Review Article

# Advances in Carbon-Based Nanomaterials: From Graphene to Quantum Dots

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## ABSTRACT

Carbon-based nanomaterials have emerged as a transformative class of materials, owing to their unique structural, electronic, optical, thermal, and mechanical properties. Since the discovery of two-dimensional graphene and one-dimensional carbon nanotubes, the field has rapidly expanded to include zero-dimensional carbon quantum dots, graphene quantum dots (GQDs), and hybrid composites. This review collates recent advances in carbon-based nanomaterials, tracing the evolution of graphene from nanotubes to quantum dots, and examines their classification, structure–property relationships, synthesis routes, characterization modalities, and application landscapes. A historical overview of carbon allotropes and nanomaterials is initially presented, and the motivation and scope of this comprehensive treatment is provided. Following the classification of materials into 0D (fullerenes, CQDs/GQDs), 1D (CNTs), 2D (graphene, graphene oxide, derivatives), and hybrid composites, the exploration focuses on how their atomic bonding ($sp^2$, $sp^3$), defects, doping, edge effects, and quantum confinement determine their performance. Synthesis strategies such as exfoliation, chemical vapor deposition (CVD), arc discharge, laser ablation, and top-down/bottom-up approaches for quantum dots have been described. Then, characterization techniques are detailed, including TEM, SEM, AFM, XRD, Raman spectroscopy, photoluminescence, UV-Vis, XPS, FTIR, and advanced time-resolved methods. Major applications are examined in energy storage and conversion, sensing, biomedicine, catalysis, the environment, and optoelectronics. Finally, challenges such as scalability, reproducibility, stability, toxicity, and integration into devices are critically discussed and future directions for hybrid systems, computational design, and multifunctional platforms are outlined. Through this review, major advances and key takeaways are synthesized, offering an outlook on the next five to ten years of carbon-based nanomaterial research and implementation.



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## Content

## 1. Introduction

Carbon is among the most versatile elements in the periodic table and is capable of forming a multitude of structural allotropes through its ability to adopt $sp^2$ and $sp^3$ hybridizations and to form extended π-conjugated networks, as well as cage and chain structures. Historically, the most common forms are graphite and diamond, each exhibiting vastly different physical and chemical properties, despite being composed solely of carbon atoms. Graphite, with $sp^2$-bonded layers of hexagonal carbon rings, offers high electrical conductivity parallel to the layers, while diamond completely $sp^3$-bonded in a three-dimensional tetrahedral network is an excellent electrical insulator and one of the hardest known materials. Over time, the discovery of new carbon allotropes and nanostructured carbon materials has expanded the landscape of carbon-based materials science [1,2]. In the mid-1980s, the discovery of $C_{60}$ (buckminsterfullerene) marked a watershed. Fullerenes have demonstrated that carbon can be assembled in closed-cage molecular forms, ushering in the field of carbon nanostructures. Subsequent research revealed that carbon nanotubes (CNTs), in the early 1990s, as cylindrical shells of graphene sheets rolled into tubes displayed remarkable mechanical strength, electrical conductivity, and unique one-dimensional quantum properties. The advent of graphene, a single atomic layer of $sp^2$-bonded carbon, around 20042005, further revolutionized the field of two-dimensional materials by offering an extraordinary combination of high carrier mobility, mechanical robustness, flexibility, and optical transparency [3,4]. Parallel to these developments, the concept of quantum confinement in zero-dimensional (0D) carbon nanostructures has emerged: Small fragments or particles of graphitic carbon or graphene derivatives, generally under approximately 10 nm in size, exhibit size-dependent optical and electronic behavior. These materials are known as carbon quantum dots (CQDs) or graphene quantum dots (GQDs) and have rapidly gained research interest due to their strong photoluminescence, tunable emissions, and biocompatibility [5]. Over the last three decades, the field of carbon-based nanomaterials has matured from fundamental curiosities (fullerenes) to sophisticated classes of materials spanning 0D, 1D, and 2D regimes (quantum dots → nanotubes → graphene) and beyond; hybrid and composite systems have become increasingly prominent. This historical progression provides the foundation for this review [6]. There are multiple reasons why carbon-based nanomaterials have captured sustained

scientific and technological interest, ranging from fundamental physics to engineering and biomedical applications. Carbon nanomaterials often exhibit extraordinary electronic, optical, mechanical, thermal, and chemical features in a single platform. For example, graphene offers exceptional in-plane carrier mobility, high optical transparency, and mechanical flexibility. CNTs exhibit high tensile strength, high aspect ratio morphology, and ballistic conduction behavior in some regimes. CQDs and GQDs provide tunable fluorescence, strong chemical stability, and excellent water dispersibility when appropriately functionalized. These multifaceted properties make carbon nanomaterials attractive in diverse fields [7, 8].

Carbon's configurational flexibility enables the formation of 0D quantum dots, 1D nanotubes, and 2D graphene sheets, each with distinct physical phenomena (quantum confinement, edge states, curvature, and defects) that can be tuned for specific applications. The ability to tailor size, shape, defects, functional groups, and hybridize with other materials adds enormous versatility. Many carbon-based nanomaterials are compatible with solution processing, chemical vapor deposition (CVD), exfoliation, or bottom-up synthesis approaches that are amenable to scaling and integration into device architectures. Their compatibility with flexible substrates, composites, and hybrid systems has broadened their applications in electronics, optoelectronics, sensors, energy storage, catalysis, biomedicine, and environmental technologies [9]. In particular, for quantum dot forms and functionalized graphene derivatives, the intrinsic carbon backbone offers lower toxicity compared to many heavy-metal quantum dots (*e.g.,* CdSe) and better chemical stability under ambient or biological conditions. This has spurred interest in bioimaging, drug delivery, biosensing, and phototherapy. At the nanoscale, carbon nanomaterials exhibit emergent physics: quantum confinement in quantum dots, Van Hove singularities in nanotubes, Dirac fermion behavior in graphene, edge and defect states in reduced-dimensional systems. These phenomena drive fundamental scientific inquiry and enable novel device concepts (*e.g.,* ultrafast photonics and quantum sensors) [10]. With a global focus on sustainability, carbon-based nanomaterials offer a strategic advantage: carbon is abundant, versatile, and amenable to many "green" synthesis routes. Their integration into energy storage (supercapacitors and batteries), environmental remediation, water purification, and sensing aligns with the goals of sustainable technology. Taken together, these motivations underscore the timely review of carbon-based nanomaterials, from graphene to quantum dots. They lie at the intersection of fundamental materials science, nanotechnology, device engineering, and applications spanning energy, environment, healthcare, and electronics [11, 12]. The major classes of carbon-based nanomaterials are organized by dimensionality, and culminating in the most recent advances in quantum-sized carbon systems. The structural features, synthesis methods (*e.g.,* CVD, exfoliation, reduction of graphene oxide), fundamental properties (electronic, mechanical, thermal, and optical), and applications (sensors, electronics, composites, and energy devices) are discussed. The aim is to highlight both the breakthroughs achieved with graphene and the remaining challenges (*e.g.,* large-area synthesis, defect control, and integration) [13]. Single-walled and multi-walled nanotubes, their structural and electronic heterogeneity (chirality, metallic vs. semiconducting behavior), synthesis routes (arc discharge, laser ablation, and CVD), properties (mechanical strength, thermal conductivity, and quantum transport), and applications (composites, field emission, sensors, and energy devices). This includes an in-depth discussion on carbon quantum dots, graphene quantum dots, and other carbon-based nanodots. Their structural origin, quantum confinement and edge effects, optical and electronic properties (photoluminescence and size-tunable emission), synthesis strategies (top-down vs. bottom-up), functionalization, and a broad range of emerging applications (bioimaging, sensing, light-emitting diodes (LEDs), photovoltaics, and catalysis) are examined [14]. Recognizing that real-world

applications increasingly rely on composite architectures, Hybrid carbon-nanomaterial systems are discussed (*e.g.,* graphene–CNT hybrids, quantum dot/carbon nanotube composites, doped carbon nanomaterials) and how they harness synergistic features. Beyond summarizing advances, the review will highlight the key characterization techniques (structural, chemical, and optical), the main bottlenecks (scalability, cost, reproducibility, and environmental/health issues), and future prospects (emerging directions such as quantum materials, heterostructures, model-guided design, and device integration) [15]. A unique theme of this review is tracing the progression from 2D → 1D → 0D carbon nanostructures, analyzing how dimensional reduction (and concomitant confinement, edge effects, curvature, and defects) influences properties and enables new functionalities. This allows the reader to appreciate how aspects discovered in graphene (2D) inform nanotube (1D) behavior and how further reduction to quantum dots leverages quantum size and surface effects [16]. By organizing the review in this way, the reader will gain a holistic understanding of the carbon-nanomaterial ecosystem, not only the individual classes, but also how they relate, evolve, and coexist in hybrid platforms. The emphasis will be balanced between fundamental material science (structure, properties, and mechanisms) and application-oriented perspectives (devices, systems, and commercial potential). Where appropriate, tables or schematics will summarize comparison metrics (*e.g.,* specific surface area, carrier mobility, and quantum yield) across the classes [17]. In particular, the section on quantum dots will reflect the most recent research attention given the explosion of interest in CQD/GQDs over the past decade. The way of developing these materials on the foundations of graphene and nanotubes are examined but has unique advantages (*e.g.,* fluorescence tunability, water solubility, and biocompatibility) and challenges (size control, precise structure–property correlation, and large-scale manufacturing) [18].

### *1.1. Dimensional evolution of carbon nanomaterials: From 2D graphene to 0D quantum dots*

Graphene (2D) has delocalized charge carriers throughout the entire extended $sp^2$ hybridized carbon lattice, leading to high mobility and exceptional conductivity, thus quantum confinement has no significant effect, and edge defects on the basal plane are negligible compared to all other effects [19]. Transitioning from graphene to 1D carbon nanostructures like nanofibers and carbon nanotubes introduce a lateral confinement in one spatial dimension. Confining the electronic states around its circumference results in an extraordinarily high sensitivity of mechanical properties to chirality, diameter, and edge defects or structural abnormalities resulting from the non-planar shape of these structures. Additionally, the presence of Edge defects and curvature effects becomes an increasingly important influence on the electronic structure of these carbon nanostructures; however, these effects do not dominate the 1D electronic structure [20].

A 0-dimensional carbon quantum dot, where the quantum dot is trapped in the three dimensions allowed to the element carbon, has discrete energy levels and bandgaps that depend on the size of the quantum dot. At this size, defects and functional groups on the edge and surface of the quantum dot dominate the electronic structure of the quantum dot, and these defects or groups are responsible for the photoluminescence because they provide sites for emission [21]. The transition from 2-dimensional to 1-dimensional to 0-dimensional quantum dots represents an evolving shift from delocalized, conductive behavior toward quantum confined optically active systems [16].

## 2. Classification of Carbon-Based Nanomaterials

Carbon-based nanomaterials (CBNs) represent a versatile and broadly studied class of materials, distinguished by their elemental composition (primarily carbon) and nanoscale dimensions (**Table 1**). The diversity of CBNs arises not only from the many allotropes of carbon (graphite, diamond, fullerenes, etc.), but also from the arrangement of carbon atoms, hybridized ($sp^2$, $sp^3$), and constrained in one-, two-, or zero-dimensional nanostructures. As many recent reviews have noted, typical categories include 0D, 1D, 2D, and hybrid/composite forms [22-26]. The structural transformation pathway of carbon-based nanomaterials, starting from a two-dimensional graphene sheet, progresses into one-dimensional carbon nanotubes, further assembling into carbon nanofibers, and finally forming zero-dimensional carbon quantum dots. This schematic highlights the diversity of carbon nanostructures and their tunable morphology, which enables unique physicochemical properties for applications in nanotechnology, electronics, and biomedical systems (**Figure 1**). The evolutionary pathway illustrated in the **Figure 1**. The transformation of carbon-based nanomaterials as they transition from a wide area as in 2D graphene, down to 1D carbon nanofibers, and then showcasing the beauty of optical activity in 0D carbon quantum dots, distinctly display how carbon nanomaterials are significantly transformed in chemical, physical and optical properties by all-through three-dimensional confinement of charge carriers, enhanced quantum confinement, as well as electrostatic edge effects respectively. As charge carriers flow through graphene (2D) and are highly delocalized across the $sp^2$ carbon plane system causing there to be excess depth defect property in the cases where the nanofiber or nanotube is now curved and/or laterally constrained this will preferentially cause additional passivation relative to the diameter of the tube *i.e.,* it causes many carbon nano-materials to become anisotropic. As these 1D forms evolve into their final state of being a 0D quantum dots their size can now have very small-step discreet energy levels, also there will be a large variation in bandgap and usually from the side/edge of this same surface, there will develop high levels of PL. Therefore, by tracing these several stages of transition from the greater dimension (2D) to the Lower dimensional range (1D) and finally to the ultimate challenge - the 0D quantum dots) In theoretical models, one can explain how/why charge carriers operate under the rules of optoelectrical, optically-based materials properties such as sensing, imaging etc.

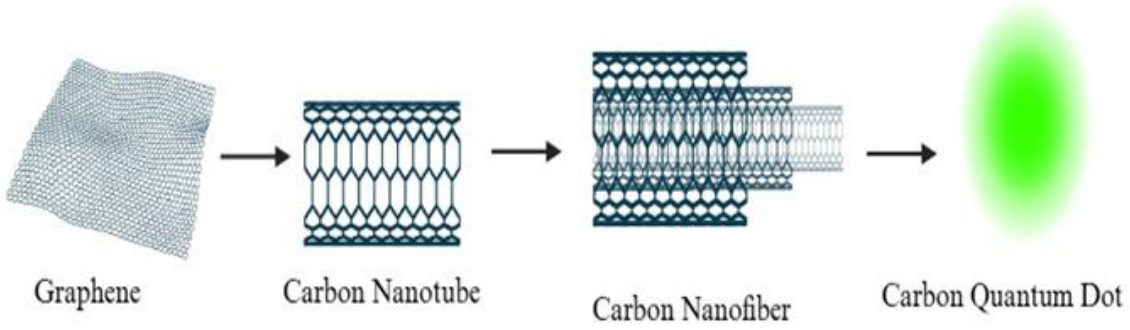


**Figure 1.** Evolution of carbon-based nanomaterials: from graphene to carbon quantum dots

**Table 1.** Classification of carbon-based nanomaterials

| Category | Dimensionality | Key examples | Structural characteristics | Major properties | Typical applications | Ref. |
|---|---|---|---|---|---|---|
| **Zero-Dimensional** | 0D (Nanoscale clusters; no extended dimensions) | Fullerenes, Carbon Quantum dots, and Graphene quantum dots | Spherical or quasi-spherical; strong quantum confinementand; discrete energy levels | High photoluminescence, tenable bandgap, good biocompatibility, and excellent electron transfer | Bioimaging, sensing, photocatalysis, drug delivery, and optoelectronics | [23] |
| **One-Dimensional** | 1D (Length, diameter) | Single-walled & Multi-walled carbon nanotubes (SWCNTs, MWCNTs) | Cylindrical $sp^2$ carbon tubes; hollow structure; and high aspect ratio | Exceptional electrical & thermal conductivity, high tensile strength, and flexibility | Nanoelectronics, reinforced composites, energy storage, sensors, and drug delivery | [24] |
| **Two-Dimensional** | 2D (Atomic-thickness sheets) | Graphene, graphene oxide (GO), reduced graphene oxide (rGO), and graphene derivatives | Single/few-layer sheets; high surface area; tenable surface chemistry; and $sp^2$ carbon network | Superior electrical/thermal conductivity, high transparency, and mechanical strength | Flexible electronics, membranes, supercapacitors, catalysis, and biomedical platforms | [27] |
| **Hybrid & Composite materials** | Multi-dimensional (0D–3D combinations) | Graphene–CNT hybrids, CQD–polymer composites, graphene–metal/oxide nanocomposites | Engineered integration of different carbon nanostructures with metals, oxides, and polymers | Synergistic enhancement of conductivity, strength, stability, and optical and catalytic behaviour | Energy devices, structural composites, photonics, sensors, and multifunctional nanoplatforms | [28] |

### *2.1. Zero-dimensional materials: fullerenes, carbon quantum dots, and graphene quantum dots*

Zero-dimensional carbon nanostructures are those in which all three spatial dimensions are constrained at the nanoscale (typically < 100 nm and often much smaller). This vanishingly small size leads to pronounced quantum confinement, surface-dominant behavior, and other nanoscopic phenomena. Fullerenes were among the earliest widely known 0D carbon nanomaterials. The classic example is C60, the "buckyball" molecule, a closed cage of 60 carbon atoms arranged in $sp^2$ hybridization, forming a truncated icosahedron. Fullerenes display interesting electron-acceptor behavior and high symmetry, and have been explored for molecular electronics, photovoltaics, and other applications. While fullerenes are not the primary focus in more recent "quantum dot"-driven carbon research, they remain relevant as a founding class of 0D carbon nanostructures [27]. Carbon quantum dots and graphene quantum dots are more recent subdivisions of zero-dimensional carbon materials. CQDs (also called carbon dots, CDs) typically consist of quasi-spherical nanoparticles with diameters less than ~10 nm, composed of $sp^2/sp^3$ hybridized carbon networks, often with oxygen, hydrogen, and nitrogen functionalization. According to Mohapatra *et al.*, based on their size, shape, and dimension, nanostructured carbon materials are classified into different

categories: 0D carbon, such as fullerenes and carbon quantum dots (CDs) [28-30]. GQDs are derived from graphene sheets cut or confined to quantum-dot sizes (typically a few nanometers in lateral dimension) and hence show both graphene-derived π-conjugated core and quantum-confinement/edge effects. A review by Speranza *et al.* listed GQDs as 0D carbon nanomaterials [31]. Size < 10 nm (for CQDs/GQDs) → strong quantum size effect, tunable bandgap/photoluminescence. Surface: A high surface-to-volume ratio and the presence of functional groups (–OH, –COOH, $–NH_2$, etc.) influence solubility, chemical reactivity, and luminescence. Electronic/optical behavior: Quantum confinement and surface states dominate the behavior. For GQDs, the combination of graphene-derived π-networks and edge states yields tenable photoluminescence. Hybridization: CQDs/GQDs often have mixed $sp^2/sp^3$ carbon domains, which differentiate them from pure graphitic $sp^2$ networks [23,32]. CQDs can be synthesized using various carbon precursors (biomass, waste, and polymers). They are promising for bioimaging, sensors, and optoelectronics because of their lower toxicity compared to that of heavy-metal quantum dots. GQDs inherit desirable graphene traits (high conductivity, π-conjugation), but are constrained to nanoscale size, leading to size-dependent optical/electronic properties. Fullerenes: While not as "bright" for photoluminescence, they introduced the carbon cage concept and still serve as model systems [33]. The 0D class of carbon nanomaterials is a rapidly evolving emerging subtype (carbonized polymer dots, heteroatom-doped CDs/GQDs) that continues to expand in scope. As Mohapatra *et al.* noted, depending on the synthesis process, CDs can be classified into three main types: CQDs, GQDs, and carbonized polymer dots (CPDs). The functional advantages (tunability, low toxicity, and chemical versatility) of 0D carbon nanomaterials make them a key pillar in the field [28].

### *2.2. One-dimensional materials: Carbon nanotubes*

One-dimensional carbon nanomaterials are those in which two spatial dimensions are confined at the nanoscale, whereas one dimension is relatively long (often microns or more). Archetypal 1D carbon nanomaterials are composed of carbon nanotubes. CNTs are cylindrical tubes of carbon with diameters typically in the nanometer range (single-walled ~1–2 nm, multi-walled tens of nanometers) and lengths reaching up to microns. They are formed by rolling graphene sheets into tubular geometries. There are two primary types: single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs). According to Mohapatra *et al.*, CNTs are 1D carbon allotropes. Since their discovery in 1991, CNTs have become a hot topic in carbon-based nanostructured material research [28]. High aspect ratio: length significantly exceeds diameter and yields delocalized carrier pathways and unique mechanical reinforcement behavior. Electronic behavior: SWCNTs can be metallic or semiconducting, depending on their chirality and diameter. Thermal and mechanical properties: exceptional strength and high thermal conductivity (along the tube axis). For instance, Zhan and Gu reviewed the thermal conduction in 1D carbon nanomaterials: Based on experimental measurements and simulations, such as CNTs. The outer wall of CNTs can be functionalized (oxidation, doping) to tailor their chemistry and compatibility with composites. SWCNTs: single graphene cylinder; chirality defines electronic type [34]. MWCNTs multiple concentric tubes, more robust mechanically, generally exhibit metallic behavior. Carbon nanofibers (CNFs): similar 1D carbon structures, although not strictly carbon nanotubes, are sometimes included under 1D carbon nanostructures. Carbon nanobuds: hybrid structures combining CNTs and fullerenes (buds) attached to nanotube walls; example of advanced 1D/0D hybridization. Owing to their strong mechanical, electrical, and thermal properties, CNTs are widely used for reinforcement in composites (polymers and

metals) as conductive fillers, electrode materials in energy storage (supercapacitors and batteries), sensors, and nanoelectronics [35]. The 1D nature provides efficient pathways for electron, phonon, and mechanical load transfer. Although, 2D graphene often steals the limelight, 1D carbon nanotubes remain vital in carbon nanomaterial research. The key challenges are achieving uniformity (chirality control in SWCNTs), reproducible synthesis, dispersion in matrices, and interface tailoring. However, their classification as a major 1D carbon nanomaterial class has been firmly established [36].

### *2.3. Two-dimensional materials: Graphene, graphene oxide, other graphene derivatives*

Two-dimensional carbon nanomaterials are those in which one dimension (thickness) is on the nanoscale (typically a few atomic layers), while the other two dimensions are extended (often microns or more). The prototypical 2D carbon material is graphene, a single (or few) layer of $sp^2$-bonded carbon atoms arranged in a hexagonal lattice. Graphene: a monolayer of carbon atoms in $sp^2$ configuration, honeycomb lattice; exceptional electrical, thermal, and mechanical properties [37]. Graphene Oxide (GO) graphene sheets functionalized with oxygen-containing groups (epoxide, hydroxyl, and carboxyl) disrupt the π-network, increase hydrophilicity, and introduce defects. Reduced graphene oxide (rGO): GO is chemically, thermally, or electrochemically reduced to partially restore $sp^2$ conjugation while retaining functional groups/defects for functionalization. Other derivatives include graphene nanoribbons (GNRs), graphdynes ($sp/sp^2$ hybrid carbon network), and other heteroatom-doped graphene sheets. Mohapatra *et al.* noted that 2D carbon, as in graphene, graphene derivatives, graphdynes, and graphitic carbon nitride (g-$C_3N_4$) fall into this category [28]. High surface area and large lateral dimensions with atomic thickness yield a very high surface-to-mass ratio (beneficial for sensing and catalysis). Electrical/thermal conduction: The in-plane conduction is excellent because of the delocalized π electrons. Mechanical strength: Graphene exhibits very high tensile strength and Young's modulus. Tunability: The properties can be tuned by defect engineering, chemical functionalization, heteroatom doping, and stacking (few-layer graphene). Edge/defect effects: because the sheet has a high aspect ratio, edges and defects play a significant role in the chemical reactivity. Layer control: The number of layers influences the band structure, carrier transport, and interlayer coupling [38]. Graphene and its derivatives have sparked wide interest across many fields, including flexible/wearable electronics, transparent conductive films, electrode materials (batteries and supercapacitors), composite reinforcements, sensors (gas and biomolecular), and membranes (water purification). The classification of 2D carbon nanomaterials is robust and expensive. The advent of graphene in 2004 (though few-layer graphitic carbon sheets existed earlier) triggered a substantial explosion in research. The versatility of 2D carbon materials stems from their planar geometry, ease of interface with other materials, and tunability. As the review by Patel et al. notes: "Carbon-based nanomaterials include graphene and its derivatives [39].

### *2.4. Hybrid and composite carbon-based nanomaterials*

Beyond pure 0D, 1D or 2D carbon nanostructures, an increasingly important category encompasses hybrid and composite carbon-based nanomaterials. These systems combine different dimensionalities, various carbon allotropes, or carbon nanostructures joined with other materials (metals, oxides, and polymers) to leverage synergistic effects. Carbon nanobuds (as mentioned above) are hybrids of 0D (fullerene) and 1D (CNT) structures. Graphene quantum dot hybrids: For example, graphene sheets with attached GQDs or CQDs combine a 2D high-conductivity plane with 0D luminescent dots [40]. 3D hierarchical structures are formed by stacking or self-assembly of 1D and 2D carbon nanostructures of graphene membranes with embedded nanotubes and foams of graphene/nanotube

networks. Although strictly 3D in architecture, the constituent building blocks are 0D/1D/2D carbon. Carbon nanostructures integrated with metals or metal oxides, for example, CNTs decorated with $TiO_2$ nanoparticles for improved photocatalysis and graphene oxide with metal nanoparticles for sensing or catalysis. Carbon-polymer composites, for example, graphene or CNTs, are dispersed in polymer matrices for mechanical reinforcement or electrical conductivity [41]. Carbon-carbon hybrids: for example, mixing graphene and CNTs in a composite to exploit planar and tubular geometries together. Carbon heteroatom-doped materials, for example, nitrogen-doped graphene and boron-doped carbon dots, while still strictly carbon nanomaterials, doping and functionalization effectively create a "composite" at the atomic level. Synergy: Different components complement each other. For example, CNTs provide excellent axial conductivity, graphene provides planar conduction, metal nanoparticles exhibit catalytic activity, and carbon networks support electron transport and structural integrity. Tuning: Composite systems allow the tuning of electronic, optical, and chemical properties beyond what pure carbon nanostructures can deliver [42]. Real-world deployment: often, pure carbon nanomaterials alone may not meet all requirements (mechanical robustness, processability, and stability); composites help bridge the gap toward applied systems. Dimensional integration: combining nano dimensional materials across length scales helps build hierarchical architectures (*e.g.,* 0D nanoparticles perched on 1D nanotubes anchored in a 2D sheet), which are beneficial for sensing, catalysis, and energy storage. Photocatalysis: carbon dots combined with metal oxide semiconductors: Mohapatra *et al.* discussed the use of CQD/GQDs in photo-Fenton or photocatalysis when integrated into composites [28]. Energy storage: graphene CNT hybrid networks are used as electrodes in supercapacitors and batteries; the carbon network provides conductive pathways and structural stability [43]. Biomedical graphene/hybrid carbon materials functionalized with biomolecules and other nanomaterials for carbon-based nanomaterials in theranostics. The composite/hybrid category is, in many ways, the frontier of carbon-nanomaterial research because the realization of devices and systems often requires multi-component architectures rather than isolated single-morphology nanostructures. The diversity of combinations (dimensions, materials, and functionalization) continues to expand [44]. **Figure 2** presents a schematic classification of major carbon-based nanomaterials, including carbon nanotubes, graphene, carbon black, carbon nanofibers, and fullerenes. Each category is depicted in its representative structural form, illustrating the diversity of the nanoscale carbon allotropes. The diagram highlights the structural variations from tubular and sheet-like morphologies to particulate and cage-like architectures, demonstrating their unique physical properties and wide-ranging applications in electronics, energy storage, catalysis, and biomedical systems.

## 3. Fundamental Structure and Properties

Carbon-based nanomaterials are among the most versatile materials in modern science. Their exceptional range of structures, from zero-dimensional fullerenes and quantum dots to one-dimensional carbon nanotubes and two-dimensional graphene, arises from the unique electronic configuration of carbon and its ability to form multiple hybridization states. The fundamental structure of these materials determines their mechanical strength, electrical conductivity, optical behavior, and chemical reactivity.

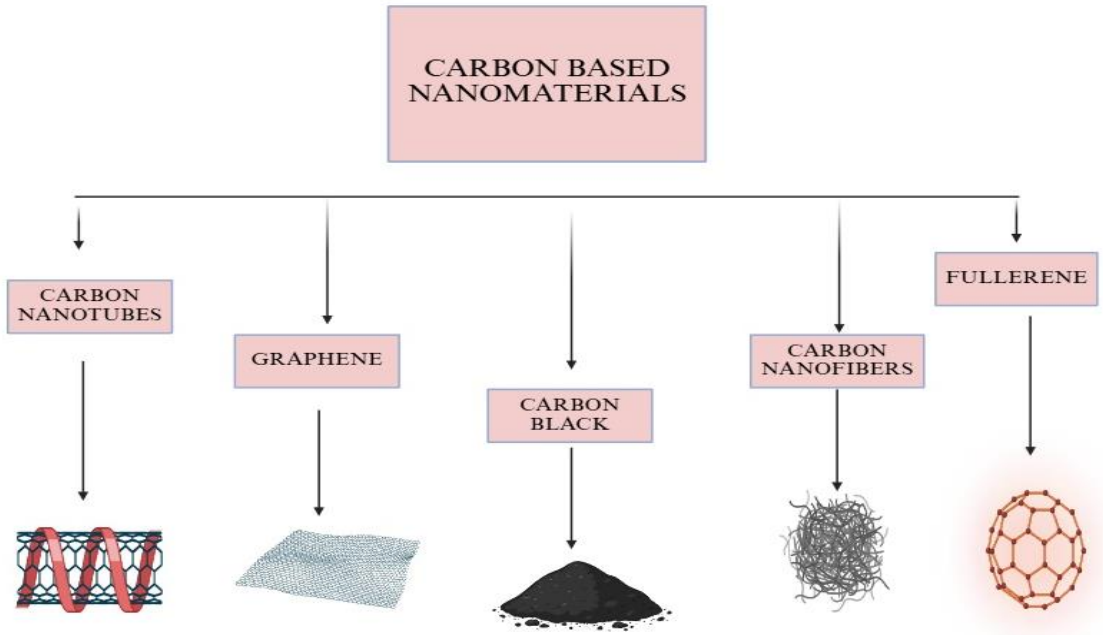


**Figure 2.** Classification of carbon-based nanomaterials and their representative structures

Understanding the relationships between structure and properties is essential for designing materials for energy storage, catalysis, sensors, electronics, and biomedical applications [45].

### *3.1. Structural characteristics ($sp^2$/$sp^3$ hybridization, edge effects, and defects)*

The remarkable diversity of carbon nanostructures originates from the ability of carbon to undergo *sp*, $sp^2$, and $sp^3$ hybridization. $sp^2$ hybridization, as found in graphene and CNTs, leads to a planar trigonal geometry where each carbon atom bonds to three others, leaving one delocalized π-electron that contributes to high electrical conductivity and strong in-plane σ-bonding. The hexagonal honeycomb lattice of graphene provides a unique combination of mechanical robustness and electronic delocalization. This structure forms the basis for all other CBNs: rolling a graphene sheet yields a CNT, wrapping it into a sphere produces fullerene, and cutting it into nanoscale fragments leads to graphene quantum dots [46]. The $sp^3$ hybridization, which is characteristic of diamond, creates a tetrahedral arrangement with strong localized σ-bonds, yielding an electrically insulating but mechanically super-hard material. Within nanocarbon systems, a partial $sp^3$ character often appears at defect sites, edges, or upon chemical functionalization (*e.g.,* oxidation in graphene oxide). This hybrid bonding significantly modifies the local electronic density, rendering such regions chemically active. Edge effects are particularly important for 2D and 0D nanocarbons. Graphene edges can be classified as *zigzag* or *armchair* types, each exhibiting distinct electronic behavior that supports localized electronic states and even magnetism, whereas armchair edges tend to be semiconducting or metallic, depending on the width. In GQDs, edges play a crucial role in photoluminescence (PL) because surface states and oxygen-containing groups can trap excitons, thereby tuning the emission wavelength and intensity [31]. Defects are key structural elements. Intrinsic point defects (vacancies, Stone–Wales defects), topological defects, and extrinsic defects

introduced by doping or irradiation affect the conductivity, mechanical stiffness, and reactivity. For example, in CNTs, a single vacancy can drastically change the band structure from metallic to semiconducting. In graphene oxide (GO), epoxide and hydroxyl functional groups introduce $sp^3$ regions that break π-conjugation, reducing conductivity, but enhancing dispersibility in polar solvents. Defects thus serve as both challenges and design opportunity sites for anchoring metal nanoparticles, enhancing catalysis, or creating desired bandgaps. The interplay between hybridization, edge configuration, and defect chemistry defines the structure-property relationship in all carbon nanomaterials [47]. Tailoring these parameters enables precise control of the mechanical, optical, and electronic performance.

### *3.2. Electronic, optical, mechanical, and thermal properties of graphene, CNTs, and CQDs/GQDs*

Electronic behavior in carbon nanomaterials arises primarily from π-electron delocalization within $sp^2$ networks. Graphene exhibits linear energy dispersion near the Dirac points (K and K′), resulting in charge carriers that behave as massless Dirac fermions. This provides graphene with an extremely high charge mobility (up to 200,000 $cm^2\ V^{-1}\ s^{-1}$) and near-ballistic electron transport at room temperature. However, its zero bandgap limits its direct use in digital logic applications. Hence, bandgap engineering through quantum confinement, doping, or bilayer stacking is often employed. In CNTs, the electronic nature (metallic or semiconducting) depends on chirality. Armchair CNTs (n = m) are metallic, while zigzag and chiral CNTs exhibit semiconducting behavior. This tunability makes CNTs promising for use in field-effect transistors, sensors, and nanoscale interconnects [48]. Carbon quantum dots, graphene quantum dots, and the strong quantum confinement of electrons and holes open discrete energy levels, leading to size-dependent bandgaps. Smaller dots show larger bandgaps and blue-shifted photoluminescence, whereas larger dots exhibit red-shifted emission. Surface functional groups further modulate the electronic structure, making CQDs and GQDs excellent materials for optoelectronic and bioimaging applications [49]. Graphene absorbs approximately 2.3% of the incident white light per layer, which is remarkably high for an atomic-thick material, owing to the interbond transitions of π-electrons. Doping or external electric fields can tune the optical conductivity, enabling transparent conductive films. CNTs exhibit unique optical transitions ($E_{11}$, $E_{22}$, etc.) that correspond to van Hove singularities in their density of states. These transitions are highly sensitive to the tube diameter and chirality. CNTs also demonstrate nonlinear optical effects, such as saturable absorption, when used in ultrafast laser systems [50]. In CQDs and GQDs, quantum confinement and surface-state emissions dominate the optical behavior. Photoluminescence can be tuned by adjusting the particle size, degree of oxidation, and heteroatom doping (*e.g.,* N, S, or P doping). Their high PL quantum yield, low toxicity, and stability make them superior alternatives to metal-based quantum dots (such as CdSe or PbS) in biological and optoelectronic devices [51].Graphene is the strongest known material with a Young's modulus of ~1 TPa and an intrinsic strength of ~130 GPa. These exceptional values arise from robust $sp^2$ bonding within the hexagonal lattice. CNTs have similar mechanical properties, exhibiting high tensile strength and flexibility; individual single-walled CNTs (SWCNTs) can sustain strains of up to 15–20% without permanent deformation. In composites, the incorporation of CNTs or graphene drastically improves mechanical stiffness, toughness, and wear resistance. For instance, polymer–CNT composites show several-fold increases in modulus and tensile strength, even at low filler loadings (<1 wt%). However, the presence of defects or poor interfacial bonding can limit mechanical reinforcement, emphasizing the importance of surface functionalization [52]. The mechanical properties of CQDs and GQDs are less significant individually but play a role in reinforcing polymer matrices or films. Their nanoscale dimensions and compatibility with aqueous

systems render them suitable for use in flexible electronics and coatings. Graphene exhibits exceptional thermal conductivity (~4,000–5,000 W $m^{-1}$ $K^{-1}$), far exceeding that of copper. This is due to efficient phonon transport in the crystalline lattice. CNTs also possess a high thermal conductivity (~3,000 W $m^{-1}$ $K^{-1}$ for individual tubes), making them attractive for thermal interface materials and heat dissipation systems. However, in bulk films or composites, phonon scattering at junctions significantly lowers effective conductivity [26]. The CQDs and GQDs have moderate thermal properties owing to phonon scattering at the boundaries and the presence of functional groups. However, their photothermal conversion efficiency is valuable for biomedical photothermal therapy and solar energy harvesting [53]. Overall, the exceptional electronic, optical, and mechanical properties of CBNs stem from their atomic-scale perfection and $sp^2$ network integrity, whereas quantum dots derive unique features from quantum confinement and surface chemistry.

### *3.3. Quantum size effects and their roles in quantum dots*

The most distinguishing feature of carbon quantum dots and graphene quantum dots is their quantum size effect, which arises when the particle dimensions become comparable to or smaller than the exciton Bohr radius (~10 nm for carbon systems). In this regime, continuous electronic energy bands break into discrete energy levels, leading to size-dependent optical and electronic properties. As the dot size decreases, the bandgap widens because the confinement energy increases according to the relation Eg∝1/R2E_g \prop to 1/R^2Eg∝1/R2, where $R$ is the QD radius of the quantum dot. This results in a blue shift in the photoluminescence spectrum for the smaller CQDs. Conversely, larger dots exhibit red-shifted emission owing to reduced confinement. This tunable emission enables multicolour luminescence in the same material system [54]. The excitons (electron–hole pairs) in the CQD/GQDs are confined within a nanometric volume, enhancing the radiative recombination probabilities. Photoluminescence can originate from intrinsic (core-state) emission, edge-state emission, or surface-defect states. The dominance of each pathway depends on the synthesis conditions and the surface passivation. For example, nitrogen-doped CQDs often show strong blue emission due to the localized energy levels introduced by N atoms [55]. CQDs exhibit excitation-dependent PL, changing emission wavelengths with excitation energy, indicating multiple emissive centres. This property is advantageous in multiplexed bio-labeling and sensors because one material can generate several emission colors under different excitations. Quantum confinement modifies the carrier mobility and transport behavior. In contrast to the delocalized π-system of graphene, electrons in CQD/GQDs are localized, leading to discrete hopping conduction and increased photostability. These confined carriers can interact strongly with surrounding molecules, enabling photoinduced charge transfer, which is crucial for photocatalysis and sensing [56]. The quantum size effect allows fine-tuning of optical absorption and emission, making CQDs ideal for LEDs, solar cells, and photodetectors. In solar cells, CQDs can serve as sensitizers, broadening the absorption across the visible spectrum and improving charge separation efficiency. The ability to engineer band alignment with other semiconductors enhances the energy transfer in hybrid architectures [57]. Overall, quantum size effects transform carbon from a semimetal (graphene) into semiconducting and luminescent forms (CQD/GQD), enabling entirely new functional regimes beyond conventional carbon materials.

### *3.4. Surface chemistry, functional groups, and doping-effects*

Surface chemistry profoundly influences the physical and chemical behaviours of carbon-based nanomaterials (**Table 2**). Due to their large surface-to-volume ratio, even slight modifications at the surface can drastically change the dispersion, optical properties, catalytic activity, and biocompatibility.

Graphene oxide (GO) and CQDs typically contain oxygen-bearing functional groups hydroxyl, epoxy, carbonyl, and carboxyl interrupt the π-conjugation network and introduce hydrophilicity. These functionalities are double-edged; while they reduce conductivity, they enable aqueous dispersion, chemical reactivity, and biomolecular conjugation. The reduction (thermal, chemical, or electrochemical) of GO partially restores conductivity by converting $sp^3$ carbons back to $sp^2$ domains, yielding reduced graphene oxide (rGO) [58]. In CQDs and GQDs, the surface functional groups act as emissive traps or passivating agents. Surface passivation with polymers (*e.g.,* polyethylene glycol) or small molecules (*e.g.,* amines) can enhance the PL quantum yield by eliminating nonradiative recombination centres. The ratio of oxygenated to graphitic regions directly determines the emission colour and stability. Doping with heteroatoms such as nitrogen, boron, sulphur phosphorus, and fluorine introduces new electronic states and alters the charge distribution within the carbon lattice [59]. Nitrogen doping adds lone-pair electrons, increasing the electron density and promoting n-type behaviour. N-doped graphene and CNTs exhibit enhanced catalytic activity toward oxygen reduction reactions (ORR) and improved capacitance in supercapacitors. In contrast, boron doping creates p-type behaviour, improving the hole conductivity and chemical reactivity. Sulphur or phosphorus doping modifies the band structure and introduces localized states that tune the photoluminescence and enhance photocatalytic performance. In CQDs and GQDs, heteroatom doping is particularly effective for controlling PL emission and introducing specific functionalities. For instance, N- and S-co-doping generates synergistic effects, improving the quantum yield and introducing red-shifted emission owing to electron-donor–acceptor interactions [60]. The interaction of CBNs with other materials, metals, metal oxides, and polymers creates hybrid interfaces that combine multiple functionalities. Anchoring metal nanoparticles (*e.g.,* Pt, Au) onto graphene or CNTs enhances the catalytic efficiency owing to synergistic charge transfer. Similarly, CQD–semiconductor composites (e.g., CQD/$TiO_2$) show enhanced photocatalytic and photovoltaic performances through effective electron injection from CQDs to $TiO_2$ [61]. Surface modification also improves compatibility with polymer matrices, allowing uniform dispersion and improved mechanical and electrical performance in the composites. Functionalization with carboxyl or amine groups facilitates covalent bonding with polymer chains, forming robust networks. Surface chemistry governs not only device performance, but also environmental and biological interactions. Hydrophilic functional groups improve the dispersibility in water and reduce cytotoxicity, making CQDs and GQDs promising for bioimaging and drug delivery. Conversely, hydrophobic or graphitic surfaces tend to aggregate and interact with cell membranes, necessitating appropriate surface design for safe biomedical use [62]. Doping and surface functionalization can modulate the bandgap, carrier type, and mobility. Substitutional doping introduces mid-gap states or shifts the Fermi level in graphene. In CNTs, dopants can switch semiconducting tubes to metallic tubes or vice versa. In CQDs, doping changes the HOMO–LUMO separation and introduces trap-assisted transitions responsible for the tunable PL. Such precise control allows tailoring electronic properties for specific applications, such as n-type CQDs for solar cells or p-type CQDs for whole transport layers. The fundamental structure and properties of carbon-based nanomaterials derive from the delicate interplay between atomic arrangement, bonding hybridization, and nanoscale phenomena [63-68]. Graphene offers high electrical and thermal conductivities, as well as exceptional mechanical strength. CNTs provide tunable electronic structure and flexibility. The CQD and GQDs exhibit quantum confinement and remarkable optical activity. The transition from extended $sp^2$ lattices (graphene) to confined quantum structures demonstrates how dimensionality controls the behavior from ballistic conduction to discrete luminescence.

Moreover, surface chemistry and doping offer additional advantages for property optimization

**Table 2.** Surface chemistry, functional groups, and doping effects in carbon-based nanomaterials

| Carbon nanomaterial | Key surface functional groups | Functionalisation techniques | Doping elements/ Methods | Resulting effects on properties | Representative applications | Ref. |
|---|---|---|---|---|---|---|
| Graphene / GO / rGO | –OH, –COOH, –C=O, epoxy groups, and hydroxyl groups | Chemical oxidation (Hummers method), plasma treatment, salinization, covalent coupling, π–π stacking, and electrochemical functionalisation | N, B, S, P, F doping via CVD, thermal annealing, plasma doping, and solvothermal reaction | Enhanced hydrophilicity, tenable bandgap, improved catalytic activity, increased dispersibility, and modified electrical conductivity | Energy storage, catalysis, membranes, sensors, and biomedical devices | [64] |
| Carbon nanotubes (SWCNTs/MWCNTs) | –COOH, –OH, –$SO_3H$, and amine groups | Acid treatment, defect engineering, fluorination, polymer wrapping, end-tipping, and diazonium chemistry | N, B, P, and S doping via arc discharge, CVD, ion implantation, and thermal treatment | Improved electron mobility, enhanced chemical reactivity, increased mechanical strength, and controlled conductivity (n-type/p-type) | Electronics, nanocomposites, drug delivery, and hydrogen storage | [65] |
| Carbon quantum dots | –OH, –COOH, amide, and amino groups | Hydrothermal/solvothermal modification, surface passivation (PEG, PEI), and microwave-assisted functionalisation | N, S, P, and B doping via bottom-up synthesis, and precursor tuning | Increased photoluminescence, tenable emission, improved quantum yield, and better biocompatibility | Bioimaging, sensing, optoelectronics, and photocatalysis | [66] |
| Graphene quantum dots | –OH, –COOH, epoxy, and amine groups | Oxidative cutting, surface passivation, ligand exchange, and polymer grafting | N, B, S, and Cl doping through hydrothermal treatment, and heteroatom precursors | Enhanced optical absorption, tenable PL (colour), improved catalytic capability, and bandgap modulation | LED devices, photodetectors, biosensors, and drug carriers | [26] |
| Fullerenes (C60, C70) | Addition of –OH, –COOH, epoxide, azide, or amine groups | Cycloaddition reactions, radical addition, nucleophilic addition, and polymer grafting | N, S, metal-doping through chemical modification, and intercalation | Increased solubility, improved electron affinity, and modified optical behaviour | Organic photovoltaics, superconductors, drug delivery, and photodynamic therapy | [67] |
| Hybrid & composite carbon nanomaterials | Mixed functional groups depending on components (metal oxides, polymers, and 2D materials) | *In situ* hybridisation, sol–gel method, layer-by-layer assembly, and grafting-to/grafting-from polymerisation | Multi-element doping (*N–S*, B–*N*, *N–P* systems) via high-temperature annealing, and solvothermal methods | Synergistic catalytic performance, tailored electronic structure, improved stability, and multifunctionality | Batteries, fuel cells, supercapacitors, and environmental remediation | [68] |

enabling multifunctional applications in electronics, photonics, catalysis, and biomedicine. A deep understanding of these fundamental aspects provides a scientific foundation for the rational design of next-generation carbon nanomaterials and hybrid architectures, driving progress toward sustainable energy technologies, advanced sensing, and quantum materials in the future [69]. Building on the structure–property relationships discussed above, the following section outlines the synthesis strategies employed to tailor the dimensionality, defects, and surface chemistry of carbon-based nanomaterials.

## 4. Synthesis Methods

The synthesis of carbon-based nanomaterials has undergone a remarkable evolution over the past three decades, driven by the need to tailor their structural, electronic, and optical properties for advanced applications. Due to their $sp^2$ and $sp^3$ hybridization flexibility, carbon materials can form diverse nanostructures, including one-dimensional nanotubes, two-dimensional graphene sheets, and zero-dimensional quantum dots. Each form requires distinct synthetic routes that influence the resulting morphology, crystallinity, defect density, and surface chemistry. This section provides a comprehensive overview of the most significant synthesis methods for graphene, carbon nanotubes, and carbon quantum dots (CQDs/GQDs), as well as emerging approaches for composite and functionalized carbon nanostructures [70].

### *4.1. Graphene production: exfoliation, chemical vapor deposition, and reduction of graphene oxide*

Graphene the archetype of 2D nanomaterials, is a single layer of carbon atoms arranged in a hexagonal lattice. Its synthesis methods can be broadly classified into top-down (breaking bulk graphite into single layers) and bottom-up (building graphene sheets atom by atom) approaches [71]. Liquid-phase exfoliation (LPE) enables scalable production by dispersing graphite in solvents such as N-methyl-2-pyrrolidone (NMP) or dimethylformamide (DMF) and applying ultrasonication. The ultrasonic energy separates graphite layers through cavitation and shear forces. The resultant dispersion can be centrifuged to collect monolayer or few-layer graphene. The efficiency of LPE depends on solvent surface energy matching with graphene (~40 $mJ/m^2$). Surfactant-assisted exfoliation using sodium cholate or SDS further improves yield and stability of graphene dispersions in water. However, LPE often produces graphene flakes with limited lateral size (100–1,000 nm) and residual defects, making it less ideal for high-performance electronic applications [72]. The CVD method is the most promising large-scale technique for producing high-quality graphene films. In this process, hydrocarbon precursors such as methane, ethylene, or acetylene are decomposed at high temperatures (900–1,100 °C) on transition metal substrates like copper or nickel. The metal surface catalyses the decomposition and facilitates carbon diffusion, leading to the nucleation of graphene layers. The growth mechanism depends on the solubility of carbon in the substrate. For instance, on Cu, which has low carbon solubility, a surface-mediated growth mechanism yields monolayer graphene [73]. Conversely, Ni supports precipitation growth, often producing multilayer graphene. After growth, the graphene film is transferred to target substrates ($SiO_2$, glass, and polymers) using polymer-assisted etching of the metal catalyst.

CVD-grown graphene exhibits high crystallinity, excellent conductivity (>$10^6$ S/m), and large domain size. Modifications such as plasma-enhanced CVD (PECVD) and low-pressure CVD (LPCVD) allow control over thickness, doping, and defect density. Challenges remain in achieving defect-free transfer and uniform large-area growth for industrial applications. Another cost-effective route involves the, which itself is produced by oxidizing graphite using the Hummers or modified Hummer's method. GO contains abundant oxygenated functional groups (epoxy, hydroxyl, and carboxyl) that

disrupt the π-conjugated network, rendering it hydrophilic and easily dispersible in water. The reduction of GO chemically (using hydrazine, ascorbic acid, or $NaBH_4$), thermally (above 800 °C), or electrochemically restores the partial conductivity and graphitic domains. The resulting material is not as pristine as CVD graphene, but offers tenable properties, ease of processing, and abundant surface functional groups that are beneficial for composites, sensors, and catalysis. Recent advances include electrochemical exfoliation, in which a graphite electrode is anodically or cathodically exfoliated in aqueous electrolytes to produce graphene sheets rapidly. This approach combines scalability, low cost, and eco-friendliness [74]. Moreover, biomass-derived graphene using natural precursors, such as sugar, cellulose, or lignin pyrolysis, represents a sustainable route for graphene production, aligned with green chemistry principles.

### *4.2. Carbon nanotube synthesis: arc-discharge, laser ablation, CVD, and growth mechanisms*

Carbon nanotubes, discovered in 1991, are cylindrical structures composed of rolled graphene sheets. They can be single-walled (SWCNTs) or multi-walled (MWCNTs) with diameters ranging from 0.7 nm to tens of nanometers. The synthesis method determines chirality, purity, and yield. The arc-discharge method was among the earliest techniques used for CNT production. This involves generating an electric arc between two graphite electrodes in an inert gas atmosphere (He or Ar) at low pressure. The high temperature (~4,000 °C) vaporizes carbon from the anode, and the vapor condenses to form CNTs on the cathode. This method yielded highly crystalline CNTs with few structural defects. Metal catalysts, such as Fe, Ni, and Co, are often incorporated to promote SWCNT formation. However, this process also produces amorphous carbon and soot, requiring extensive purification using acid treatments or filtration. Moreover, arc discharge offers limited control over tube diameter and alignment, restricting its large-scale applicability [75]. In the laser ablation method, a high-power laser is used to vaporize a graphite target containing transition metal catalysts under inert gas at ~1,200 °C. Carbon vapor condenses on a cooler collector to form CNTs. This technique yielded high-purity SWCNTs with narrow diameter distributions. The laser parameters, power, pulse duration, and target composition control nanotube morphology. Despite the production of high-quality CNTs, laser ablation is energy intensive and costly, making it less favorable for commercial production. This remains valuable for fundamental studies, where uniformity is crucial. The chemical vapor deposition technique dominates large-scale CNT synthesis. In this process, hydrocarbons (methane, acetylene, and ethanol) are decomposed over metal catalysts (Fe, Co, and Ni) supported on substrates such as $SiO_2$, $Al_2O_3$, or MgO at 600–900 °C. The catalyst particles act as nucleation centres, where carbon atoms dissolve, diffuse, and precipitate as nanotubes[76]. CVD allows excellent control over tube length, diameter, and alignment by adjusting the temperature, gas flow, and catalyst size. Variants include the standard thermal CVD method for vertically aligned CNT arrays. Plasma-enhanced CVD (PECVD) uses plasma to enable low-temperature growth and control alignment. Floating catalyst CVD involves injecting catalyst precursors (*e.g.,* ferrocene) directly into the gas phase, which is suitable for continuous CNT fibre production. The growth mechanism involves either base growth or a tip-growth model. During base growth, the catalyst remains anchored to the substrate while CNTs grow upward; during tip growth, the catalyst lifts off as the CNT elongates. CVD offers scalability, tunability, and compatibility with the device integration. Nevertheless, challenges, such as chirality control, purity, and uniformity, remain under active research. Recent advances have included aerosol-assisted CVD for continuous CNT synthesis and biogenic precursors (*e.g.,* ethanol and plant oils) as eco-friendly carbon sources. Additionally, template-assisted growth using nanoporous alumina or zeolites enables diameter and orientation control, thereby expanding the applicability of CNTs in electronics and membranes [77].

### *4.3. Quantum dots (CQDs, GQDs): top-down vs bottom-up approaches; size control; doping; and surface modification*

Carbon quantum dots and graphene quantum dots are zero-dimensional nanostructures (<10 nm) exhibiting unique photoluminescence due to quantum confinement and edge effects. Their synthetic approaches fall into two major categories: top-down (fragmentation of bulk carbon materials) and bottom-up (molecular assembly). Top-down methods involve cutting larger carbon structures (graphite, graphene, carbon fibres, and soot) into nanoscale dots via physical or chemical means. Acid oxidation is the most common process, where precursors are treated with strong acids ($H_2SO_4$/$HNO_3$) to cleave carbon bonds and introduce oxygenated groups that improve water solubility and fluorescence [78]. The electrochemical oxidation of graphite or graphene electrodes in neutral electrolytes offers a greener alternative, yielding size-controlled GQDs. Laser ablation and arc discharge have also been used, although they require sophisticated equipment. Top-down methods offer simplicity and high yield, but often produce QDs with broad size distributions and surface defects, necessitating post-synthesis purification or passivation. Bottom-up synthesis involves the carbonization of small organic molecules or polymer precursors through thermal, hydrothermal, or microwave-assisted reactions. Common precursors include citric acid, glucose, urea, and polyethylene glycol [79]. Hydrothermal/solvothermal synthesis: organic molecules were heated (150–250 °C) in sealed autoclaves, triggering dehydration and carbonization into nanodots. The reaction time and pH influenced the size and surface states of the QDs. Microwave-assisted synthesis: provides rapid and uniform heating, drastically reducing reaction times (minutes instead of hours). Pyrolytic methods: The high-temperature decomposition of carbon-rich precursors, such as citric acid, yields luminescent CQDs. Bottom-up routes allow precise control of composition and doping [80]. CQDs (using amine precursors) show enhanced PL quantum yield and electron-donating behavior, whereas S or P-doped CQDs exhibit tenable emission and catalytic activity.

The optical properties of QDs depend critically on their particle size, edge structure, and surface chemistry. Size control was achieved by adjusting the precursor concentration, reaction time, and temperature. Smaller QDs (<5 nm) show blue-shifted emission owing to stronger quantum confinement. Surface passivation via organic ligands (polyethyleneimine, PEG, and amines) reduces the surface traps and enhances photoluminescence. Functionalization also enables bioconjugation in bioimaging and sensing applications. Heteroatom doping introduces additional electronic states that alter the bandgap and emission behavior. Nitrogen doping enhances the PL intensity and electron mobility. Sulfur or phosphorus doping modifies the redox potential and catalytic properties. Co-doping creates synergistic effects that improve optical and electrochemical characteristics. These engineered QDs have emerged as efficient materials for LEDs, sensors, photocatalysis, and bioimaging [81]. **Figure 3** illustrates the two primary synthetic pathways for the generation of carbon quantum dots. The top-down approach involves breaking down bulk carbon precursors, such as carbon black, graphite oxide, and carbon nanotubes, through energy-driven transformation and oxidative processes. The subsequent surface passivation and reduction steps yield nanoscale carbon quantum dots. The bottom-up approach starts with molecular precursors, such as polycyclic aromatic hydrocarbons, which undergo ionization, formation of reactive species (ions, radicals, and electrons), and condensation to form carbon clusters. This schematic highlights the key reaction stages and precursor types that enable controlled CQD synthesis for diverse applications in sensing, imaging, and nanomedicine.

#### *Synthesis routes dictate final dot properties*

The attributes of carbon quantum dots are determined through the method of synthesis as illustrated in the synthesis routes in **Figure 3** by

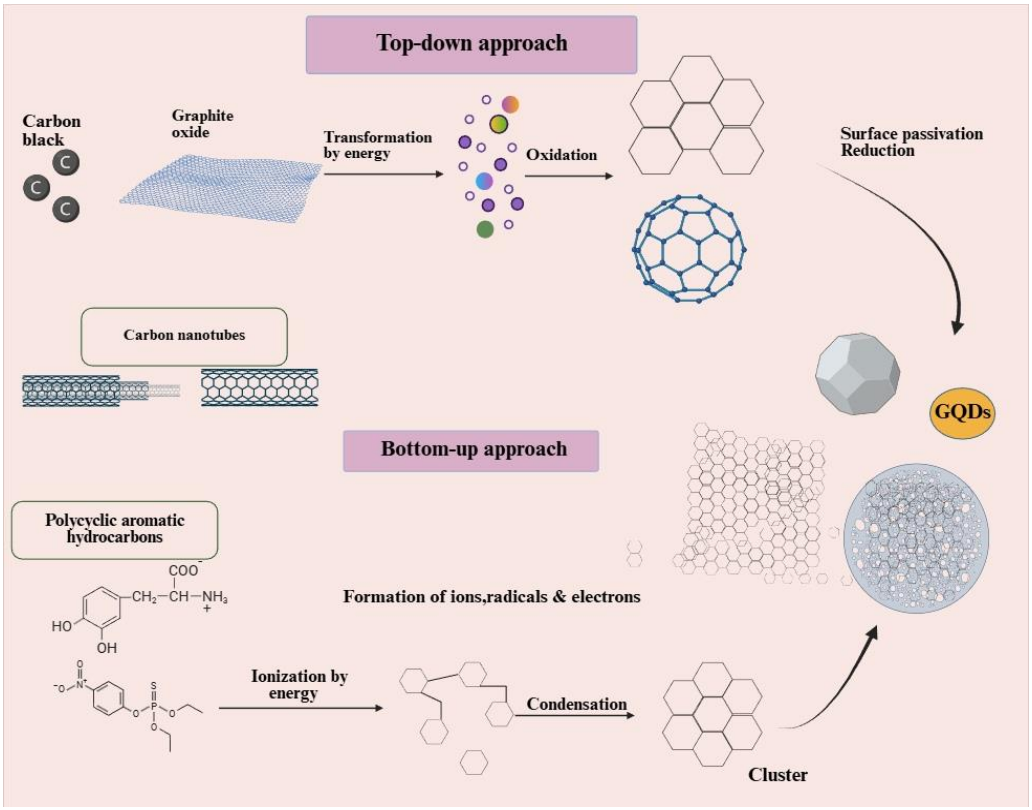


**Figure 3.** Synthesis strategies of carbon quantum dots: top-down and bottom-up approaches

manipulating the size, crystallinity, defect density, and surface chemistry of the final product. In the top-down synthesis route, extreme fragmentation of a larger bulk carbon precursor either by oxidation or through some high-energy pathology forms a large quantity of edge defects along with oxygenated functional groups on the surface, all of which result in non-uniformity of size, and therefore, the resulting photoluminescence is dominated by surface defect states. In contrast, the bottom-up synthesis route uses a molecular precursor as the starting point and builds from there by way of controlled condensation and carbonization of the resulting compounds, which allows for greater uniformity of size, tunable capacity for doping, and passivated surfaces, thereby producing carbon quantum dots that exhibit long-range and more stable photoluminescence compared to those produced via the top-down route. Ultimately, the synthesis method fundamentally dictates the structural characteristics of the carbon quantum dots, which in turn dictate their electronic and optical behaviors.

### *4.4. Composite synthesis and functionalization*

The integration of carbon nanomaterials into composite structures enhances their mechanical strength, stability, and multifunctionality. Combining graphene, CNTs, or QDs with metals, metal oxides, or polymers leads to synergistic effects arising from the interfacial interactions. Hybrid composites are synthesized via *in situ* chemical growth, sol–gel processing, or electrophoretic deposition. For instance, graphene–metal oxide composites (*e.g.,* graphene $TiO_2$) show enhanced photocatalytic activity due to charge separation facilitated by the conductivity of graphene. Similarly, CNT polymer composites display superior mechanical flexibility and electrical conductivity and are applicable in flexible electronics and energy devices. CQDs or GQDs incorporated with graphene or CNTs yield hybrid nanostructures

with high surface areas and photoluminescence. Such composites are synthesized via solution blending, electrostatic assembly, or hydrothermal methods. For example, GQD graphene composites improve charge transport in solar cells, whereas CQD CNT hybrids enhance the sensitivity of electrochemical sensors. Functionalization, either covalent (via carboxyl or amine linkages) or non-covalent (π–π stacking, van der Waals interactions), is crucial for dispersion, compatibility, and targeted applications. Covalent functionalization introduces chemical stability but can disrupt conjugation. Non-covalent modification preserves the electrical properties while offering versatility for biomolecular attachment. Emerging techniques, such as plasma treatment, click chemistry, and supramolecular assembly, provide new routes for controlled functionalization, which are essential for biomedical and catalytic applications [82]. The composite synthesis and functionalization of the carbon-based nanomaterials are listed in **Table 3**. To verify the effectiveness of these synthesis routes and correlate structural features with functional performance, comprehensive characterization techniques are essential.

**Table 3.** Composite synthesis and functionalisation of carbon-based nanomaterials

| Composite type | Carbon component(s) | Synthesis / Fabrication techniques | Functionalisation strategies | Enhanced properties achieved | Representative applications | Ref. |
|---|---|---|---|---|---|---|
| Carbon–Polymer Composites | Graphene, CNTs, CQDs, and GQDs | Solution mixing, melt blending, *insitu* polymerization, electrospinning, and layer-by-layer assembly | Surface oxidation, polymer grafting, covalent coupling (amidation, esterification), π–π stacking, and surfactant-assisted dispersion | Improved mechanical strength, enhanced electrical conductivity, increased thermal stability, and controlled optical emission | Flexible electronics, conductive films, wear-resistant coatings, biomedical scaffolds, and drug delivery | [68] |
| Carbon–Metal Nanocomposites | Graphene, CNTs, CQDs | Electrochemical deposition, hydrothermal growth, solvothermal reaction, microwave-assisted synthesis, and CVD metal decoration | Metal nanoparticle anchoring via heteroatom doping, thiol/amine functionalisation, and electrostatic interaction | Enhanced catalytic activity, improved charge transport, plasmonic effects, and magnetic behaviour | Fuel cells, electrocatalysis, photocatalysis, biosensors, and magnetic imaging | [83] |
| Carbon–Metal Oxide Composites | Graphene, rGO, and CNTs | Sol–gel method, hydrothermal/solvothermal synthesis, atomic layer deposition (ALD), and template-assisted growth | Oxygen functional groups for anchoring, surface hydroxylation, and heteroatom doping (N, S, and B) | High surface area, increased redox activity, enhanced electron mobility, and improved cycle stability | Supercapacitors, lithium-ion batteries, gas sensors, and environmental remediation | [84] |

| Composite type | Carbon component(s) | Synthesis / Fabrication techniques | Functionalisation Strategies | Enhanced Properties Achieved | Representative Applications | Ref. |
|---|---|---|---|---|---|---|
| Carbon–Ceramic Composites | Graphene and CNTs | Spark plasma sintering, hot pressing, sol–gel processing, slurry infiltration, and thermal spraying | Surface roughening, silane coupling agents, and ceramic nanoparticle embedding | High-temperature stability, improved fracture toughness, and lightweight structural integrity | Aerospace parts, thermal barrier coatings, and friction materials | [85] |
| Carbon–Biomolecule/Biopolymer Composites | CQDs, GQDs, GO, and CNTs | Self-assembly, aqueous blending, freeze-drying, hydrogel formation, and bioconjugation reactions | PEGylation, peptide/protein conjugation, DNA immobilization, and carboxyl/amino-functionalisation | Increased biocompatibility, targeted delivery, enhanced fluorescence, and controlled drug release | Tissue engineering, bioimaging, targeted therapeutics, and biosensors | [86] |
| Carbon–2D Material Hybrids | Graphene + $MoS_2$, $WS_2$, h-BN, and MXenes | Liquid-phase exfoliation, van der Waals stacking, electrostatic assembly, and interfacial growth | Heterostructure engineering, doping, and surface passivation | Synergistic electron transfer, tenable bandgap, and high catalytic and sensing performance | Photodetectors, transistors, heterogeneous catalysis, and multi-functional coatings | [87] |
| Carbon-Based Multicomponent Ternary/Quater | CNT–graphene–metal oxides, Graphene– and polymer–metal | Layered assembly, hybrid sol–gel, multi-step hydrothermal synthesis, and hierarchical templating | Stepwise functionalisation, multi-doping, and interface engineering | Ultra-high conductivity, enhanced structural stability, and synergistic catalytic/optical performance | Energy storage systems, electromagnetic shielding, and advanced photonic devices | [88] |

## 5. Characterization Techniques

Characterization plays a central role in understanding the structure, composition, optical behavior, and surface chemistry of carbon-based nanomaterials. Because materials such as graphene, carbon nanotubes, carbon quantum dots, graphene quantum dots, fullerenes, and hybrid structures differ widely in dimensionality, defects, and surface functional groups, no single technique can reveal their properties. Instead, a combination of microscopy, spectroscopy, crystallographic analysis, and electrochemical tools is required to gain a comprehensive understanding. Over the last two decades, the development of advanced characterization methods has significantly improved researchers' ability to control material quality, optimize synthesis, and expand the application potential of nanomaterials. This section provides a detailed overview of the major characterization approaches, highlighting their principles, strengths, limitations, and relevance to carbon-based nanostructures [89].

### *5.1. Structural characterization: TEM, SEM, AFM, XRD, and Raman spectroscopy*

Structural characterization plays a crucial role in understanding the morphology, crystallinity, defect density, and atomic-level arrangement of carbon-based nanomaterials ranging from

graphene and carbon nanotubes to carbon and graphene quantum dots (CQD/GQD). Transmission electron microscopy (TEM) is one of the most powerful tools for visualizing nanostructures on the atomic scale. In graphene, TEM reveals layer numbers, grain boundaries, and edge defects, whereas in CNTs, it helps determine the tube diameter, wall number, and chirality. High-resolution TEM (HRTEM) further enables the direct observation of lattice fringes and crystalline domains in quantum dots. Scanning electron microscopy (SEM), although lower in resolution than TEM, provides essential information on surface morphology, particle aggregation, film uniformity, and microstructural features, which are particularly important for CNT mats, graphene films, and composite nanomaterials [90]. Atomic force microscopy (AFM) offers nanoscale topographical imaging and is especially valuable for measuring the thickness of graphene layers, identifying the surface roughness, and analyzing the size distribution of CQDs and GQDs when deposited on substrates. X-ray diffraction (XRD) is widely used for evaluating crystallinity, interlayer spacing, and graphitic ordering. The (002) peak of graphene and graphite derivatives indicates the degree of exfoliation or reduction, while in CNTs and carbon dots, XRD helps to determine amorphous versus crystalline carbon domains [91]. Raman spectroscopy is one of the most characteristic tools for carbon materials owing to its sensitivity to disorder, defects, strain, and electronic structure. The D, G, and 2D bands provide insight into graphitization, $sp^2$ hybridization, defect density, and layer number. In CQDs and GQDs, Raman spectra help to differentiate between graphitic cores and amorphous carbon regions. Collectively, TEM, SEM, AFM, XRD, and Raman spectroscopy form a complementary toolkit that allows researchers to correlate structural features with functional properties, enabling more precise control over the synthesis methods and performance optimization across carbon-based nanomaterials [92].

### *5.2. Optical/electronic characterization: UV-Vis, photoluminescence, and electrochemical methods*

Optical and electronic characterization techniques are crucial for evaluating the light absorption, emission behavior, and charge transfer properties of carbon-based nanomaterials such as graphene, carbon nanotubes, carbon quantum dots, and graphene quantum dots. UV–Visible (UV–Vis) spectroscopy is commonly used to analyze electronic transitions and band structure features. Graphene and its derivatives exhibit characteristic π–π* transitions associated with $sp^2$ carbon networks, whereas CNTs show absorption features related to van Hove singularities. CQDs and GQDs display broad UV–Vis absorption extending into the visible region owing to quantum confinement and surface states [93- 95].

Photoluminescence spectroscopy provides key insights into the emission properties of CQDs and GQDs, which arise from size-dependent quantum confinement, edge effects, and surface functional groups. Variations in the emission wavelength and intensity reflect the particle size, surface passivation, and defect states, making PL analysis essential for optoelectronic and bioimaging applications [33, 96].

Electrochemical techniques, such as cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), were employed to investigate the charge-transfer behavior, redox activity, and conductivity. Graphene and CNTs exhibit fast electron-transfer kinetics, whereas CQDs and GQDs enhance the electrochemical performance when integrated into composite electrodes. Together, these techniques provide a comprehensive assessment of the optical and electronic functionalities of carbon-based nanomaterials [97,98]. Despite the advances in characterization, significant challenges remain in translating these materials from laboratory-scale studies to reliable and scalable real-world applications.

## 6. Structure Property Relationships in Carbon-Based Quantum Dots

Optical properties are determined by the number of and types of defects introduced into the GQD during its production. A common method of producing GQDs is through a chemical oxidative method, *i.e.,* using strong oxidants like nitric acid or sulphuric acid, to sever extended graphene sheets into small segments of nanometre size. This is achieved by the method of unselective bond cleavage for the introduction of many edge defects, oxygenated functional groups, and lattice defects [99]. The result of this is that the $sp^2$ carbon bonding is disrupted by radicals forming along the edges of the sheets where the σ bonds have been broken, generating edge defects on the surface of the sheets and creating a deficiency in π conjugation, resulting in localised electronic excitations within the energy gap of the band width of the GQD from which the dominant radiative recombination is generated [100]. The presence of defect-induced electronic states or excitations affects the nature of excitation dependent photoluminescence, broadening of emission spectra, and red-shifting of emission compared to 'more crystallised' GQDs; it is oftentimes the case that photoluminescence is primarily driven by the surface and edge defect states as opposed to quantum confinement effects as in the case of more crystallised materials [101]. The production of GQDs through 'bottom-up' molecular carbonization processes will typically yield a lower quantity of structural defects and fewer non-ideal edge terminations, resulting in a more confined emission breadth with an increased photoluminescent quantum yield, compared to the photoluminescent quantum yields obtained from 'top-down' synthesis. This example demonstrates how the use of a specific method of synthesis embeds the defect chemistry of the GQD and thus influences the photophysical characteristics of the emitted light [102].

### *6.1. Trade-offs between electrical conductivity and photoluminescence in carbon-based nanomaterials for sensor applications*

In different parts of this document, there are many different mentions of various types of sensors. The choice of the nanomaterial that will be used for your sensor application is important in terms of size and shape. A two-dimensional $sp^2$-carbon graphite lattice, such as that of graphene, is a very good conductor of electricity. Because it has a very low intrinsic noise level, it can help us to detect the presence of an analyte by sensing perturbations. In terms of low noise levels and efficient transduction layers, CQDs are noteworthy. CQDs are made of amorphous carbon, but have many surface functional groups [13]. When combined together, CQDs can be effectively used to optically sense many different types of analytes. GQDs are produced from partially graphitic carbon using chemical and physical processes. Thus, GQDs provide a good trade-off between the two-dimensional ($sp^2$) structure of graphene and the low intrinsic noise levels of CQDs, which provide the best of both worlds.

These differences highlight an inherent trade-off between structure and property concerning composites [103]. In other words, a material that is designed for maximum electrical sensitivity typically lacks optical activity; conversely, a material with a high degree of luminescence usually does not perform well electrically. As a result, many modern sensor designs use hybrids composed of graphene, which is an excellent conductor, and either CQDs or GQDs, which are photoluminescent. Hybridization allows for the creation of 'multifunctional sensors,' enabling greater sensitivity and versatility in operation [104].

## 7. Challenges, Limitations, and Future Perspectives

Carbon-based nanomaterials, including graphene, carbon nanotubes, fullerenes, carbon

quantum dots, and graphene quantum dots, have emerged as transformative materials because of their exceptional electronic, thermal, optical, and mechanical properties. Despite significant breakthroughs, broad industrial adoption remains limited. Translating laboratory performance into real-world applications requires overcoming a complex series of fundamental, technological, economic, and environmental challenges. This section provides a detailed analysis of the key obstacles and outlines possible future research directions to ensure sustainable and scalable development of carbon-based nanomaterial technologies.

### *7.1. Scalability, reproducibility, and cost-effectiveness of synthesis*

#### *7.1.1. Limitations in large-scale production technologies*

One of the most persistent challenges is the difficulty in scaling up the synthesis process while preserving the quality and uniformity of the materials. Techniques such as chemical vapor deposition, laser ablation, and arc discharge can yield high-quality graphene and CNTs; however, they require high temperatures, controlled atmospheres, and expensive catalysts. These factors make industrial-scale production costly and energy intensive. For graphene, large-area growth through CVD often leads to heterogeneous grain sizes, grain boundaries, wrinkles, and defects that significantly alter electrical conductivity. Similarly, CNT synthesis frequently suffers from undesired variations in the chirality, diameter, length, and wall number. Such inconsistencies limit the use of CNTs in electronics, where the precise tuning of semiconducting versus metallic behavior is essential.

#### *7.1.2. Reproducibility and batch-to-batch consistency*

Reproducibility of the properties across different batches is another major concern. Small variations in the precursor purity, catalyst composition, deposition times, and furnace parameters often lead to measurable differences in the material quality. For example, CNTs may exhibit different chiralitites or impurity levels, graphene grown under slightly different conditions may have variations in defect density. CQDs synthesized by top-down methods often show wide size distributions, affecting their optical bandgaps and quantum yields and hindering their commercialization in the electronic and biomedical sectors, where reliability and standardization are mandatory.

#### *7.1.3. Purification, separation, and defect control*

Even after the synthesis, many carbon nanomaterials require extensive purification. CNTs commonly contain metal catalyst residues and amorphous carbon that must be removed for biological or electronic applications. The processes used for acid treatment, ultrasonication, and high-temperature oxidation frequently introduce further defects, reducing the material performance. Controlling the defect density in graphene is challenging because some defects are unintentionally introduced during transfer from substrates, mechanical handling, or chemical treatments. In quantum dots, achieving precise control over the size distribution is essential because the optical properties depend directly on quantum confinement. However, synthesis methods often produce polydisperse populations, necessitating additional separation steps, such as centrifugation, chromatography, or dialysis.

### *7.2. Stability, toxicity, and environmental and health concerns*

#### *7.2.1. Chemical and structural stability issues*

Carbon-based nanomaterials often exhibit limited stability under operational conditions: graphene is oxidized at high temperatures or in oxidative environments. CNTs may degrade under UV exposure or in biological fluids. CQDs and GQDs sometimes suffer from fluorescence quenching owing to aggregation or chemical reactions at their surfaces. Maintaining stability without sacrificing functionality is particularly

challenging for applications in sensors, catalysis, and biomedicine, where the environmental conditions may vary significantly.

#### *7.2.2. Interactions with biological systems and potential toxicity*

Although many carbon nanomaterials are considered to be relatively biocompatible, concerns persist regarding their cytotoxicity, biodistribution, and long-term accumulation. Key challenges include the presence of metal residues from catalysts that can cause oxidative stress in cells. Sharp structures (*e.g.,* CNTs) may induce inflammation or damage the cell membranes. Surface functional groups influence protein adsorption and immune response in complex ways. The long-term fate of nanomaterials in tissues, the blood, and organs is not fully understood. CQDs and GQDs are less toxic than heavy-metal quantum dots (such as CdSe); however, their surface chemistry can still affect cellular processes. In vivo studies remain limited, and standardized toxicological testing protocols are urgently needed.

#### *7.2.3. Environmental impact and waste management*

The increasing production of nanomaterials raises questions regarding their environmental footprint. Manufacturing processes generate chemical waste, including strong acids, solvents, and catalysts. Furthermore, the disposal of nanomaterial-containing electronic devices or biomedical products can introduce persistent nanoparticles into soil or water systems. The environmental behavior of carbon nanomaterials is complex and they may interact with organic matter, heavy metals, or microbes. They can undergo slow transformation or degradation, forming unknown byproducts. Their small size allows mobility in ecosystems, raising concerns regarding bioaccumulation. Therefore, sustainable production and safe disposal must become central considerations for future development.

### *7.3. Integration into devices and real-world systems*

#### *7.3.1. Challenges in device fabrication and material compatibility*

Even when high-quality carbon nanomaterials are available, their integration into functional devices is difficult. Their unique nanoscale characteristics often lead to challenges, such as poor adhesion to substrates, difficulty in controlling orientation and alignment, challenges in forming stable electrical contacts, aggregation during processing stages, and limited compatibility with existing microfabrication protocols. For graphene, transferring large-area sheets onto desired substrates without tearing, folding, or contamination remains problematic. CNTs require alignment for high-performance transistors or sensors; however, large-scale alignment still lacks precision and reproducibility.

#### *7.3.2. Interfacing with electronic and optical components*

Electronic devices require highly controlled and defect-free interfaces. Variations in the thickness, doping level, and contact resistance can drastically affect the performance. Specific issues include the zero bandgap of graphene, which limits its use in digital electronics without additional bandgap engineering. CNTs often contain mixtures of metallic and semiconducting tubes, which complicates their use in logic circuits. Quantum dots incorporated into LEDs or bioimaging systems must maintain a high quantum yield and stability under illumination. Engineering scalable integration strategies, such as printing, roll-to-roll manufacturing, directed assembly, and hybrid device architectures, remains a major area of ongoing research.

#### *7.3.3. Reliability, consistency, and long-term performance*

For real-world applications, the long-term performance of carbon nanomaterials must be predictable. CNT networks may undergo structural rearrangement under heat or humidity. CQDs may photobleach over time, which reduces their utility in optical applications. Composite materials often exhibit poor interfacial bonding or degradation. Reliability testing under operational conditions (*e.g.,* temperature, humidity, and mechanical cycling) is essential for understanding aging, degradation pathways, and performance losses.

### *7.4. Emerging directions: quantum materials, hybrid systems, multi-functional platforms, and computational modeling*

#### *7.4.1. Quantum materials and next-generation electronics*

Carbon nanomaterials are increasingly being studied for applications in quantum technologies that offer ballistic transport and tunable electronic properties for quantum Hall devices. CNTs have been explored for use in single-photon generation, qubits, and quantum sensors. GQDs and CQDs exhibit size-tunable band gaps and photoluminescence, making them attractive for quantum communication and bioimaging. However, the use of these materials in quantum devices requires unprecedented control over the purity, defect density, and surface state parameters, which are very challenging to regulate in bulk production. Future research must focus on atomic-precision synthesis and defect engineering strategies.

#### *7.4.2. Hybrid and composite systems*

To overcome the intrinsic limitations of individual materials, researchers are increasingly combining carbon nanomaterials with metals, polymers, semiconductors, and oxides. Hybrid systems can provide enhanced conductivity, enhanced mechanical strength, improved charge-transfer properties, and tunable optical and catalytic characteristics. Examples include graphene/metal oxide electrodes for batteries, CNT/polymer composites for flexible electronics, and CQD-decorated graphene sheets for photocatalysis. Despite their promise, hybrid systems pose new challenges for controlling interfaces, ensuring uniform dispersion, and maintaining long-term stability. The complexity of multicomponent structures also complicates their mass production.

#### *7.4.3. Multi-functional platforms*

Carbon nanomaterials are well suited for the development of multi-functional systems capable of performing several tasks simultaneously, such as sensing, energy conversion, and signal processing. For example, a graphene-based sensor can detect molecules while simultaneously harvesting energy from the environment. CQD systems can combine imaging, drug delivery, and therapeutic functions in a single nanosystem. CNT networks can act as both structural reinforcements and electrical pathways in the composite materials. Developing such platforms requires advanced engineering of the surface chemistry, functional groups, and device architectures. The challenge lies in achieving synergetic performance without compromising individual functionalities.

#### *7.4.4. Computational modeling and AI-driven materials discovery*

Modern computational tools offer unprecedented opportunities to accelerate research, and density functional theory (DFT) helps predict the electronic and optical properties. Molecular dynamics simulations guide the synthesis and processing steps. Machine-learning algorithms can optimize experimental parameters, predict toxicity, or design novel material structures. AI-driven automated laboratories may enable rapid screening of thousands of synthetic routes. Computational modeling will play an increasingly central role in bridging the gap

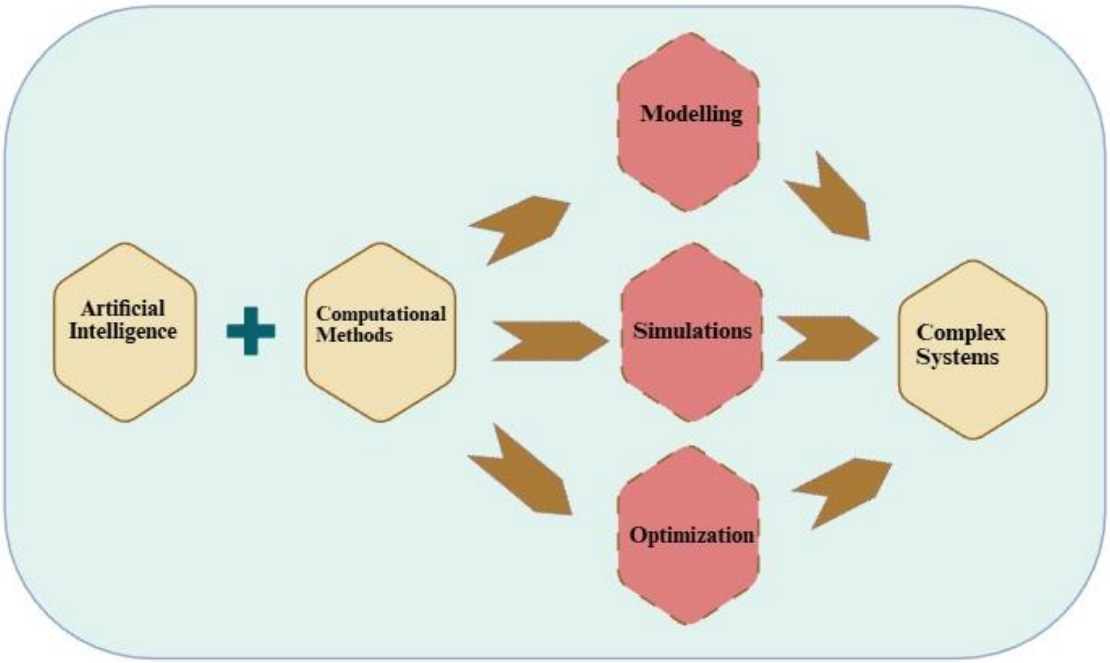


**Figure 4.** Integration of AI and computational methods for complex system analysis

between fundamental science and practical applications. However, the accurate modeling of defects, interfaces, and quantum behaviors remains a difficult task that requires further theoretical advances. The conceptual framework in **Figure 4** demonstrates how artificial intelligence (AI), combined with advanced computational methods enables the analysis and understanding of complex systems. The integration of AI tools with computational techniques drives three critical processes: modeling, simulations, and optimization. These interconnected processes support the study of highly dynamic and multifaceted systems, allowing researchers to predict behavior, refine system performance, and generate data-driven solutions.

## 8. Conclusion

This review highlights the fact that the properties and performance of carbon-based nanomaterials are strongly governed by dimensionality-dependent factors. For 0D carbon materials, such as CQDs and GQDs, surface chemistry, functional groups, and heteroatom doping are the dominant factors controlling the optoelectronic behavior, photoluminescence efficiency, and biocompatibility. In 1D CNTs, chirality, diameter, and defect density primarily dictate the electronic transport, optical transitions, and mechanical performance. For 2D graphene-based materials, the crystalline domain size, defect concentration, and interlayer interactions are the key parameters influencing conductivity, mechanical strength, and thermal transport. Across all dimensions, the interplay between $sp^2/sp^3$ hybridization, quantum confinement, and surface functionalization defines structure–property relationships. Despite substantial progress in synthesis and characterization, several critical challenges remain, particularly in achieving scalable, cost-effective, and reproducible production with precise control over the size, defects, and composition. Future research should prioritize green synthesis strategies, AI-assisted design and optimization, and improved stability and toxicity assessments to enable reliable industrial translation. From an application perspective, carbon-based

nanomaterials show the strongest potential in energy storage and conversion, optoelectronics, sensing, and biomedical technologies, where their tunable electronic, optical, and surface properties offer clear performance advantages. In particular, hybrid and composite architectures are expected to play a key role in overcoming the current material limitations and enabling multifunctional device platforms.

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## Conflict of Interest

There is no conflict of interest exists.

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