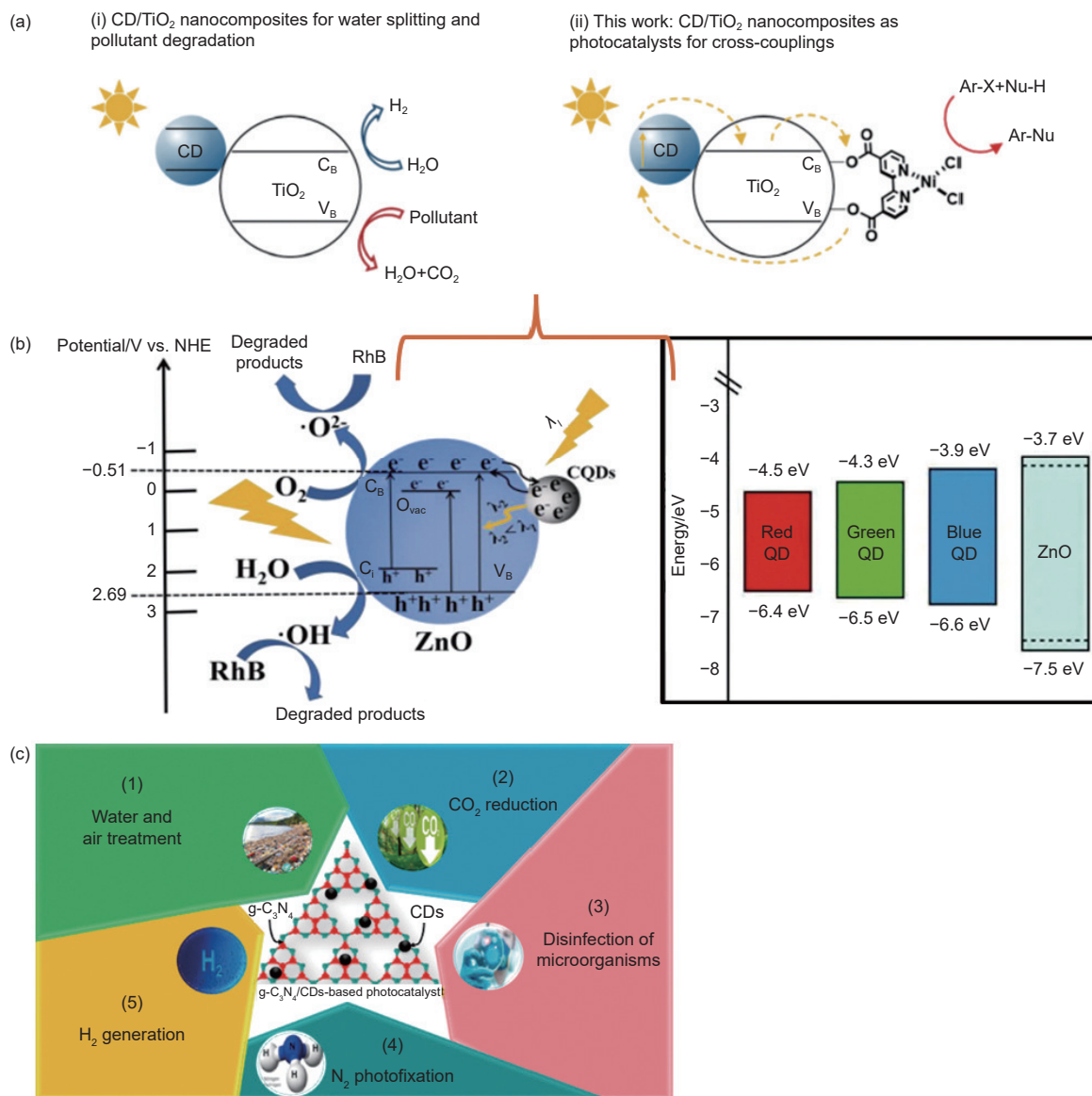


Fig. 6 (a) Schematic representation of CD/TiO<sub>2</sub> nanocomposites as (i) photocatalysts for water splitting, pollutant degradation and (ii) metallaphoto-catalytic carbon heteroatom cross-couplings<sup>[102]</sup>. Copyright 2021, Royal Chemistry Society. (b) Possible photodegradation mechanism of RhB over the CQDs/ZnO composite<sup>[103]</sup>. Copyright 2023, American Chemical Society. (c) Schematic representation of the multifunctional applications of g-C<sub>3</sub>N<sub>4</sub>/carbon dot (CDs)-based photocatalysts, including (1) water and air treatment, (2) CO<sub>2</sub> reduction, (3) disinfection of microorganisms, (4) N<sub>2</sub> photofixation, and (5) H<sub>2</sub> generation<sup>[104]</sup>. Copyright 2020, Elsevier

energy-level mapping, and life-cycle analysis to establish robust design principles for next-generation carbon-based hybrids<sup>[108]</sup>.

## 6 Environmental remediation applications

Environmental pollution, particularly of water systems, is a critical global challenge due to the annual discharge of billions of tons of industrial and domestic waste<sup>[109]</sup>. CDs have recently emerged as

highly promising nanomaterials for this purpose due to their superior properties, including broad-spectrum light absorption, upconversion luminescence, and excellent electron transfer capabilities<sup>[110]</sup>. Their straightforward synthesis, low energy requirements, and compatibility with solar energy make CDs a viable and attractive solution for environmental cleanup. This chapter details the fundamentals of CDs, their synthesis, the mechanisms of CDs-based photocatalysis, and their applications in environmental remediation<sup>[111]</sup>.

CDs are metal-free, renewable photocatalysts used for decontaminating organic pollutants in wastewater. They provide tunable light absorption and good stability in water. CDs directly absorb photons and promote electrons to higher energy levels, generating charge pairs when illuminated by visible light. Their carbon-altered core can promote charge separation, preventing recombination. This results in a highly efficient production of oxidants such as hydroxyl and superoxide radicals which degrade contaminants<sup>[112]</sup>. Electrons drive dissolved oxygen reduction to superoxide radicals ( $\bullet\text{O}_2^-$ ), and holes either oxidize water or hydroxyl groups giving origin to hydroxyl radicals ( $\bullet\text{OH}$ ). Oxygen radicals, such as superoxide, may be converted into hydrogen peroxide and further  $\bullet\text{OH}$  radicals thereby achieving a synergistic action to degrade the pollutants to innocuous chemicals such as  $\text{CO}_2$  and  $\text{H}_2\text{O}$ <sup>[113]</sup>.

The attack by  $\bullet\text{OH}$  and  $\bullet\text{O}_2^-$  radicals targets the chromophoric center of the MB molecule, breaking the conjugated system responsible for its color and cleaving the heterocyclic rings. Similarly, rhodamine B (RhB), a xanthene dye, is degraded through N-deethylation, chromophore destruction, and ring-opening, all mediated by ROS generated from photoexcited CDs. Beyond dyes, CDs are effective against persistent and toxic pollutants like phenol. The degradation of phenol involves hydroxylation of the aromatic ring by  $\bullet\text{OH}$  radicals, forming catechol, hydroquinone, and benzoquinone as intermediates, which are further oxidized and cleaved into aliphatic carboxylic acids before final mineralization to carbon dioxide and water<sup>[114]</sup>. The versatility of CDs in degrading a wide spectrum of pollutants underscores their potential as a robust, eco-friendly, and effective photocatalyst for advanced oxidation processes in environmental cleanup.

Fig. 7a shows the CDs/MIL-88B(Fe)/ $\text{Bi}_2\text{S}_3$  heterojunction photocatalyst. The diagram uses an energy level diagram (with potentials in eV versus the normal hydrogen electrode, NHE) to show how the combination of three materials CDs, a metal-organic framework (MIL-88B(Fe)), and bismuth sulfide

( $\text{Bi}_2\text{S}_3$ ) creates a system for efficient charge separation upon light absorption. Photogenerated electrons ( $e^-$ ) in the  $\text{Bi}_2\text{S}_3$  semiconductor are excited from the valence band ( $V_B$ , +0.91 eV) to the conduction band ( $C_B$ , -0.29 eV). These electrons then transfer to the CDs, which have a lowest unoccupied molecular orbital (LUMO) level at -0.2 eV, a suitable potential for reducing oxygen to generate reactive superoxide radicals. Simultaneously, the photogenerated holes ( $h^+$ ) left in the  $V_B$  of  $\text{Bi}_2\text{S}_3$  transfer to the highest occupied molecular orbital (HOMO) of MIL-88B(Fe) at +2.13 eV, which has a sufficiently positive potential to directly oxidize water or pollutants, with the pathway for generating hydroxyl radicals ( $\bullet\text{OH}$ ) also indicated. The proposed photocatalytic mechanism for hydrogen production (Fig. 7b) using the CdSQDs/ $\text{Bi}_2\text{S}_3$  nanocomposite and  $\text{Na}_2\text{SO}_3/\text{Na}_2\text{S}$  sacrificial agents is illustrated in Fig. 6b. Under simulated solar light, both narrow-bandgap components are excited. Their inherent  $C_B$  and  $V_B$  positions are 0.11 eV/1.43 eV for  $\text{Bi}_2\text{S}_3$  and -0.66 eV/1.72 eV for CdSQDs. However, the high photon energy of solar irradiation further elevates their excited-state potentials to approximately -1.53 and -1.31 eV, respectively.

## 7 Renewable energy applications of carbon dots

A particularly effective strategy for enhancing overall water splitting efficiency is the construction of Z-scheme photocatalytic systems, which mimic natural photosynthesis<sup>[117]</sup>. These systems facilitate superior charge separation and retain strong redox potentials, making them ideal for the simultaneous evolution of  $\text{H}_2$  and  $\text{O}_2$ <sup>[118]</sup>. In contrast to conventional Type-II band alignment, a direct Z-scheme heterojunction is engineered to preserve the highest redox potentials of the constituent photocatalysts, thereby mimicking the essential charge transfer pathway of natural photosynthesis<sup>[119]</sup>. This configuration typically involves two semiconductors with staggered band positions like a Type-II system<sup>[120]</sup>. However, the charge migration mechanism is fundamentally different. Upon photoexcitation, instead of electrons and

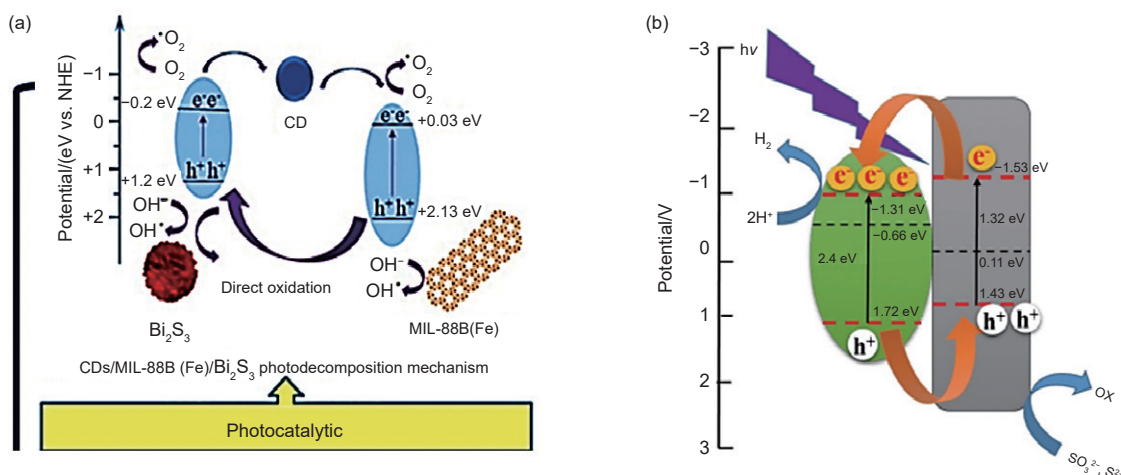


Fig. 7 (a) Possible photodecomposition mechanism for CDs/MIL-88B (Fe)/Bi<sub>2</sub>S<sub>3</sub> nanocomposite under LED light<sup>[115]</sup>. Copyright 2021, Elsevier. (b) Plausible photocatalytic mechanism of CdS/CdS/Bi<sub>2</sub>S<sub>3</sub> nanocomposite<sup>[116]</sup>. Copyright 2019, Springer

holes migrating to the lowest  $C_B$  and highest  $V_B$ , respectively, a direct interfacial charge recombination occurs between the less useful charge carriers<sup>[121]</sup>. Specifically, the photogenerated electrons in the semiconductor with the lower (less negative) reduction potential readily recombine with the holes in the semiconductor with the lower (less positive) oxidation potential. This selective recombination pathway effectively quenches the low-energy charges while isolating the most energetically potent electrons in the higher  $C_B$  and the most powerful holes in the higher  $V_B$ . Consequently, the system maintains strong driving forces for both reduction and oxidation reactions simultaneously. This architecture is particularly advantageous for applications such as overall water splitting and CO<sub>2</sub> reduction, which demand both highly reductive electrons for proton or CO<sub>2</sub> reduction and highly oxidative holes for water oxidation. The CdS/Bi<sub>2</sub>S<sub>3</sub> nanocomposite discussed herein exemplifies this principle, where the interface facilitates the recombination of Bi<sub>2</sub>S<sub>3</sub> electrons with CdS holes, thereby preserving the highly negative photoexcited electrons in CdS for efficient hydrogen evolution<sup>[122]</sup>.

### 7.1 CO<sub>2</sub> reduction

CDs are widely studied as photocatalysts, commonly for degrading organic molecules. However, their most significant potential lies in more complex reactions like CO<sub>2</sub> reduction and water splitting. The mechanism is attributed to the electrons released after

light absorption. This is supported by experiments where adding noble metals to CDs captured these electrons, which quenched fluorescence but boosted CO<sub>2</sub> reduction efficiency. A key finding was that the yield of CO<sub>2</sub> reduction products surprisingly depends on the concentration of CO<sub>2</sub> itself. In the experiment, researchers adjusted CO<sub>2</sub> concentration by varying its pressure in a high-pressure optical cell containing an aqueous solution. They used gold-doped CDs as the visible-light photocatalyst and isopropanol as a sacrificial electron donor (Fig. 8).

### 7.2 Solar cells and DSSCs

C-dots can improve dye-sensitized solar cells (DSSCs) by sensitization or co-sensitization<sup>[124–125]</sup>. They are standalone sensitizers which can cover a broad range of UV-vis region and inject electron into the semiconductor oxides (NiO<sup>[124]</sup>/ZnO<sup>[126]</sup>/TiO<sub>2</sub><sup>[127]</sup>) upon excitation. As co-sensitizers to the conventional dyes, the C-dots can help energy injections by Förster Resonance Energy Transfer (FRET)<sup>[4]</sup>, enhance spec-

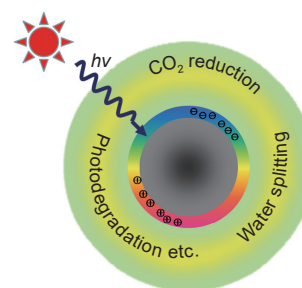


Fig. 8 Cartoon illustration of photocatalytic energy conversion applications of CDots<sup>[123]</sup>. Copyright 2019, AIP Publishing

tral response and reduce competitive absorption. They also facilitate charge separation, reduce recombination losses, and contribute to the light harvesting and charge transfer offers better PCE.

The schematic illustration in Fig. 9a below represents the charge transfer mechanism in a C-dot/N719/NiO-based dye-sensitized solar cell (DSSC). Upon visible-light irradiation, carbon dots (C-dots) act as photosensitizers, absorbing photons and exciting electrons from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). The excited electrons are subsequently injected into the  $C_B$  of NiO, facilitating charge separation and photocurrent generation. Meanwhile, holes remaining in the C-dots are transferred to the N719 dye, suppressing electron-hole recombination and enhancing charge transport efficiency. The red crosses indicate undesirable electron recombination pathways: (1) between injected electrons and oxidized species at the NiO/C-dot interface, (2) between electrons in C-dots and triiodide ( $I_3^-$ ) ions, and (3) between the HOMO level of C-dots and  $I_3^-$  species in

the electrolyte. The iodide/triiodide ( $I^-/I_3^-$ ) redox couple serves to regenerate the oxidized dye molecules, closing the catalytic cycle. This synergistic interaction between C-dots, N719 dye, and NiO enhances light harvesting, promotes efficient charge separation, and minimizes recombination losses, leading to improved photovoltaic performance under visible light.

The schematic diagram in Fig. 9b illustrates the charge transfer and separation mechanism in a C-dot/N719/ZnO/NiO heterojunction-based photoelectrochemical cell under solar illumination. Upon visible-light irradiation, the C-dots and N719 dye serve as dual sensitizers, effectively harvesting photons and exciting electrons from their HOMO to LUMO energy levels. The excited electrons are injected sequentially from the LUMO of C-dots into the conduction band ( $C_B$ ) of ZnO, and subsequently to the  $C_B$  of NiO, facilitating efficient charge transport toward the external circuit to generate photocurrent. Meanwhile, the photogenerated holes ( $h^+$ ) in the HOMO of N719 are transferred to the valence band ( $V_B$ ) of NiO, promot-

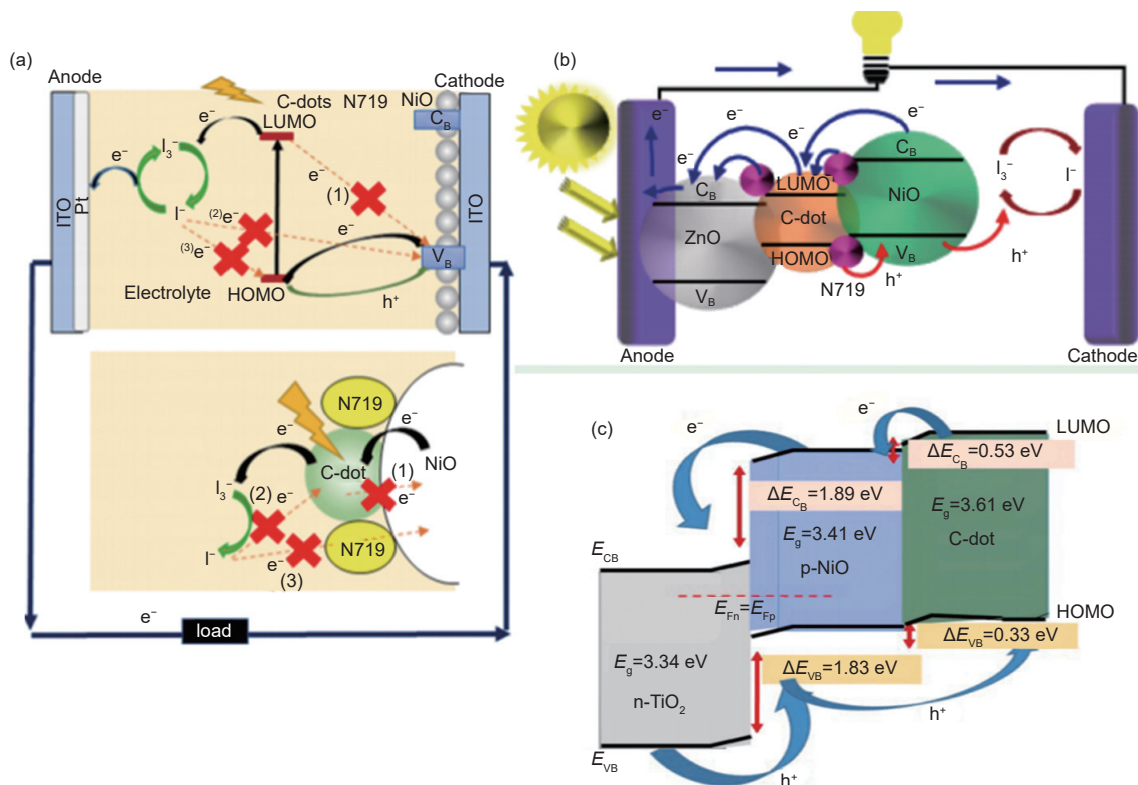


Fig. 9 DSSCs mechanism of Carbon dots with (a) NiO<sup>[124]</sup>, Copyright 2020, American Chemical Society (b) ZnO<sup>[128]</sup>, Copyright 2020, American Chemical Society and (c) TiO<sub>2</sub><sup>[129]</sup>, Copyright 2023, Elsevier

ing charge separation and suppressing recombination. The iodide/triiodide ( $I^-/I_3^-$ ) redox couple in the electrolyte regenerates the oxidized dye and completes the catalytic cycle by transferring electrons back to the anode. The synergistic effect among ZnO, C-dots, NiO and N719 dye broadens the light absorption range, enhances interfacial charge transfer, and improves overall solar-to-electric conversion efficiency through effective suppression of electron-hole recombination pathways.

The schematic energy band diagram in Fig. 9c illustrates the charge transfer mechanism across the n-TiO<sub>2</sub>/p-NiO/CD heterojunction, demonstrating efficient charge separation and transport under photoexcitation. The CDs, having a bandgap of 3.61 eV, act as visible-light sensitizers, facilitating electron excitation from the HOMO to the LUMO upon illumination. The photogenerated electrons in the LUMO of C-dots are transferred to the conduction band ( $E_{CB}$ ) of p-NiO and subsequently to n-TiO<sub>2</sub>, driven by the favorable conduction band offsets ( $\Delta E_{CB} = 0.53$  eV and 1.89 eV, respectively). Meanwhile, holes ( $h^+$ ) migrate in the opposite direction from the valence band ( $E_{VB}$ ) of TiO<sub>2</sub> to that of NiO and further to the HOMO of C-dots guided by the valence band offsets ( $\Delta E_{VB} = 0.33$  and 1.83 eV). This cascade-type band alignment effectively promotes directional charge migration, minimizes electron-hole recombination, and en-

hances the separation of photoinduced charge carriers. The matched Fermi levels ( $E_{Fn} = E_{Fp}$ ) between TiO<sub>2</sub> and NiO establish a strong internal electric field at the interface, further supporting efficient charge transport, making this heterostructure highly favorable for applications in photocatalysis and solar energy conversion.

Carbon dots serve as excellent sensing platforms due to their tunable fluorescence, high sensitivity, and selective response to various analytes through mechanisms such as fluorescence quenching (static/dynamic), the inner filter effect, or fluorescence enhancement. As shown in Table 4, CDs demonstrate remarkable versatility and performance across multiple domains, as evidenced by their application in bioimaging, energy, photocatalysis, and antibacterial therapy. In bioimaging, CDs derived from natural precursors such as aloe vera, honey, and chitosan exhibit high quantum yields (up to 31.2%) and excellent photostability, enabling prolonged imaging in HeLa cells, zebrafish, and bacterial systems. For energy applications, CDs enhance device efficiency and longevity, achieving a power conversion efficiency of 8.7% in solar cells, a high specific capacity in lithium-ion batteries, and exceptional cyclic stability in fuel cells. In photocatalysis, they drive efficient degradation of pollutants (e.g., 98% methylene blue removal) and CO<sub>2</sub>

**Table 4 Application, stability/efficiency of C-dots**

Bioimaging applications of carbon dots				
Cell/organism	Precursor	Quantum yield/%	Photostability	Ref.
HeLa cells	Aloe vera	24.6	>2 h continuous	[130]
MCF-7 cells	Honey	31.2	>90% intensity after 1 h	[131]
Zebrafish	Chitosan	19.8	3 h continuous	[132]
Bacterial cells	Tulsi leaves	22.1	Superior to FITC	[133]
Energy applications of carbon dots				
Solar cells	Garlic	PCE: 8.7%	500 h, 90% retention	[134]
Lithium-ion batteries	Grass	1250 mAh g <sup>-1</sup> after 100 cycles	200 cycles, 85% capacity	[40]
Fuel cells	Chitosan	Onset potential: 0.91 V	10 000 cycles stable	[135]
Photocatalytic applications of carbon dots				
Methylene blue degradation	Banana peel	98% in 60 min	5 cycles, 90% efficiency	[136]
Cr(VI) to Cr(III) reduction	Grass	95% in 90 min	8 cycles stable	[137]
CO <sub>2</sub> reduction	Coffee grounds	84% conversion to CH <sub>3</sub> OH	50 h stable	[138]
Antibacterial applications of carbon dots				
<i>E. coli</i>	Neem leaves	85% reduction	98% wound closure in 14 days	[139]
<i>S. aureus</i>	Banana peel	78% reduction	Complete healing in 10 days	[140]
MRSA	Garlic	92% reduction	2× faster than control	[141]

conversion with sustained activity over multiple cycles. Additionally, CDs display potent antibacterial effects against pathogens like *E. coli* and MRSA, promoting wound healing and demonstrating potential for therapeutic use. Their synthesis from renewable biomass, coupled with high efficiency, stability, and multifunctionality, positions CDs as promising sustainable nanomaterials for advanced technological and biomedical applications.

## 8 Conclusions, challenges and prospects

The origin and applications of biomass-assisted B-CDs are described in this review as being promising nanomaterials. Sustainable fabrication of tunable nanocarbons is summarized. Eco-friendly synthesis methods, such as hydrothermal, pyrolysis, solvent and ultrasonic methods, allow the sustainable preparation of nanocarbons. The treatments improve the optical and electronic properties of B-CDs for different purposes. B-CDs are effective photocatalysts for pollutant degradation, possess antibacterial activity during wastewater treatment, and are widely used as photocatalysts in water splitting for hydrogen generation. They are good bio-imaging agents due to their biocompatibility and luminescence. Due to the versatility of B-CDs, tremendous applications have been realized such as in energy, environment and biomedical fields.

Although the synthesis has improved, challenges in scaling up C-dot technology remain<sup>[142–143]</sup>. The bottleneck is the diversity and incomparable natural precursors, which make it difficult to control the size, surface functionalization, and optical properties of B-CDs, hindering understanding of property relationships and large-scale reproducibility. B-CDs suffer from high charge recombination and poor visible light absorption, resulting in a relatively low hydrogen generation efficiency for photocatalytic water splitting than the inorganic counterpart<sup>[144]</sup>. Furthermore, the long-term photostability, reusability and environmental application of CDs in practice should be further explored<sup>[145]</sup>. The trend future should be from experi-

ence synthesis to design knowledge-based and package integration. Machine learning based “process structure property” studies will be indispensable for predicting the precursor-synthesis combination, which would yield the desired B-CDs with specific bandgap and surface states. Doping with heteroatoms (N, S, and P) or creating heterojunctions with semiconductors (g-C<sub>3</sub>N<sub>4</sub>, TiO<sub>2</sub>) promote charge separation and photocatalytic activity for environmental purification or hydrogen production<sup>[146]</sup>. The development of scalable, continuous-flow synthesis approaches according to green chemistry is a prerequisite for homogeneity. In addition, researching the potential non-toxic multifunctional B-CD analogs in theranostics for photoimaging, antibacterial therapy and targeted drug delivery may contribute to personalized treatment because of their good biocompatibility<sup>[147]</sup>.

The future lies in moving beyond empirical synthesis towards intelligent design and hybrid integration. Advanced “process structure property” studies, powered by machine learning, will be crucial for predicting optimal precursor-synthesis combinations to yield B-CDs with tailored bandgaps and surface states. Purposeful heteroatom doping (e.g., with N, S, P) and the construction of heterojunctions with other semiconductors (e.g., g-C<sub>3</sub>N<sub>4</sub>, TiO<sub>2</sub>) are key strategies to enhance charge separation and boost photocatalytic activity for both environmental remediation and hydrogen generation<sup>[146]</sup>. For real-world impact, the focus must shift to scalable, continuous-flow synthesis processes that maintain green chemistry principles while ensuring homogeneity. Finally, the exploration of B-CDs as non-toxic, multifunctional agents in theranostics combining their bioimaging, antibacterial, and targeted drug delivery capabilities represents a vibrant frontier for personalized medicine, leveraging their unique biocompatibility derived from natural source<sup>[147]</sup>.

## Author contributions

Habtamu F Etefa contributed to the conceptualization, methodology, investigation, formal analysis, visualization, writing—original draft preparation, and

review and editing of the manuscript. Francis B. Dejene provided supervision, project administration, approval of the final version, financial support, and administrative assistance. All authors have read and approved the final version of the manuscript.

### Conflicts of interest

The authors declare no conflict of interest.

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