

Processing-Defined Nanodiamonds: Material-State Control for Reliable Function

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Abstract: Nanodiamonds have attracted increasing interest owing to their unique optical, spin, thermal and chemical properties, enabling emerging applications in quantum technologies, biomedical diagnostics, thermal management and electrochemical sensing. However, the reported performance of nanodiamonds varies considerably among studies because synthesis routes, purification processes, defect populations, surface chemistry and interfacial structures generate distinct material states. A processing-defined material-state perspective is proposed to understand how these coupled characteristics determine functional properties and application performance. This perspective highlights that nanodiamond functionality is not governed by isolated parameters, but by the coupled evolution of defects, surfaces and interfaces during processing. Representative applications demonstrate that different functions require distinct material-state configurations, involving trade-offs among spin coherence, fluorescence stability, interfacial heat transfer and charge-transfer behaviour. Achieving reliable nanodiamond technologies therefore requires application-oriented optimization, standardized material-state reporting and reproducible processing strategies. This framework provides a pathway toward rational design and scalable integration of nanodiamonds for advanced functional applications.

Keywords: nanodiamonds; processing-defined material state; defect engineering; surface and interface engineering; quantum sensing

1. Introduction

Nanodiamonds are a distinctive class of zero-dimensional (0D) carbon nanomaterials that combine the structural robustness of the sp³-bonded diamond lattice with the pronounced influence of nanoscale surfaces, defects and interfaces [1,2]. Their diamond cores provide chemical stability, photostability and a wide bandgap, whereas particle size, surface reconstruction and termination, impurity and defect populations, and the surrounding interfacial environment become increasingly important as the particle dimensions decrease [3,4]. These characteristics support functions including quantum sensing, fluorescence imaging and diagnostics, thermal transport in composites, and electrochemical interface modification [5,6]. Importantly, these functions are not determined by the diamond lattice alone, but by the specific particle, defect, surface and interfacial state established during formation and subsequent processing. Nanodiamonds should therefore be considered heterogeneous functional material systems rather than a single material class defined only by nanoscale size or synthetic origin.

Nanodiamonds have already been reviewed from several complementary perspectives. Recent reviews have addressed nanodiamond production, surface modification and physicochemical characterization [3], biomedical and theranostic applications [7–11], engineering and energy-related nanodiamond coatings [12], and fluorescent-



nanodiamond quantum and biosensing [13,14]. These studies provide increasingly comprehensive accounts of synthesis, functionalization, properties and application-specific developments. Notably, the most recent biomedical reviews have begun to integrate multiple stages from synthesis and surface functionalization to physicochemical properties, biological applications and safety evaluation [9–11]. However, these analyses are often organized within particular application domains or functional themes. A complementary need is to compare nanodiamonds across different origins and applications using complete processing history as the basis for defining a measurable, multidimensional material state. The present review therefore focuses on how processing sequences establish combinations of particle, structural, defect, surface and interfacial characteristics, how these states evolve during subsequent treatment, and how they determine application-specific functional performance and reporting requirements.

However, the term “nanodiamond” often conceals substantial materials heterogeneity. Common labels are themselves based on different criteria: “detonation” and “HPHT-derived” describe material origin or formation history, whereas “fluorescent nanodiamond” denotes a defect-enabled functional state. Such labels therefore identify only part of a material’s history or function and should not be interpreted as complete descriptions of its physicochemical state [15]. Materials grouped under these labels may all contain nanoscale diamond crystals, yet differ markedly in primary particle size and particle-size distribution [16], impurity background, defect-related lattice perturbation and colour-centre population [17], and surface chemistry and the associated spin environment [18]. Even nanodiamonds derived from the same parent material can retain substantial size polydispersity after milling and require subsequent fractionation to isolate more narrowly defined particle populations [16]. Likewise, defect engineering and surface processing can markedly alter the optical and spin properties of fluorescent nanodiamonds without changing their nominal material label. These differences are not secondary details. They determine whether nominally similar particles exhibit reproducible optical, spin, colloidal or interfacial behaviour under the intended operating conditions. Thus, nominal nanodiamond labels do not uniquely define either material identity or functional performance.

In this review, “processing history” refers to the ordered sequence of material formation and subsequent treatments, including purification, size reduction and fractionation, defect creation and annealing, surface reconstruction, functionalization, and final assembly or integration. We use “processing-defined material state” not to introduce a new set of material descriptors, but to denote the measurable joint configuration of particle and structural characteristics, impurity and defect populations, surface chemistry, and interfacial or assembly characteristics established at a particular stage of that processing history. “Functional properties” refer to the responses that emerge from this state, such as optical and spin stability, colloidal behaviour, charge-transfer characteristics or interfacial transport, whereas “application performance” denotes task-level outcomes measured under specified operating conditions, such as sensing sensitivity, detection limit, imaging reliability or effective composite thermal conductivity. The distinction is therefore sequential rather than terminological: processing history describes what has been done to the material, material state describes what the material has become, functional properties describe how that state behaves, and application performance describes how effectively it performs the intended task. This framework extends the conventional structure-property-application relationship by retaining processing provenance and processing sequence as explicit variables, thereby enabling nominally similar nanodiamonds reached through different processing pathways to be compared on the basis of their measured states rather than their labels alone.

This heterogeneity also explains why nanodiamond performance cannot be inferred directly from the properties of bulk diamond. At reduced dimensions, the high surface-to-volume ratio amplifies the influence of surface reconstruction, non-diamond carbon, adsorbates and nearby impurities, while functional defects become increasingly sensitive to their local chemical and magnetic environment. Here, we use “coupled evolution” in an operational sense: it does not imply a single universal microscopic interaction among defects, surfaces and interfaces, but rather that these state variables frequently change non-independently during processing and jointly influence functional behaviour. Reduced particle dimensions, for example, bring colour centres closer to the surface, where magnetic surface noise, charge fluctuations and lattice strain increasingly constrain spin relaxation and charge stability [19]. Surface processing provides a direct example of this non-independence. Oxidation and silica coating of fluorescent nanodiamonds altered surface functional groups and sp^2 -carbon content while increasing the NV longitudinal relaxation time from $320 \pm 9 \mu s$ to $1.00 \pm 0.06 ms$; modelling further showed that increasing shell thickness introduces a competing sensor-target separation penalty, with an optimum thickness on the order of 1 nm for the system studied [18]. Consistently, core-shell engineering has been shown to suppress deleterious surface states and improve NV spin coherence in individual nanodiamonds [20]. These examples show that processing acts on a multidimensional material state rather than on isolated descriptors. Optimizing defect density, surface chemistry or interfacial structure independently can therefore obscure trade-offs that emerge only when their combined evolution is considered.

Accordingly, this review focuses primarily on particulate nanodiamonds as zero-dimensional carbon materials and examines how their functional states are established and transformed through processing. Rather than providing an exhaustive catalogue of synthesis methods or applications, we organize the discussion around the sequence from material formation and post-processing to state evolution, functional properties and application performance. Representative examples from quantum sensing, fluorescence imaging and diagnostics, thermal transport and electrochemical sensing are used to illustrate how different application requirements impose distinct material-state constraints and processing trade-offs. Particular emphasis is placed on characterization, reporting and state traceability, which are essential for meaningful comparison and reproducibility across studies. The overall processing-state-function framework and the corresponding processing chain are summarized schematically in Figure 1.

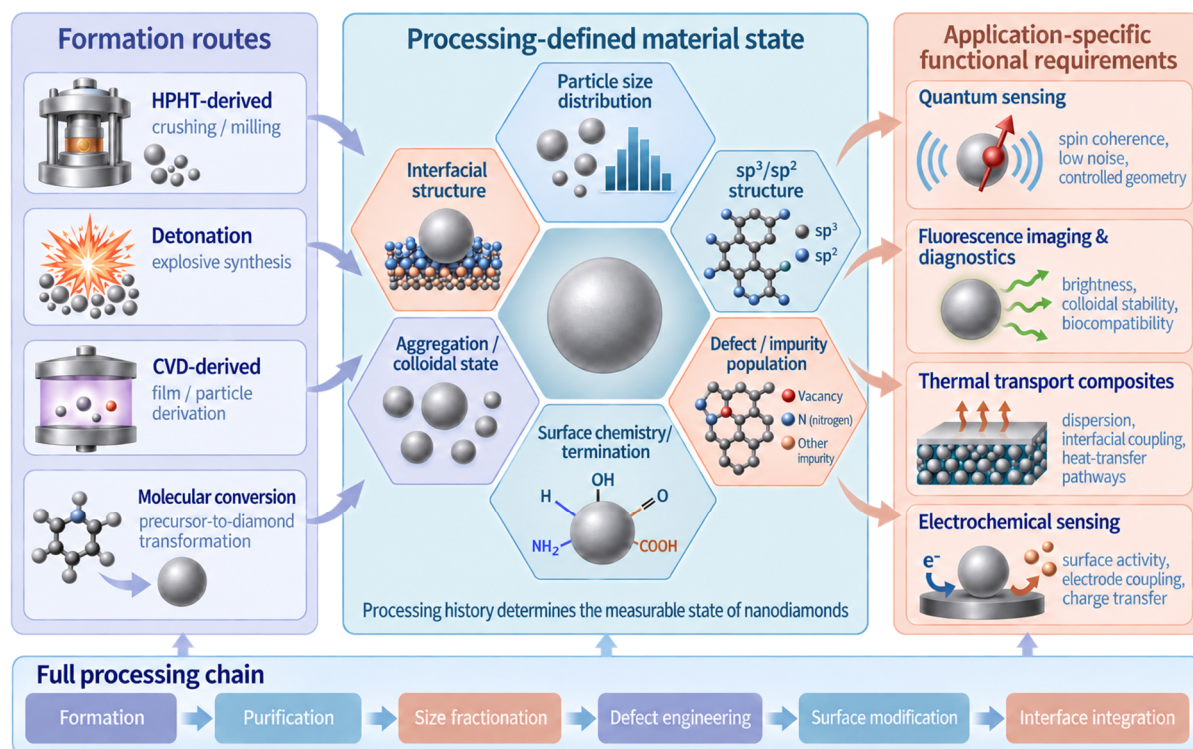


Figure 1. Processing-chain engineering of nanodiamonds.

2. Processing Routes and the Establishment of Initial Nanodiamond States

Nanodiamond formation routes establish the initial particle, structural, impurity and surface states on which subsequent processing acts. Rather than providing an exhaustive catalogue of synthesis methods, this section compares representative routes according to how the nanoscale diamond lattice is established: inheritance from pre-existing diamond through top-down size reduction, formation from condensed or molecular non-diamond carbon, or nucleation from reactive gas-phase carbon species. The comparison focuses on the initial material-state signatures established during formation, whereas purification, fractionation, defect engineering, surface reconstruction and functionalization are treated separately in Section 3. Table 1 summarizes the dominant formation variables, initial material states and principal downstream requirements of these routes.

Table 1. Representative nanodiamond formation routes and their initial-state characteristics.

Formation Logic	Representative Route/Processing Conditions	Initial-State Signature	Main Limitation	Refs.
Top-down derivation	- HPHT-derived milling - Size fractions ~10/25/35 nm	- Inherited core; polydisperse particles - Newly created surfaces	Size/surface control required	[16,21]
Rapid conversion	- Detonation - Aggregation detectable at ~0.1 μs	- Few-nm crystallites; formation-stage aggregation - Heterogeneous carbon/defects	Deaggregation/purification required	[22–24]

Table 1. Cont.

Formation Logic	Representative Route/Processing Conditions	Initial-State Signature	Main Limitation	Refs.
Rapid conversion	- Liquid-confined laser processing - Ethanol/fs laser or graphite/liquid-N₂	<5 nm particles - Route-dependent defect/optical state	Limited comparability	[25,26]
Rapid conversion	- Flash Joule heating - Ms-scale pulse, fluorine-assisted, ~1 s conversion	- Ultrafast formation - Pulse-dependent phase selection	Size/residual species/yield control	[27,28]
Precursor-directed formation	- Adamantane/nanographene 12–13 GPa, 1200–1300 °C or e-beam	2–5 nm particles - Precursor-guided size/surface/defects	Scale-up/recovery limited	[29–32]
Gas-phase nucleation	- HFCVD/H₂-CH₄ microplasma - Plasma chemistry/power	- Mixed carbon phases - Plasma-dependent nucleation	Phase/size/yield control immature	[33–35]

2.1. Top-Down Derivation from Pre-Existing Diamond

Top-down processing derives nanodiamonds from a pre-existing diamond lattice rather than nucleating diamond from a non-diamond carbon precursor. Parent crystals are reduced to nanoscale dimensions through mechanical fragmentation and milling. In this route, the term “HPHT-derived” identifies the origin of the parent diamond but does not fully define the resulting nanoparticle state. Crystal quality, isotope composition and impurity content are largely inherited from the parent crystal, whereas mechanical fragmentation establishes the particle-size distribution and generates new surfaces whose composition and structure may differ substantially from those of the parent crystal. Top-down processing therefore preserves important characteristics of the parent lattice while introducing a new particle population and surface state during nanosizing.

Achieving a narrowly defined nanoparticle state remains a central challenge for top-down nanodiamond production. Chang et al. emphasized that reliable preparation and isolation of ultrasmall nanodiamonds with simultaneously controlled size, surface composition and lattice defects remain difficult, motivating greater control over both formation and post-formation selection [21]. This limitation is directly illustrated by recent fractionation experiments. Recent work by Finas et al. showed that milled nanodiamonds originating from the same parent material could be separated into populations centred at approximately 10, 25 and 35 nm, illustrating that a common source label can contain substantially different particle populations [16]. Thus, the product of top-down derivation should be regarded as a particle population whose usable state is determined not only by the parent diamond and milling conditions, but also by the subsequent selection of particle-size fractions.

The principal advantage of top-down derivation is the inheritance of a pre-existing crystalline core and impurity background from the parent diamond. Its principal limitation is that mechanical fragmentation simultaneously generates a polydisperse particle population and newly created surfaces whose state may no longer reproduce that of the parent crystal.

2.2. Direct Formation from Non-Diamond Carbon

Direct-transformation routes create a new nanoscale diamond lattice from non-diamond carbon rather than inheriting it from a pre-existing diamond crystal. For comparison of the initial states established during formation, these routes can be considered in two groups. Rapid-conversion routes use transient mechanical, optical or electrothermal energy to drive carbon reorganization on short time scales, whereas precursor-directed routes use structurally defined molecular carbon sources to constrain nucleation and particle dimensions. This distinction is used here to compare how different formation pathways establish the initial nanodiamond state, rather than as an exhaustive classification of synthesis methods.

Rapid Conversion Routes

Among rapid carbon-conversion routes, detonation synthesis remains a mature route for nanodiamond powder production. Importantly, aggregation can develop during the formation process itself rather than arising only from subsequent powder handling. Time-resolved small-angle X-ray scattering by Hammons et al. detected hierarchical nanodiamond aggregation as early as approximately 0.1 μs after the detonation front, on a time scale comparable to particle formation [22]. The precursor chemistry also influences the state established during detonation. Shames et al. compared nanodiamonds produced from different explosive compositions and observed

variations in the relative carbon populations associated with the diamond core and surrounding carbon, together with differences in paramagnetic-defect characteristics [23]. More recently, Oleynik et al. identified structural features consistent with a two-stage graphite-to-diamond transformation and proposed a martensitic contribution to detonation-nanodiamond formation [24]. Taken together, these studies indicate that detonation establishes not only nanoscale diamond crystallites but also an aggregation state, carbon-phase heterogeneity and defect background during formation.

Liquid-confined energy deposition provides a more flexible route for converting molecular or graphitic carbon precursors into particulate nanodiamonds. Nee et al. demonstrated the direct formation of sub-5-nm nanodiamonds from ethanol under femtosecond laser irradiation, attributing nucleation to carbon species generated within the confined laser-induced plasma [25]. Using a different precursor and liquid environment, Cazzanelli et al. subsequently produced fluorescent nanodiamonds by pulsed laser ablation of graphite in liquid nitrogen, demonstrating that diamond formation and NV-related optical functionality can be introduced within the same laser-processing route [26]. Together, these studies show that the precursor, energy-deposition mode and confining liquid participate jointly in determining the initial particle and defect state. However, the substantial differences in precursor chemistry and laser conditions among reported routes make direct state-to-state comparison difficult.

Flash Joule heating extends rapid carbon conversion from transient mechanical or optical excitation to electrically driven electrothermal processing. Chen et al. demonstrated that flash Joule heating could induce ultrafast carbon phase evolution and enable nanodiamond-related phase control [27]. More recently, Du et al. approach to coke-derived feedstocks using fluorine-assisted flash Joule heating, producing nanodiamonds within approximately 1 s (Figure 2A–E) [28]. After post-treatment, the product approached 100% phase purity with an approximately 8% yield, while calculations indicated that fluorine-induced electronic redistribution promotes interlayer C–C bond formation during conversion. Together, these studies show that FJH is not only an ultrafast carbon-conversion route but also one in which pulse conditions and chemical assistance can influence phase selection during nanodiamond formation. However, comparison with established nanodiamond sources still requires fuller characterization of particle-size distributions, residual species, defect populations and batch-to-batch reproducibility.

Precursor-directed transformation introduces a different strategy in which molecular structure, rather than post-synthesis size selection alone, participates directly in determining nanodiamond nucleation and dimensions. Earlier studies had already shown that adamantane derivatives can act as molecular precursors or seeds under HPHT conditions. Ender et al. investigated the early stages of seeded nanodiamond growth from adamantane derivatives and showed that decomposition of the accompanying carbon source leads to alkylation of the diamondoid precursor before diamond growth [29]. Kudryavtsev et al. subsequently synthesized ultrasmall 2–5 nm nanodiamonds directly from adamantane at 12 GPa and approximately 1300 °C and identified a strongly hydrogenated surface state through characteristic C–H vibrational signatures [30]. Fu et al. converted adamantane into 2–4 nm cubic nanodiamonds under electron irradiation (Figure 2F–H) [31]. Time-resolved TEM further revealed the evolution of adamantane-derived intermediates into nanodiamonds (Figure 2I). Electron irradiation at 80–200 keV and 100–296 K produced nanodiamonds within tens of seconds, while time-resolved TEM directly captured the evolution from adamantane oligomers to spherical nanodiamonds. Together, these studies trace a progression from molecularly seeded HPHT growth to direct observation and activation of precursor-to-diamond conversion, establishing molecular structure as an active variable in nanodiamond formation rather than simply a carbon source.

Liang et al. extended precursor-directed control to hydrogen-terminated molecular nanographenes, which were converted at 13 GPa and 1200 °C into ultrasmall, monodisperse and highly crystalline nanodiamonds with a narrow size distribution of approximately 3–4 nm (Figure 2J–L) [32]. HRTEM revealed highly crystalline nanodiamonds with a single surface reconstruction (Figure 2K), while analysis of the particle population gave an average diameter of 4.0 ± 1.4 nm (Figure 2L). Spatially resolved EELS further identified the reconstructed surface as sp^2 -rich and no thicker than approximately 0.5 nm. Graphite remained largely unchanged under comparable pressure and temperature conditions, indicating that the molecular organization of the precursor, rather than the external conditions alone, governed nucleation and particle dimensions. In situ diffraction further showed rapid, quantitative conversion of the molecular nanographene, whereas graphite remained kinetically trapped under the same conditions [32]. Notably, the same platform enabled one-step incorporation of silicon- and germanium-based colour centres, yielding SiV^- - and GeV^- -containing fluorescent nanodiamonds without ion implantation, irradiation or post-synthetic defect activation. This result extends precursor-directed formation from control of particle size and surface reconstruction toward direct control of defect composition during nanodiamond formation.

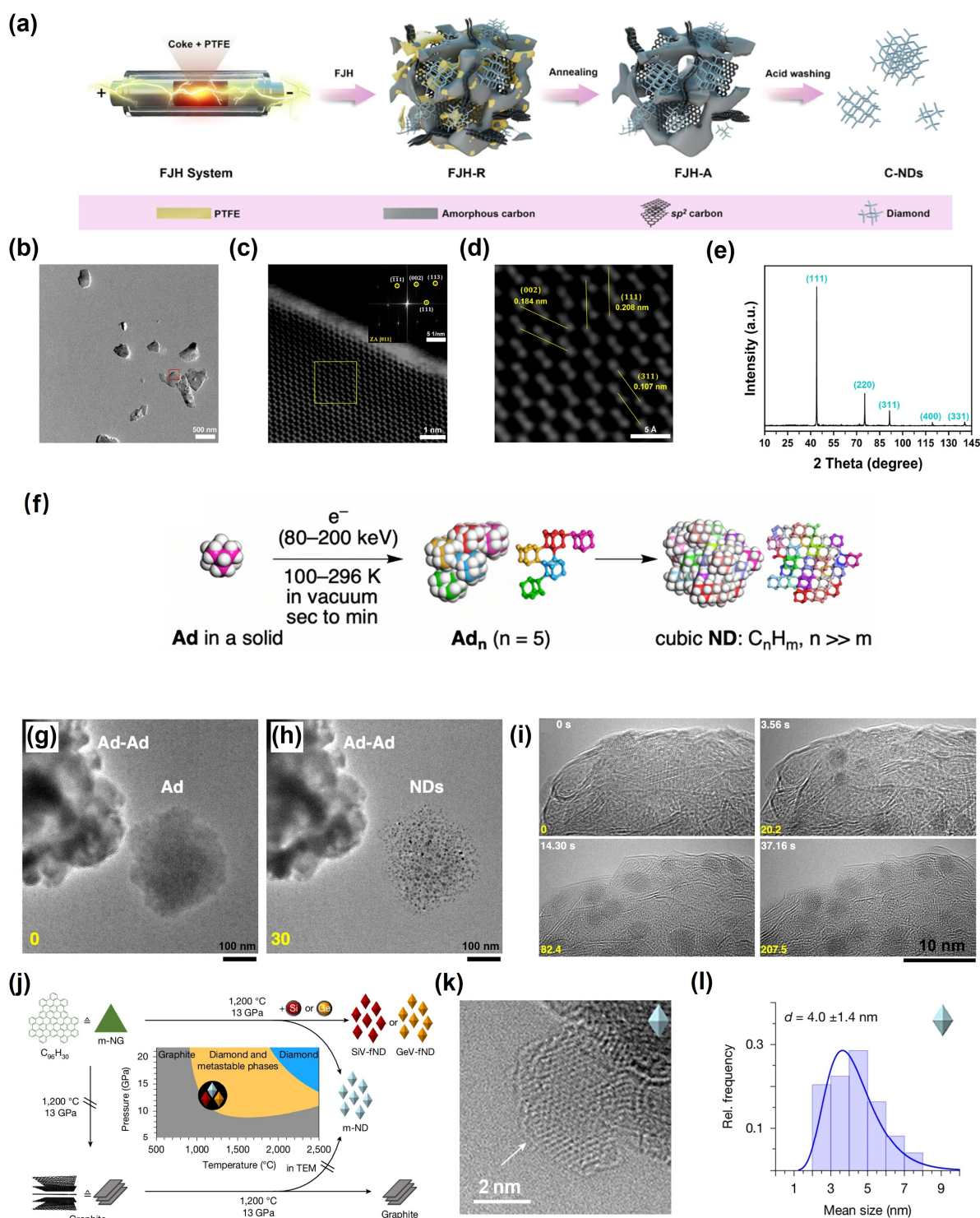


Figure 2. Selected recent routes for direct nanodiamond formation from non-diamond carbon. **(a–e)** Fluorine-assisted flash Joule heating for rapid nanodiamond formation. Reprinted with permission from ref. [28]. Copyright 2025, American Chemical Society. **(f–i)** Electron-beam-induced conversion of adamantane into cubic nanodiamonds. Reprinted with permission from ref. [31]. Copyright 2025, The American Association for the Advancement of Science. **(j–l)** HPHT conversion of molecular nanographene into ultrasmall molecular nanodiamonds, including colour-centre incorporation. Reprinted from ref. [32] (2026, Springer Nature), under the terms and conditions of the Creative Commons CC BY 4.0.

Direct-transformation routes therefore span two distinct but complementary strategies for establishing the initial nanodiamond state. In rapid-conversion routes, transient energy input and reaction chemistry drive diamond formation but can simultaneously establish aggregation, carbon-phase heterogeneity and defect backgrounds. Precursor-directed routes instead introduce structural information before nucleation, allowing molecular geometry, hydrogen content and precursor composition to participate directly in controlling particle dimensions, surface

reconstruction and, increasingly, defect incorporation. The key distinction is therefore where material-state control enters the formation pathway. Across both groups, diamond-phase confirmation alone is insufficient to define the resulting nanodiamond state. Particle-size distribution, aggregation, residual non-diamond carbon or reaction species, impurity and defect content, and surface composition must also be established. Subsequent purification, fractionation, deaggregation and surface modification can further transform these initial states and are discussed separately in Section 3.

2.3. Gas-Phase Nucleation and Plasma-Assisted Growth

Gas-phase routes differ from top-down derivation and condensed-phase transformation by nucleating diamond nanoparticles directly from reactive carbon species in hydrogen-containing CVD or plasma environments. Kim et al. provided direct evidence of gas-phase particulate formation during hot-filament CVD, identifying cubic diamond together with hexagonal diamond, n-diamond and other carbon phases within the captured nanoparticle population [33]. Jia et al. subsequently showed that, in an H_2/CH_4 microwave microplasma, the populations of H atoms, C_2 and CH_3 and the applied microwave power were closely associated with the appearance of the diamond phase [34]. More recently, Siby et al. demonstrated that high H-atom densities, moderate gas temperatures and appropriate hydrocarbon concentrations favour nanodiamond nucleation, whereas excessive hydrocarbon abundance shifts the products toward soot, transpolyacetylene and other sp^2 -rich phases [35]. These studies collectively show that gas-phase nanodiamond formation is governed by a competition among hydrogen activity, reactive-carbon availability and plasma energy rather than by nominal gas composition alone.

The main value of this route is therefore its potential to control nanodiamond nucleation directly through plasma chemistry without relying on a pre-existing diamond crystal or a condensed molecular precursor. At present, however, the particulate products remain heterogeneous in phase and comparatively under-characterized in terms of particle-size distribution, yield, population uniformity and recovery. Gas-phase growth should therefore be regarded as an emerging formation strategy that provides useful insight into formation-level state control, rather than as a mature alternative to established nanodiamond powder-production routes.

3. Processing-Induced Evolution of Nanodiamond Material States

The formation routes discussed in Section 2 establish the initial particle, structural, impurity/defect and surface states of nanodiamonds, but post-formation processing can substantially transform that state before the particles reach their final application. This section therefore organizes processing by the operation performed—defect creation and annealing, purification and surface reconstruction, nanosizing and fractionation, and functionalization, coating and interface formation—rather than by individual material properties. Each operation is evaluated according to the intended change, the accompanying changes in other state variables, and the resulting functional trade-offs. In this sense, “coupled evolution” refers to the non-independent modification of defect, surface, particle and interfacial characteristics during processing, rather than to a single universal microscopic interaction.

3.1. Defect Creation and Annealing

Irradiation-annealing treatments are widely used to create optically active NV centres, but their outcome depends on the full processing sequence rather than on vacancy generation alone. Boudou et al. established an early route in which HPHT microdiamonds were irradiated and annealed before high-energy milling, demonstrating that colour-centre formation can be completed in the comparatively intact parent crystal before nanosizing [36]. Subsequent studies showed that annealing itself introduces a substantial trade-off. Nunn et al. found that increasing the annealing temperature from 900 to 1600 °C improved T_1 and T_2 in surviving micrometre-scale particles and removed rapidly relaxing spins, but simultaneously reduced NV concentration and caused substantial particle loss, particularly for the smallest particles [37]. Oshimi et al. further showed that high-quality spin performance could be achieved by combining ^{12}C enrichment, controlled nitrogen content, electron irradiation and annealing, yielding 0.6–1.3 ppm NV^- centres with mean T_1 and T_2 values of 0.68 ms and 3.2 μs , respectively (Figure 3A) [17]. Together, these studies show that defect engineering is governed by the interaction among parent-crystal composition, vacancy production, annealing and processing order; increasing vacancy generation or annealing severity does not monotonically improve the final spin-active state.

The central processing objective is therefore not to maximize colour-centre density, but to establish a defect population that remains optically stable and spin coherent. The annealing and impurity-control studies above show that improved relaxation or ODMR performance can coincide with lower NV concentration or material yield [17,37]. The sensitivity of the functional state to irradiation conditions is further illustrated by Flinn et al., who exposed pre-existing FNDs to 80–200 keV electron beams and observed energy- and fluence-dependent loss of

photoluminescence and sensing contrast even when SAED and EELS indicated no major bulk-lattice damage [38]. These results indicate that irradiation and annealing should be evaluated by the balance among useful NV formation, residual or newly activated defects, spin-bath suppression, optical stability and particle survival. The optimum processing condition is therefore application dependent and cannot be defined by NV concentration alone.

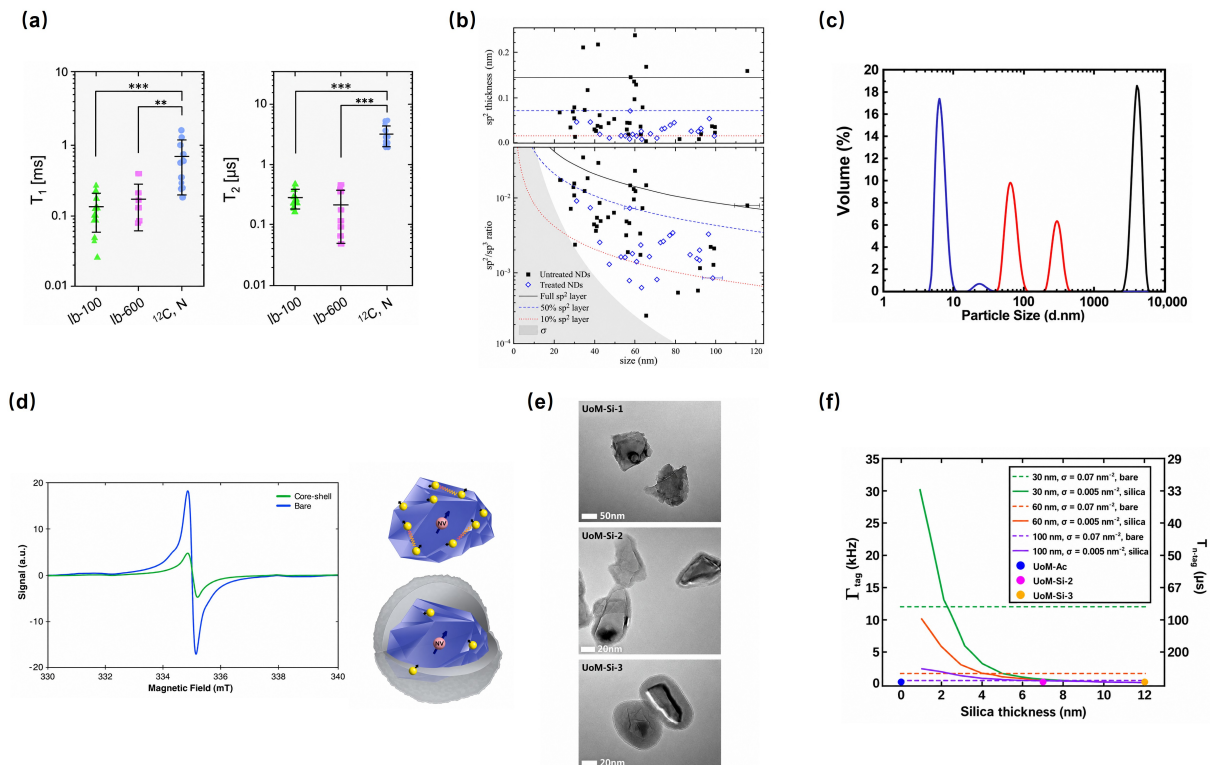


Figure 3. Processing-induced evolution of nanodiamond material states. (a) Spin properties of quantum-grade nanodiamonds enabled by controlled defect engineering. Reprinted with permission from ref. [17] (2024, American Chemical Society), under the terms and conditions of the Creative Commons CC BY 4.0. (b) Reduction of graphitic sp^2 surface content after chemical treatment. Reprinted with permission from ref. [39] (2024, Elsevier Ltd.), under the terms and conditions of the Creative Commons CC BY 4.0. (c) Hydrodynamic-size evolution during chemical deaggregation of detonation nanodiamonds. Reprinted with permission from ref. [40] (2022, the Royal Society of Chemistry), under the terms and conditions of the Creative Commons CC BY 3.0. (d) Comparison of spin responses between bare and silica core-shell nanodiamonds. Reprinted with permission from ref. [20] (2025, PNAS), under the terms and conditions of the Creative Commons CC BY 4.0. (e) TEM images showing tunable silica shell formation around fluorescent nanodiamonds; (f) Simulated dependence of sensing performance on silica-shell thickness, highlighting the trade-off between surface passivation and NV-target distance. Reprinted with permission from ref. [18] (2025, American Chemical Society), under the terms and conditions of the Creative Commons CC BY 4.0.

3.2. Purification and Surface Reconstruction

Purification of nanodiamonds simultaneously alters non-diamond carbon content and surface chemistry, with consequences for colloidal, optical and spin behaviour. Purification should therefore not be regarded simply as removal of unwanted carbon or inorganic impurities, because oxidative and chemical treatments simultaneously reconstruct the particle surface. Ardhayanti et al. recently demonstrated this coupling in detonation nanodiamonds: salt-assisted air oxidation at 450 °C selectively removed graphitic impurities while preserving the diamond lattice, whereas subsequent Fenton treatment introduced hydrophilic surface functionalities and improved colloidal stability [41]. At the single-particle level, Hamilton et al. showed that chemically treated milled nanodiamonds contained only about 10% of the graphitic sp^2 coverage measured on untreated particles, yet substantial particle-to-particle variation remained after treatment (Figure 3B) [39]. Such residual heterogeneity is functionally relevant because the surface carbon removed or reconstructed during purification can also modify the electronic and magnetic environment experienced by embedded colour centres. Ryan et al., for example, found that borane-reduced 50 nm nanodiamonds exhibited approximately twice the NV spin-relaxation time of thermally oxidized particles, with spectroscopy linking the change to conversion of double-bonded sp^2 carbon into C-O and C-H

surface environments [42]. Purification and surface reconstruction are therefore inseparable at the nanoscale: a treatment selected to increase phase purity also establishes a new chemical, colloidal and spin environment.

The functional consequence of surface reconstruction depends on which surface state is created, rather than on purification severity alone. Ryan et al. showed that a reduced surface could provide longer NV relaxation than a thermally oxidized surface [42], whereas Peng et al. found that air annealing efficiently removed paramagnetic surface spins and markedly reduced their contribution to the longitudinal relaxation of internal P1 centres [43]. Although P1 and NV centres are distinct defects, the latter result provides independent evidence that thermal surface treatment can suppress a magnetic-noise source without changing the identity of the internal lattice defect. More recently, Pasternak et al. demonstrated a complementary electronic effect: removal of hydrogen termination increased SiV⁻ fluorescence by more than 50% for nanodiamonds below approximately 100 nm, corresponding to an effective near-surface region of about 6 nm in which hydrogen-induced charge redistribution affected the SiV charge state [44]. These results show why surface state cannot be reduced to a single descriptor such as “oxidized”, “reduced” or “hydrogen terminated”. Different treatments simultaneously alter non-diamond carbon, termination, paramagnetic surface defects and near-surface charge transfer, and the optimum reconstructed state therefore depends on whether the required function is spin relaxation, charge-state stability, fluorescence or subsequent interfacial chemistry.

3.3. Nanosizing, Deaggregation and Fractionation

Nanosizing and deaggregation alter the particle population presented to an application without necessarily changing the dimensions of the primary diamond crystallites. This distinction is especially important for detonation nanodiamonds, whose few-nanometre primary particles can persist as much larger aggregates in suspension. Terada et al. showed that a combined air-oxidation and boiling-acid treatment could chemically deaggregate detonation nanodiamonds to stable single-digit-nanometre dispersions without relying on high-power sonication or bead milling (Figure 3C) [40]. However, deaggregation does not imply that a suspension becomes structurally uniform. Kuschnerus et al. compared detonation nanodiamonds subjected to different post-synthesis treatments and found persistent hierarchical chain-like and cluster aggregates in aqueous media, with aggregate morphology and fractal characteristics varying with the treatment history [45]. These results show that “particle size” in a processed nanodiamond sample can refer to at least three distinct quantities—primary crystallite size, aggregate size and hydrodynamic size—and processing may change these quantities differently.

Fractionation introduces a different form of state control because it does not primarily modify individual particles; instead, it selects which part of a polydisperse population is retained. Finas et al. demonstrated this directly for milled nanodiamonds, separating material from the same source into populations centred at approximately 10, 25 and 35 nm by centrifugation-based size sorting [16]. The protocol could be applied to both oxidized and hydrogenated particles, demonstrating the versatility of fractionation-based population control. Taken together, these results indicate that the “size” reported for a nanodiamond sample is often a processing-defined population property rather than a direct consequence of the formation route alone.

The particle population produced by deaggregation or fractionation is not necessarily preserved under operating conditions. Kuschnerus et al. showed that aqueous detonation-nanodiamond dispersions can reorganize into distinct hierarchical aggregate morphologies even after different purification and deagglomeration treatments [45]. More recently, Volkova et al. demonstrated that the structure and stability of concentrated detonation-nanodiamond dispersions depend strongly on both particle concentration and electrolyte content, with increasing ionic strength promoting coagulation, viscosity changes and structured sedimentation [46]. Thus, a narrowly fractionated powder or water dispersion does not by itself define the working particle state. The relevant state is the population present under the concentration, ionic strength and medium used for the intended measurement or application.

3.4. Functionalization, Coating and Interface Formation

Surface functionalization converts a purified nanodiamond surface into an interface that can operate in a specific chemical, biological or physical environment. The relevant objective is therefore not simply to attach a terminal group, but to create an interface that remains accessible, colloidally stable and compatible with the optical or spin state of the particle. Recent work on particulate nanodiamonds illustrates this multivariable requirement. Głowacki et al. grafted hyperbranched polyglycerol onto approximately 140 nm nanodiamonds and showed improved colloidal stability across a wide pH range, concentrated phosphate-buffered saline and physiological media, together with suppression of non-specific protein adsorption while retaining strong fluorescence [47]. Using a different functionalization strategy, Laube et al. employed electron-beam-induced radiation chemistry to graft fluorene and 9,10-dimethylantracene onto fluorescent nanodiamonds, producing stable molecular

conjugates while preserving distinguishable emission from the grafted dye and the internal NV centres [48]. Together, these studies show that successful functionalization must be judged by the combined state of the surface layer, particle dispersion and retained internal optical functionality rather than by grafting yield alone.

Coating and core-shell formation can modify not only the outer chemical interface but also the magnetic and electronic environment experienced by near-surface colour centres. Zvi et al. showed that silica core-shell nanodiamonds exhibited substantially longer qubit coherence times than bare particles, with T_2 increasing from approximately 1.1–35 μs in bare nanodiamonds to 52–87 μs in core-shell particles; the coated particles also showed a 1.9-fold increase in luminescence (Figure 3D) [20]. Barzegaramiriolya et al. independently found that oxidation followed by silica coating increased the ensemble T_1 of approximately 100 nm FNDs from $320 \pm 9 \mu\text{s}$ to 1.00 ± 0.06 ms, while modelling showed that thicker shells improve surface passivation but simultaneously increase the sensor-target separation; for the system studied, a shell thickness on the order of 1 nm maximized predicted magnetic sensitivity (Figure 3E,F) [18]. These studies provide direct evidence that an interfacial layer can improve the internal spin environment of a nanodiamond while imposing a geometric penalty on sensing proximity. Coating design should therefore be optimized as a coupled interface problem rather than treated as a universally beneficial passivation step.

Overall, these studies reveal that post-formation processing of nanodiamonds should not be interpreted as a sequence of isolated optimization steps. Irradiation and annealing determine the defect landscape, purification reconstructs the surface chemical environment, nanosizing and fractionation redefine the particle population, and functionalization establishes the final interface with the surrounding medium. These processes are strongly coupled because each operation modifies not only the targeted parameter but also the subsequent accessibility and stability of other material states. Therefore, the functional performance of nanodiamonds is ultimately determined by the integrated evolution of defect, surface, particle and interfacial states rather than by a single processing parameter.

4. Application-Directed Material-State Requirements and Performance Trade-Offs

The preceding sections established that nanodiamond formation and post-processing generate a multidimensional material state comprising particle population, defect and impurity content, surface chemistry and interfacial structure. In this review, material state does not represent a new category of descriptors, but rather the processing-dependent configuration of existing structural, chemical, defect and interfacial characteristics that collectively governs functional behaviour. Whether a particular state is advantageous can only be judged against the function to be performed and the conditions under which that function is measured. Residual sp^2 carbon and surface-associated spins, for example, may increase magnetic noise in quantum sensing, whereas conductive carbon or surface oxygen groups can participate in adsorption and charge-transfer processes at electrochemical interfaces. Likewise, a coating that improves colloidal stability or suppresses surface noise may simultaneously increase hydrodynamic size or sensor-target separation. Material quality is therefore application-dependent rather than universal, because the optimal combination of defect, surface and interfacial characteristics varies with the targeted function and operating environment.

This section uses representative particulate-nanodiamond applications to examine how specific combinations of material-state variables translate into functional properties (such as spin coherence, fluorescence stability, interfacial heat transfer and charge-transfer behaviour) and, ultimately, task-level performance. Quantum sensing places stringent requirements on colour-centre population, spin bath, surface noise and sensor-target geometry. Fluorescence imaging and diagnostics additionally depend on brightness, dispersion, biomolecular accessibility and behaviour in complex media. Thermal composites require control of particle organization and interfacial heat transfer, whereas electrochemical sensing depends on particle coverage, surface chemistry and electrical connectivity to the supporting electrode. For each application, the discussion therefore distinguishes (i) the material-state variables that must be controlled, (ii) the functional properties through which they act, and (iii) the performance metrics required to evaluate the final system.

4.1. Quantum Sensing Applications

Colour centres in nanodiamonds provide optically readable spin states for detecting magnetic fields, temperature variations and local magnetic fluctuations. Their nanoscale mobility enables measurements in environments difficult to access with bulk diamond sensors, but the same reduction in dimensions introduces additional sensitivity to particle-to-particle variation, surface-associated noise and colour-centre environment. Quantum-sensing performance therefore does not arise from the presence of NV centres alone, but from the combined state of the defect population, surrounding spin bath, particle surface and sensor-target geometry. These variables are coupled because modifying one component often changes the others; for example, reducing particle size can improve access to nanoscale targets while simultaneously increasing surface-induced noise, whereas

interface protection can suppress fluctuations but alter sensing distance. Accordingly, parameters such as colour-centre concentration, defect depth, particle size, aggregation state and surface termination should not be optimized independently; instead, they must be considered as coupled material-state variables determined by the processing history of the nanodiamond.

Spin relaxometry provides a representative example of how nanodiamond material state determines sensing capability. Early studies by Tetienne et al. showed that reducing nanodiamond size from approximately 100 to 10 nm caused a pronounced decrease in NV longitudinal relaxation time, revealing the increasing contribution of surface-associated magnetic fluctuations as colour centres approach the particle boundary [49]. Subsequent studies demonstrated that nanodiamond relaxometry can detect external spin fluctuations and biomolecular magnetic signals under ambient conditions [50,51]. These studies defined the fundamental sensing principle but also exposed a central materials challenge: reducing the distance between the sensing centre and the target enhances interaction strength while simultaneously increasing sensitivity to surface and interfacial noise.

Recent developments have therefore shifted from demonstrating detectability toward engineering a reproducible quantum-grade material state. Oshimi et al. demonstrated that high-performance fluorescent nanodiamonds require simultaneous control of isotope composition, nitrogen background, vacancy conversion and residual paramagnetic spin noise, rather than simply increasing colour-centre density [17]. This transition highlights that quantum-sensing performance is governed by the entire processing history—from parent diamond selection and defect engineering to the final particle state—rather than by a single optical or spin parameter.

Beyond the intrinsic defect state, quantum sensing performance is also determined by how the nanodiamond interface interacts with its surrounding environment. Surface passivation and interfacial layers can reduce fluctuations originating from the particle boundary [18]. Core-shell and silica-coated nanodiamonds further demonstrate that interface protection can improve spin stability while introducing a proximity trade-off [20]. The optimal interface is consequently not the one that maximizes surface isolation alone, but the one that balances noise suppression with target coupling.

A related challenge arises from the spatial relationship between nanodiamond probes and their measurement targets. In biological environments, particle uptake, intracellular localization and aggregation can introduce uncertainty in sensor–target distance, making the measured response dependent not only on the nanodiamond state but also on its positioning configuration. Xu et al. addressed this limitation by electrically trapping and manipulating individual nanodiamonds on a glass nanopipette inside living cells, converting probe location from an uncontrolled variable into an experimentally defined parameter (Figure 4A) [52]. Such approaches highlight that the effective sensing unit is not only the processed nanodiamond particle, but the nanodiamond together with its interface, positioning strategy and readout geometry.

Taken together, these studies show that quantum-grade nanodiamonds cannot be defined by a single parameter such as particle size, NV concentration or fluorescence brightness. Instead, sensing performance emerges from the coupled evolution of defect state, surface environment, particle population and measurement geometry. Different sensing modes impose different material-state requirements: relaxometry requires a low and reproducible magnetic-noise background, thermometry requires stable resonance response and controlled measurement perturbation, whereas intracellular sensing additionally requires predictable particle localization and interface compatibility.

Beyond standalone nanodiamond probes, advanced quantum platforms require integration strategies that preserve colour-centre properties while improving photon collection and device accessibility. This represents a further extension of material-state engineering, where defect environments must be coordinated with optical confinement structures and fabrication-induced perturbations. Diamond nanophotonic platforms have demonstrated SiV integration into cavities and waveguides for enhanced light-matter interaction and photon extraction [53]. Inverse-designed photonic structures further enable control of optical modes and emitter-photon coupling [54]. Hybrid integration strategies can separate emitter requirements from photonic architectures [55]. Heterogeneous GaP-diamond integration further demonstrates this approach [56]. Recent deterministic diamond nanophotonic interfaces with optically accessible electronuclear spin registers further highlight the importance of combining defect engineering, nanofabrication and optical integration [57].

To enable meaningful comparison across studies, quantum-sensing reports should therefore characterize not only optical outputs but also the underlying material state, including particle size and aggregation behaviour, colour-centre population, spin-bath information, surface termination or coating state, and the relevant ODMR-derived metrics (e.g., T_1 , T_2 and sensitivity). These parameters provide the necessary link between processing history, nanodiamond state, functional properties and application-level performance, and form the basis for the application-oriented characterization framework summarized later in this review.

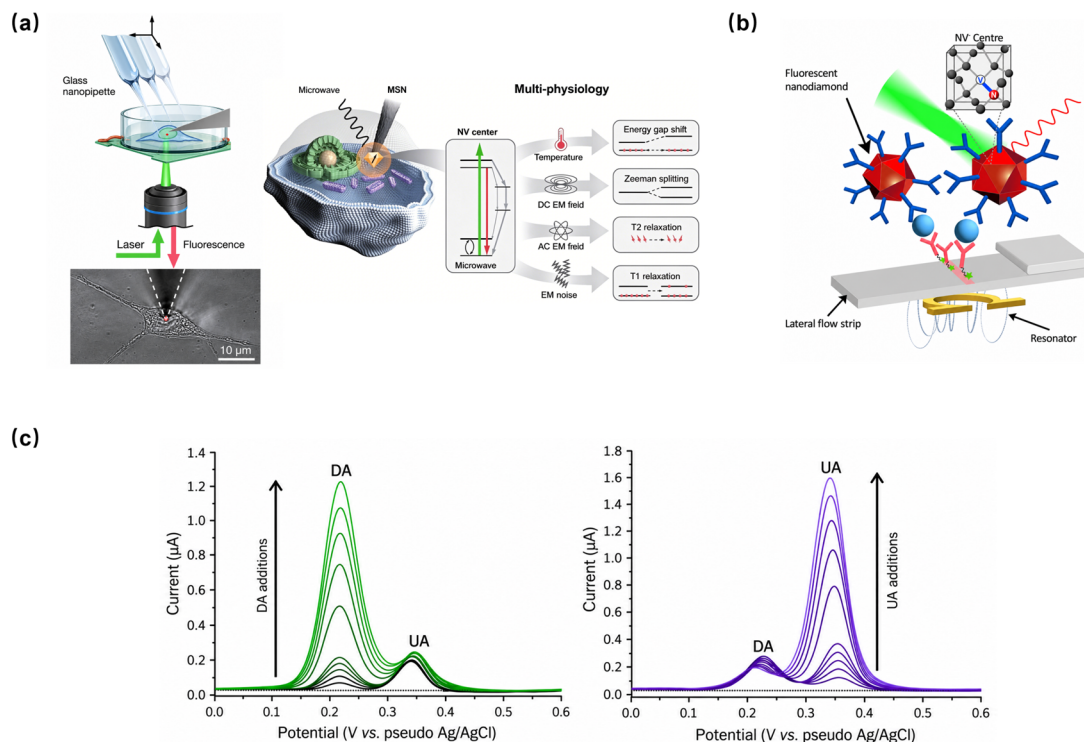


Figure 4. Application-dependent performance of nanodiamonds. **(a)** Quantum sensing using a manipulable single nanodiamond probe. Reprinted with permission from ref. [52] (2025, Oxford University Press on behalf of China Science Publishing & Media Ltd.) under the terms and conditions of the Creative Commons CC BY 4.0. **(b)** Fluorescent-nanodiamond-based lateral-flow sensing for quantum-enhanced diagnostics. Reprinted with permission from ref. [58] (2025, Springer Nature), under the terms and conditions of the Creative Commons CC BY 4.0. **(c)** Electrochemical sensing using nanodiamond-modified electrodes. Reprinted with permission from ref. [59] (2019, Springer Nature), under the terms and conditions of the Creative Commons CC BY 4.0.

4.2. Fluorescence Imaging and Biological Diagnostics

Fluorescence imaging exploits the optically stable emission of colour centres in nanodiamonds without requiring the long spin-relaxation times or narrow ODMR responses needed for quantum sensing. However, reliable biological imaging depends on more than intrinsic fluorescence brightness. Particle size distribution, aggregation behaviour, defect-related optical stability, surface chemistry and colloidal state collectively determine whether fluorescent signals can be maintained after dispersion, functionalization and exposure to biological environments. Diagnostic platforms impose additional requirements, including selective molecular recognition, compatibility with assay environments and sufficient signal contrast against biological backgrounds. This requirement makes biomedical imaging another example where application performance is governed by the coupled evolution of particle, surface and colloidal states. Therefore, the relevant imaging material is not simply an emissive nanodiamond particle, but a processing-defined fluorescent probe whose optical and physicochemical state remains compatible with the intended biological measurement.

Early studies established the basic imaging advantages of fluorescent nanodiamonds while also revealing the importance of particle preparation. Yu et al. provided an early demonstration that fluorescent nanodiamonds could combine bright emission with negligible photobleaching and low cytotoxicity [60]. Chang et al. subsequently produced fluorescent nanodiamonds in larger quantities by helium-ion irradiation of synthetic diamond nanocrystallites and demonstrated three-dimensional tracking of individual particles in cells using one- and two-photon fluorescence microscopy [61]. These early demonstrations also highlighted that imaging performance is strongly influenced by the state of the nanodiamond particle population. Smaller particles provide more localized labels and may enter cells more readily, but generally contain fewer emitters and exhibit a greater contribution from surface-related fluorescence. Larger particles generate stronger optical signals but are more likely to aggregate, sediment or remain confined within endosomal compartments. Therefore, fluorescence brightness alone does not fully define an optimal imaging probe; particle size distribution, emitter population, surface state and colloidal stability should be considered together, as these factors influence signal intensity, localization accuracy and measurement reliability in biological environments.

Surface functionalization provides a route to adapt nanodiamonds for biological environments, but its role extends beyond simply improving water dispersibility or enabling molecular conjugation. For fluorescence imaging, the

functionalized interface becomes an additional component of the probe state because it regulates interactions with proteins, cells and surrounding biological media. Polymer, silica and biomolecular coatings can modify aggregation behaviour, surface charge and biological recognition, thereby influencing fluorescence accessibility, cellular localization and imaging reproducibility [3,4]. The relevant design objective is therefore not maximum surface modification, but a controlled interface that preserves optical performance while providing predictable biological interactions.

Diagnostic applications introduce additional requirements because nanodiamonds must maintain reliable fluorescence signals within chemically and biologically complex environments. Unlike conventional fluorescence labels, where signal intensity is often the primary consideration, nanodiamond-based diagnostics require simultaneous control of optical stability, surface recognition and assay compatibility. Miller et al. demonstrated that microwave-modulated fluorescence readout from nanodiamonds could enhance diagnostic sensitivity by reducing background interference in lateral-flow assays, highlighting the importance of integrating optical readout strategies with the intrinsic properties of the nanodiamond probe [62]. More recently, DeCruz et al. extended this concept toward clinical translation by developing a quantum-enhanced nanodiamond rapid test for SARS-CoV-2 antigen detection, demonstrating that probe-state control and signal amplification strategies can improve diagnostic performance in complex biological samples (Figure 4B) [58]. These studies indicate that nanodiamond diagnostics depend not only on fluorescence intensity but also on maintaining a reproducible probe state throughout the entire assay process, including particle functionalization, target recognition and signal readout.

4.3. Thermal Transport in Nanodiamond Composites

The high intrinsic thermal conductivity of diamond does not translate directly into high thermal conductivity in a nanodiamond composite. Heat transport is interrupted by particle aggregation, polymer-rich gaps and interfacial thermal resistance at nanodiamond-matrix and particle-particle contacts. Studies of epoxy, poly (vinyl alcohol), cellulose, polyethylene and aramid-based composites collectively show that effective thermal transport emerges from processing-controlled particle organization and interfacial coupling rather than filler loading alone. The amount of nanodiamond required therefore varies widely among systems and cannot be interpreted independently of dispersion, matrix structure, composite density and interfacial thermal resistance.

At relatively low filler contents, surface chemistry mainly affects thermal transport by controlling dispersion and particle-matrix interfacial coupling with the polymer. Ozone treatment followed by tetraethylenepentamine grafting suppressed aggregation of 5–10 nm nanodiamonds in epoxy; at an optimized loading of 0.5 wt%, the functionalized particles increased thermal conductivity by 34.1% relative to the composite containing untreated nanodiamonds, while also improving fracture toughness [63]. Hydroxylated nanodiamonds in poly (vinyl alcohol) provide a useful comparison: interactions between the modified surface and polymer chains were most influential at lower loading, suggesting that direct filler contact became increasingly important as the nanodiamond fraction approached 90 wt%, where a thermal conductivity of $18.98 \text{ W m}^{-1} \text{ K}^{-1}$ was reported [64]. These results show that improved particle-matrix compatibility is beneficial when particles remain separated, whereas continuous particle contacts become increasingly important when high absolute thermal conductivity is targeted.

Thermal pathways can be established through hierarchical assembly, hybrid fillers and matrix orientation. Nanofibrillated cellulose has been used to disperse low fractions of nanodiamond within an organized film structure [65], whereas nanodiamonds attached to exfoliated h-BN can bridge neighbouring platelets and improve heat transfer between otherwise separated two-dimensional fillers [66]. In aramid-nanofibre films, electrostatic modification and gelation-induced assembly produced a connected network with in-plane and through-plane thermal conductivities of 30.99 and $6.34 \text{ W m}^{-1} \text{ K}^{-1}$, respectively, at 50 wt% nanodiamond loading [67]. A different mechanism operated in solid-state-drawn ultra-high-molecular-weight polyethylene containing only 2 wt% functionalized nanodiamonds, which reached $60 \text{ W m}^{-1} \text{ K}^{-1}$ along the drawing direction [68]. In the latter case, the high conductivity arose primarily from polymer-chain orientation and crystallization, with the nanodiamonds assisting structural organization and interfacial compatibility. Across these systems, nanodiamonds may function as conductive particles, bridges between larger fillers or promoters of matrix organization; the final conductivity therefore reflects the architecture created during processing rather than the filler content alone.

Comparisons among nanodiamond composites should therefore include processing history, filler volume fraction, primary and aggregate sizes, surface treatment, dispersion procedure, porosity, composite density and the direction in which thermal conductivity is measured. Additional application-relevant parameters, such as mechanical reliability, electrical insulation and thermal cycling stability, should also be considered when evaluating practical thermal management systems. Studies of diamond-containing liquid-metal interfaces provide additional insight into wetting and interfacial heat-transfer mechanisms [69], although these systems should not be directly compared with nanodiamond-filled polymers because of differences in filler dimensions and heat-transfer geometry [70,71].

4.4. Electrochemical Sensing and Electrode Architecture

Electrochemical performance is not determined by the presence of diamond alone, but by how diamond-derived interfaces are electrically coupled and chemically exposed within the electrode architecture. Nanodiamonds may alter analyte adsorption, mass transport, electrode fouling and the spatial distribution of electroactive sites, but their contribution depends on whether they are electrically connected to the underlying electrode. Surface sp^2 carbon, oxygen-containing groups, particle coverage and the conductivity of the supporting material may all influence the measured response. An increase in current should therefore not automatically be interpreted as intrinsic electrocatalysis by the nanodiamonds.

Studies of nanodiamond-modified carbon electrodes illustrate the diversity of these mechanisms. Functionalized detonation nanodiamonds deposited on tetrahedral amorphous carbon improved the dopamine detection limit from 10 μM to 50 nM, while the surface termination and deposition method also affected the electrochemical response and cell compatibility [72]. Nanodiamond coatings on carbon-fibre microelectrodes similarly increased neurotransmitter sensitivity and reduced electrochemical and biological fouling, although coating morphology varied with particle size and surface chemistry [73]. High-purity sp^3 nanodiamonds on screen-printed graphite provide a contrasting case: because the particles were essentially nonconductive, moderate surface coverage improved dopamine and uric-acid detection mainly by modifying mass transport and exposing a distributed graphite microelectrode network, whereas excessive deposition blocked electron transfer (Figure 4C) [59]. An optimum loading of approximately 140 ng cm^{-2} produced detection limits of 0.57 and 0.89 μM for dopamine and uric acid, respectively. Collectively, these studies show that particle coverage, surface carbon structure and electrical connection to the supporting electrode determine whether nanodiamonds act through adsorption, antifouling, local redox processes or geometrical restructuring of the electrode surface.

Nanostructured conductive-diamond electrodes provide complementary evidence for the importance of electrode geometry, although they should be distinguished from particulate nanodiamond modifiers. Reactive-ion etching of heavily boron-doped diamond produced nanograss arrays with more accessible reaction sites and faster electron transfer [74], while increasing the thickness of porous boron-doped diamond changed its morphology and dopamine-detection performance [75]. Substrate pretreatment provides another level of control: lapping, electropolishing and chemical etching of titanium substrates altered the morphology and surface chemistry of subsequently grown Ti-doped diamond, and the controlled introduction of oxygen-containing groups lowered the dopamine detection limit from 6000 to 600 nM [76]. These studies indicate that porosity, thickness, surface termination and the structure of the underlying substrate can be as important as nominal diamond composition.

Across particulate nanodiamond coatings and nanostructured conductive-diamond electrodes, the central trade-off is between increasing the accessible interface and preserving efficient electron transfer. Nanodiamond modifiers and conductive diamond electrodes therefore require different optimization strategies: the former rely primarily on controlled surface interactions and electrode coupling, whereas the latter depend more strongly on conductive pathways, morphology and electrochemical stability. Sparse particle coverage or controlled porosity can improve analyte adsorption, mass transport and exposed reaction sites, whereas excessive deposition may block electron transfer or increase background signals. Surface oxygen groups and residual sp^2 carbon may further influence adsorption and charge transfer, but their effects depend on the analyte and electrode architecture. Electrode processing should therefore be selected according to the intended sensing mechanism rather than simply maximizing particle loading or surface area. The application-dependent material-state requirements, recommended characterization strategies and corresponding functional relevance are summarized in Table 2, highlighting that nanodiamond performance is governed by coupled structural, chemical and interfacial characteristics rather than isolated parameters.

Table 2. Application-dependent material-state requirements and recommended characterization strategies for nanodiamonds.

Application	Critical Material-State Variables	Recommended Characterization	Functional Relevance
Quantum Sensing	• Colour-centre population; nitrogen and impurity background • Spin-bath environment • Particle size and aggregation • Surface termination or coating state	• Photoluminescence spectroscopy • ODMR measurements (T_1, T_2, sensitivity) • EPR • TEM/DLS • XPS or FTIR	Stable spin coherence, reliable quantum readout and high sensing sensitivity

Table 2. Cont.

Application	Critical Material-State Variables	Recommended Characterization	Functional Relevance
Fluorescence Imaging and Diagnostics	• Fluorescence-emitter population • Particle size distribution • Aggregation behaviour • Surface chemistry • Colloidal stability	• Photoluminescence spectroscopy • TEM/DLS • XPS/FTIR • Zeta-potential analysis • Biological compatibility assays	Stable optical emission, biological compatibility and reliable signal detection
Thermal Transport Composites	• Particle dispersion • Primary and aggregate size • Surface functionalization • Filler-matrix interaction • Interfacial thermal resistance	• SEM/TEM • DLS • Raman/XPS for surface state • Thermal conductivity measurements • TDTR or thermal boundary conductance measurements	Efficient heat-transfer pathways and enhanced composite thermal conductivity
Electrochemical Sensing	• Surface termination • sp²/sp³ carbon ratio • Particle coverage • Electrode interface structure • Electrical connectivity	• Raman spectroscopy • XPS • SEM/TEM • Electrochemical impedance spectroscopy (EIS) • Cyclic voltammetry (CV)	Efficient charge transfer, high sensitivity and selective analyte detection

5. Standardization and Outlook

5.1. Establishing Standardized Material-State Reporting

Although nanodiamonds have demonstrated diverse functionalities across quantum sensing, biomedical diagnostics, thermal composites and electrochemical systems, direct comparison among studies remains challenging because reported performances are often determined by different material states generated during synthesis and post-processing. Variations in particle size distribution, defect and impurity populations, surface termination, aggregation behaviour and interfacial structures can substantially modify functional properties even when nominal nanodiamond materials appear similar. Therefore, future studies should report nanodiamond characteristics using a standardized material-state description, including the relevant structural, chemical, defect, surface and interfacial descriptors together with appropriate characterization methods, rather than relying on isolated parameters such as particle size or fluorescence intensity.

Such reporting should establish clear connections between processing history, resulting material state and application-relevant performance. Essential information should include synthesis origin, purification and annealing treatments, primary and hydrodynamic particle size, defect or impurity characteristics, surface chemical state, aggregation behaviour and interface conditions with surrounding materials. These parameters provide the basis for interpreting differences in spin coherence, optical stability, thermal transport or electrochemical response across different application scenarios. These descriptors should be quantified using application-relevant characterization approaches, such as optical and spin-resonance measurements for quantum functions, chemical and colloidal analyses for biological applications, thermal-interface measurements for heat-transfer systems, and electrochemical analyses for sensing platforms.

Beyond material characterization, performance evaluation should also be normalized according to application-specific criteria. Quantum sensing studies should correlate defect and surface environments with spin coherence and sensitivity, whereas imaging and diagnostic studies should consider fluorescence stability, biological compatibility and signal reliability. Similarly, thermal and electrochemical applications require consistent evaluation of interfacial thermal resistance and charge-transfer behaviour, respectively. Establishing such standardized reporting frameworks will enable more meaningful comparison across nanodiamond platforms and accelerate the rational design of application-specific material states.

5.2. Application-Oriented Optimization and Trade-Offs

The concept of an optimal nanodiamond material state is inherently application-dependent. A material configuration that enhances one functionality may introduce limitations in another, because defect populations, surface chemistry, particle dimensions and interfacial structures influence multiple properties simultaneously.

Therefore, nanodiamond optimization should be guided by application-specific requirements rather than by maximizing individual parameters such as defect concentration, fluorescence intensity or thermal conductivity alone.

For quantum sensing, improving colour-centre density or reducing the distance between sensing centres and external targets can enhance signal strength, but these approaches may also increase magnetic noise or surface-induced decoherence. Similarly, surface coatings can improve colloidal stability and suppress fluctuations, while simultaneously increasing probe size and reducing target accessibility. For fluorescence imaging and diagnostics, highly emissive and chemically stabilized nanodiamonds are desirable, yet excessive surface modification may alter biological interactions or increase hydrodynamic dimensions.

Thermal and electrochemical applications present different optimization criteria. In thermal composites, increasing nanodiamond loading and promoting particle connectivity can establish efficient heat-transfer pathways, but aggregation and increased interfacial resistance may limit practical improvements. In electrochemical sensing, surface functionalization and electrode coupling enhance charge-transfer processes and analyte interactions, whereas uncontrolled surface states can reduce reproducibility. These examples demonstrate that nanodiamond performance results from balancing competing requirements among structural, chemical and interfacial characteristics.

Consequently, future nanodiamond development should move beyond material-centred optimization toward application-oriented design strategies, where processing conditions are deliberately tailored to generate the material state required for a specific function. Such an approach provides a rational pathway for improving reproducibility, comparing different nanodiamond platforms and translating laboratory-scale demonstrations into reliable technologies.

5.3. Future Directions toward Scalable Nanodiamond Technologies

Future advances in nanodiamond technologies will depend not only on discovering new functionalities but also on establishing reproducible routes for controlling material states at relevant scales. Although nanodiamonds have demonstrated unique advantages in quantum sensing, biomedical diagnostics, thermal management and electrochemical applications, the transition from laboratory demonstrations to practical technologies remains limited by variations in synthesis, purification, surface modification and integration processes.

A major direction is therefore the development of scalable and controllable manufacturing strategies. Improvements in detonation and high-pressure high-temperature-derived nanodiamond production, together with more precise purification and defect-engineering approaches, are required to reduce batch-to-batch variations. Similarly, scalable surface modification methods should enable controlled chemical states while maintaining particle dispersibility and functional compatibility with target environments. Establishing material-state databases will further facilitate the rational selection of nanodiamond states for specific applications.

Future application development will also require closer integration between nanodiamond materials and device architectures. Quantum technologies will benefit from improved coupling between colour centres, optical structures and sensing environments, whereas biomedical applications require reliable surface engineering and regulatory-compatible platforms. Thermal and electrochemical applications will require scalable assembly strategies that maintain interfacial quality and performance consistency. Rather than pursuing a single universal nanodiamond platform, future technologies will likely rely on application-specific material states optimized for different functional requirements.

Through the combination of standardized characterization, scalable processing and application-driven design, nanodiamonds may evolve from versatile laboratory materials into reproducible functional platforms. This transition will require coordinated efforts in synthesis control, interface engineering and device integration, providing a pathway toward reliable nanodiamond technologies across diverse application fields.

Author Contributions

W.Z.: Conceptualization, Investigation, Data curation, Visualization, Writing—original draft, Writing—review & editing; M.G.: Writing—review & editing; Q.C.: Conceptualization, Supervision, Project administration, Writing—review & editing. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

During the preparation and revision of this manuscript, the authors used ChatGPT (OpenAI) to assist with language polishing and improving the clarity and readability of the text. After using these tools, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

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