Proceedings of the 4th International Conference on Mathematical Physics and Computational Simulation
DOI: 10.54254/2753-8818/2026.33629

Spin-Active Defect Engineering in Hexagonal Boron Nitride for Room-Temperature Single-Photon Emission and Coherent Spin Control

Botao Zheng

Department of Materials Science and Engineering, National University of Singapore, Singapore, Singapore
e1713744@u.nus.edu

Abstract. Hexagonal boron nitride (h-BN) has emerged as a versatile quantum material platform that combines an ultrawide bandgap (UWBG), a two-dimensional van der Waals (vdW) structure, and exceptional chemical stability. These features make h-BN an attractive host for point defects that can act as single-photon emitters (SPEs) and, in certain cases, spin-active centers. This review examines h-BN from three connected perspectives: the structural and electronic properties of the material platform, the nature and engineering of the quantum emitters, and the integration of these optically and spin-active defects into functional quantum components. Particular emphasis is placed on the atomic and electronic structures of the proposed defects, controlled fabrication and engineering approaches, and the resulting optical and spin-related functionalities. Demonstrated applications in integrated quantum photonics, electrical control, and sensing are also summarized, together with the major bottlenecks that still limit practical deployment. Overall, h-BN is argued to be valuable not merely as a host of quantum emitters, but also as a platform where defect physics, material synthesis, and device engineering and integration can be linked. The future of h-BN quantum technology will depend on moving beyond emitter discovery toward defect design supported by theoretical screening, targeted creation, correlative characterization and device-aware optimization.

Keywords: Hexagonal boron nitride, Defect structure engineering, Single-photon emitters, Coherent spin control, Quantum device integration

1. Introduction

Quantum defects hosted by wide-bandgap or ultrawide-bandgap materials have become one of the central building blocks of modern quantum science because they offer localized states that are optically addressable and even spin manipulable. Unlike conventional host materials such as diamond and silicon carbide (SiC), which have established the broader promise for solid-state quantum emitters and spin qubits, the hexagonal boron nitride (h-BN) is attracting growing interest as an alternative host with an ultrawide bandgap of about 6 eV for hosting defect states, and a two-dimensional van der Waals (vdW) structure that can be exfoliated to atomic thickness, transferred

DOI: 10.54254/2753-8818/2026.33629

onto diverse substrates, incorporated into heterostructures, and interfaced directly with external fields and architectures.

Interest in h-BN accelerated after the discovery of room-temperature single-photon emission from its defect centers. Since then, the field has expanded rapidly from the initial observation of bright emitters to more detailed investigations of their photophysics, spin-related behavior, and device integration. First-principles studies have proposed a wide landscape of candidate defect structures, yet direct assignment remains challenging because many distinct structures can produce similar optical signatures. As a result, the investigation of h-BN is not only about discovering bright emitters, but also understanding, reproducing, and tuning the defect origin to match specific quantum applications. The challenge is made intricate by the 2D nature of h-BN, which strongly affects both the opportunities and the challenges of defect engineering, as later discussion reveals.

Studying the h-BN platform for quantum defects thus requires a multi-level perspective: from structure-property mapping at the material level, to defect engineering at the function level, to practical evaluation of performance metrics at the device level. This review follows the exact logic. It first outlines the materials properties that make h-BN a compelling host for optically and spin-active defects, then examines the structures and engineering of those defects, before discussing the optical physics and spin functionalities of h-BN defects as emitters, and finally addressing device integration with an emphasis on design challenges and rules. The key point is that h-BN is not only as a material hosting interesting defects, but also an emerging device platform with potential of linking atomic-scale structures and physics to scalable, functional architectures. h-BN would realize its full value when defect identities and formation, optical and spin properties, and device performance are under a coherent and predictive framework.

2. Material properties of hexagonal boron nitride

Boron nitride was first synthesized from potassium cyanide (KCN) and boric acid (H_3BO_3) via combustion reaction. Later, more stable BN was achieved using boron compounds and alkali metal amides with refined synthetic conditions and post-synthesis treatments. Since then, a series of precursors such as boron halide, B_2H_6, ammonia borane, and borazine have been utilised; various synthesis techniques including mechanical exfoliation, chemical vapor deposition (CVD), and plasma-enhanced atomic layer deposition (PEALD) have also been developed to improve thermal and chemical stability.

It is well established that boron nitride has four basic crystalline phases: hexagonal boron nitride (h-BN), rhombohedral boron nitride (r-BN), cubic boron nitride (c-BN), and wurtzite boron nitride (w-BN). Additional modifications include turbostratic boron nitride (t-BN), amorphous boron nitride (a-BN) and various alternative-dimensional h-BN nanostructures. Among all boron nitride modifications, h-BN has the most thermodynamically stable form under ambient conditions, and is by far the most promising and versatile material for applications in electronics and optoelectronics.

Hexagonal boron nitride (h-BN) consists of vertically stacked sp^2-bonded honeycomb layers held weakly by van der Waals (vdW) forces, with boron and nitrogen atoms in adjacent layers aligned directly above one another, creating a stacking sequence of AA' as shown in Figure 1. Similar to its carbon counterpart, h-BN crystallizes in a hexagonal system of the space group $P6_3/mmc$, with its lattice parameters (a = 2.5038 Å, c = 6.661 Å) in close approximation with graphite (a = 2.464 Å, c = 6.707 Å). In the 2D h-BN structure, both boron and nitrogen atoms adopt sp^2 hybridization to form three strong in-plane σ bonds with neighboring atoms, while the unhybridized $2p_z$ orbitals orient out-of-plane and overlap to form π bonds, resulting in a fully filled valence band and an ultrawide bandgap of about 6 eV. Detailed information on the band structure of h-BN is given in Figure 2.

DOI: 10.54254/2753-8818/2026.33629

Apart from rendering h-BN intrinsically insulating, the ultrawide bandgap makes the material an ideal host for defects to introduce various optical transition energies into its bandgap. The strong B-N bonding also provides excellent chemical and physical protection for defects residing within the structure.

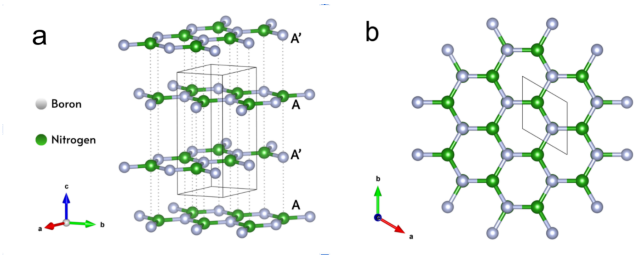

Figure 1. (a) Crystal structure and (b) atomic arrangement in (001) basal plane of h-BN constructed from the relaxed structure calculated using FHI-aims [1]. Initial relaxations were performed with PBE functional, followed by optimization at the HSE06 level, yielding a = 2.4900 Å, c = 6.5144 Å

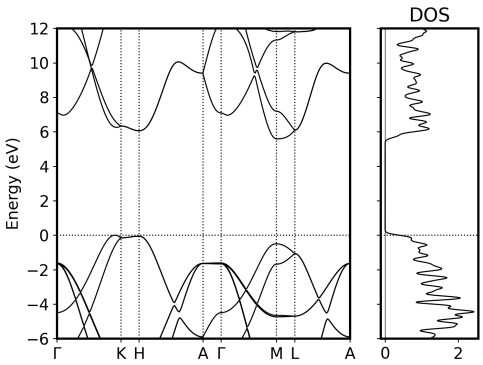

Figure 2. Band structure and density of states (DOS) of h-BN calculated using FHI-aims based on HSE06 functional, yielding an indirect bandgap of ~5.59 eV and a direct bandgap of ~6.09 eV [1]

The layered structure and chemical inertness make h-BN an excellent platform for van der Waals hetero-integration with graphene, transition metal dichalcogenides (TMDs) and other 2D materials to achieve tunable interfacial electronic and optical properties while minimizing dangling bonds or interface charge traps. In pursuit of ultrathin h-BN for efficient extraction of quantum emission and excellent coupling to photonic architectures, epitaxy growth on Cu, Ni or CuNi substrates with borazine or ammonia borane as precursor, and thermal CVD of ultrathin h-BN films at 1000°C using ammonia borane have been demonstrated. The weak interlayer vdW forces also allow various exfoliation methods such as mechanical exfoliation, liquid-phase exfoliation, intercalation-assisted exfoliation and mechanical ball milling. While mechanical exfoliated h-BN with reduced damage or contamination is typically preferred for hosting stable quantum emitters, CVD-grown h-BN is becoming increasingly competitive and dominant with scalable area, layer control and tunable defect incorporation.

3. Defects as spin-active centers: structure and engineering

Point defects in crystals are the fundamental units for quantum applications. Depending on its geometry, symmetry and charge state, a defect may behave as a radiative center, spin-carrying states or trap. Strong localization of defect states is especially essential for quantum photonics since

DOI: 10.54254/2753-8818/2026.33629

strongly localized orbitals favour atom-like optical transitions, narrow spectral features, and well-defined spin manifolds.

Compared to the well-established nitrogen-vacancy (N_V^-) centers in diamond, defect centers in h-BN are particularly attractive by combining room-temperature photon emission and spin functionality with low dimensionality and versatile integrability, yet experimentally observed single photon emitters (SPEs) in h-BN are typically understudied with the lack of information on detailed atomic and electronic structures. Uncovering the microstructure origins will allow for further theoretical predictions, defect-specific engineering and device optimization.

3.1. The atomic and electronic structures of defect centers

Since direct experimental identification of candidate defects remains difficult, first-principles studies have played a central role in predicting the atomic and electronic structures of defects. Hybrid functionals such as HSE06 and CAM-B3LYP are widely used to optimize geometries and evaluate formation energies, charge-transition levels and spin configurations, which help relate candidate defects to experimental observed optical and spin signatures.

To date, a wide range of defect centers in h-BN has been proposed and investigated. Intrinsic vacancies and interstitials (V_B, V_N, B_i, N_i) represent the simplest possibilities, and extrinsic impurities such as substitutional carbon (C_B, C_N) further introduce complexity to the crystal. Beyond isolated defects, many defect complexes have been suggested as spin-active centers, including vacancy-derived complexes such as V_N-C_B, V_B-C_N and V_B-C_N-C_B, interstitial- derived complexes such as B_i-C_B, B_i-C_N and N_i-C_N, and substitutional complexes such as C_B-C_N, C_{2B}-C_N-C_B and C_{6O}. A more comprehensive list of defect families is given in Figure 3. However, not all defect structures are thermodynamically stable. Formation energies depend on chemical potential, charge state and geometries. Isolated defects tend to self-stabilize into more complex forms, such as dimerization of vacancies, electron pairing of C_B-C_N, charge compensation and dangling bond passivation of C_BV_B-nH, pseudo-Jahn-Teller distortion of V_B-C_N, and π delocalization of C_{3B}-C_N [2-5].

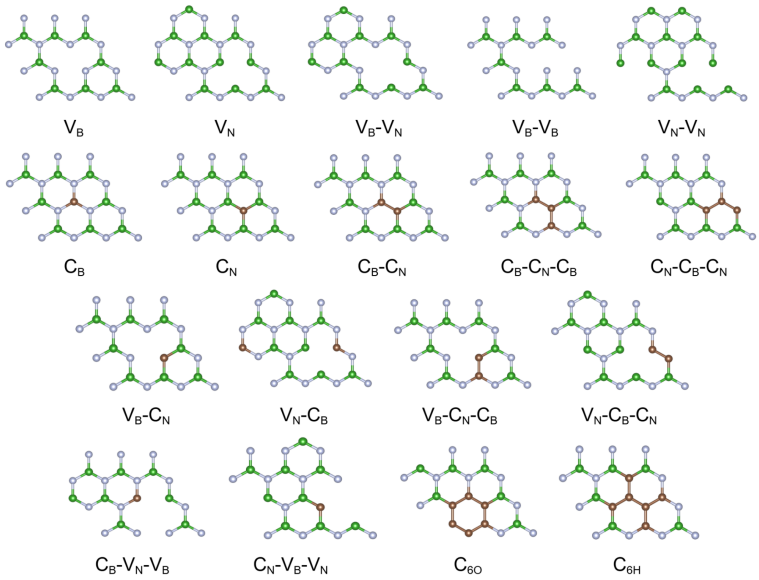

Figure 3. The atomic structures of vacancy and carbon defect centers commonly reported in literatures (green for boron, grey for nitrogen, brown for substitutional carbon)

DOI: 10.54254/2753-8818/2026.33629

Both intrinsic and extrinsic defects exhibit active, localized midgap orbitals, charge-transition levels, and charge-state-dependent occupancy. However, experimentally relevant defects are frequently dominated by impurities and defect complexes, while native vacancies, interstitials and antisites are either thermodynamically or energetically unstable. Substitutional carbon is of particular chemical and electronic importance, with many first-principles studies on carbon-related defect complexes indicating that coupling between neighboring defect orbitals can generate richer manifolds of singlet and triplet states, thereby altering ZPL energies, and in some cases, giving rise to spin-selective optical transitions. While many bright emitters have been associated with carbon-derived complexes, the microscopic identities have not yet been unambiguously resolved and remain theoretical candidates. Within the defect landscape, the negatively charged boron vacancy (V_B^-) remains the best-established example of a defect whose localized in-gap manifold supports a triplet ground state, a triplet excited state and optically detected magnetic resonance, making it a benchmark spin-active center in h-BN [6].

3.2. Formation and engineering of defects centers

For h-BN to become a practical quantum platform for SPEs, reproducible creation, deliberate engineering and precise identification of desirable defects must be realized. The key variables are not only the defect type, but also the location, concentration and charge state of the defect, as well as the local chemical and mechanical environment. Therefore, both growth chemistry and post-growth processing have become important parts of defect engineering.

Defects in h-BN can form spontaneously or be introduced intentionally during crystal growth. Nonstoichiometric growth condition modifies the relative formation energies and equilibrium concentrations of defects, with sublattice selectivity of the same defect type observed in many studies: C_N, C_BC_N and $C_NC_BC_N$ are typically favored under B-rich conditions, while C_B, C_BC_N and $C_BC_NC_B$, are energetically preferred under N-rich conditions [2,3,7]. Kinetically, precursor chemistry, growth temperature, parasitic gas-phase reactions and growth interruption schemes also influence crystal quality and defect incorporation. A further lever is the growth mode: by controlling grain sizes via hydrogen- or oxygen-assisted growth, catalyst and substrate engineering, grain-boundary-related defects are suppressed [3,8,9]. Thus, growth conditions influence not only the film quality, but also the defect identities in the as-grown h-BN.

Post-growth processing techniques provide a comprehensive and versatile toolbox to further create, activate or transform defect centers. Thermal annealing can activate quantum emitters at a temperature over 850°C, is not applicable to temperature-sensitive substrates and lacks spatial determinism. More techniques are developed with different balances of spatial control, collateral damage and chemical specificity, as evaluated in Figure 4. Laser writing uses focused, high-energy, femtosecond lasers to induce bright, stable quantum emitters with efficiency and minimal damage. Plasma treatment bombards the lattice with accelerated ions in the plasma, followed by thermal treatment for lattice reconstruction and site-specific defect formation. Electron-beam irradiation activates defects at chosen locations with submicrometric accuracy, reproducible quantum emission, and better penetration. Ion implantation is more versatile for target defect chemistry and can achieve spatially localized quantum emitters, but causes severe lattice damage. Nanoindentation utilizes localized stress to deform lattice and trigger defect formation, producing site-specific emitters that could be scaled to large arrays.

DOI: 10.54254/2753-8818/2026.33629

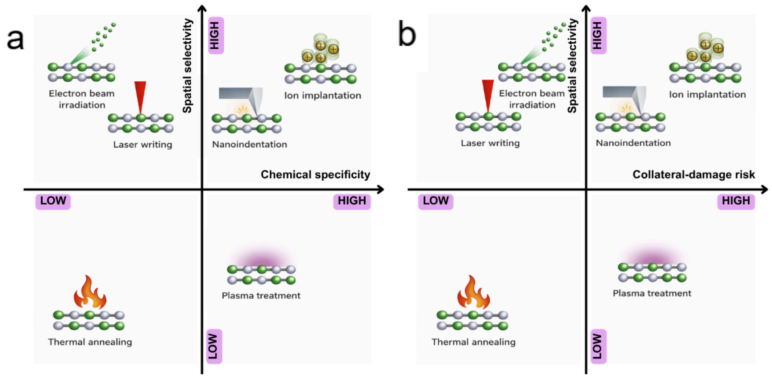

Figure 4. Schematic diagram of 6 common post-synthesis processing approaches evaluated in terms of(a) Spatial selectivity - Chemical specificity and (b) Spatial selectivity - Collateral damage risk

Beyond the established synthesis and post-synthesis methods, emerging defect engineering strategies are seeking to target defect specificity or site-deterministic creation more directly. Liu et al. showed that methane-assisted CVD can regulate surface carbon concentration in monolayer h-BN, Tang et al. demonstrated carbon-defect transition by substrate-controlled carbon supply tuning, and Wu et al. reported site-controlled carbon implantation as a more position-controlled, type-specific engineering approach [10-12]. Atomic-scale engineering and strain modulation of individual defects in h-BN via combined STM/AFM approaches are recently explored, though it remains far less mature than controlled growth or implantation [13].

4. Optical properties and spin-photon coupling

Since the demonstration of room temperature h-BN single-photon emission in 2016, the field has expanded into a broader program covering optical and spin coherence, spectral tuning, spin-photon interfaces and device integration. The appeal of h-BN lies in the possibility of combining single-photon emission with spin addressability in the versatile 2D platform, and the quality of this combination defines the progress.

4.1. Principles of quantum emission in hexagonal boron nitride

Similar to other solid-state emitters, SPEs in h-BN behave like a non-ideal two-level atomic system in a crystal matrix with significant coupling to the solid-state environment, reflected in the emission spectrum by a sharp zero-phonon line (ZPL) corresponding to pure electronic transition, accompanied by a broad phonon sideband (PSB) as a result of vibronic coupling. Polarization-resolved studies suggest that absorption and emission dipoles are not always perfectly aligned, indicating that optical transitions in h-BN may involve multilevel pathways rather than a strict two-states configuration-coordinate picture.

Three optical excitation schemes, as shown in Figure 5(a), are commonly discussed. Resonant excitation, where the excitation energy precisely matches that of the optical transition, is the most efficient scheme due to the huge absorption cross section at the ZPL. The excitation and emission lights are separated by wavelength or by polarity: Spectral filtering collects photons in the PSB window at the cost of coherence, while cross-polarizing the two lights yield purer and more coherent photons at the ZPL. Stokes excitation involves an excitation energy higher than the optical transition and phonon-assisted relaxation before emission. This yields higher purity but lower coherence, since the wide PSB allows for larger spectral separation between excitation and emission, but its

DOI: 10.54254/2753-8818/2026.33629

inefficiency requires higher excitation power that causes local heating and linewidth broadening. Contrary to Stokes excitation, Anti-Stokes excitation uses laser energies lower than the optical transition and absorbs extra phonons to assist excitation. The lower-energy pump can better suppress spectral diffusion compared to Stokes excitation, and the involvement of phonons allows selective excitation of target defect centers.

A photon is emitted when an electron decays from the excited state back to the ground state. The average time the electron stays in the excited state is the excited-state lifetime. A shorter lifetime suggests higher repetition rate, but also a greater tendency of non-radiative transition and linewidth broadening. SPEs found in h-BN typically have a lifetime of ~1-3 ns, which is shorter than many color centers such as NV^- in diamond (~12-22 ns) and V_{Si} in SiC (~5 ns). Mashnoon et al. pushes its lifetime further below 0.5 ns via Purcell enhancement in pursuit of ultra-brightness, while Xu et al. extended its lifetime to 1.9 ns via two-photon excitation to improve emission stability and coherence [14,15]. Despite the short lifetime, emitters in h-BN have a high radiative decay percentage, or quantum efficiency, up to 87±7%, which also surpasses most group-IV centers in diamond (typically reported to be ~ 30%). These superior optical properties make SPEs in h-BN one of the brightest solid-state emitters, attracting continuous research on improving coherence, purity and photostability.

Similar to absorption, photon emission spans some energy range, with the highest intensity at the ZPL (responsible for ~ 70% of the emission) and the rest within the PSB window at lower energies, as depicted in Figure 5(b). Single-photon character is commonly verified by Hanbury Brown–Twiss measurements of the second-order autocorrelation function, $g^{(2)}(\tau)$, in which an antibunching dip at zero delay ($g^{(2)}(\tau) < 0.5$) confirms single-photon emission. For h-BN SPEs, $g^{(2)}(\tau) < 0.1$ is achievable by creating one dominant emitter through in situ doping, ultrasonic nanoindentation, or single-pulse laser writing while suppressing emitters or contaminants that contribute to background fluorescence via thermal annealing. Beyond purity, spectral measurements also provide access to lifetime, spectral diffusion, linewidth, and ZPL fraction that are key metrics in determining the emission quality and specific application.

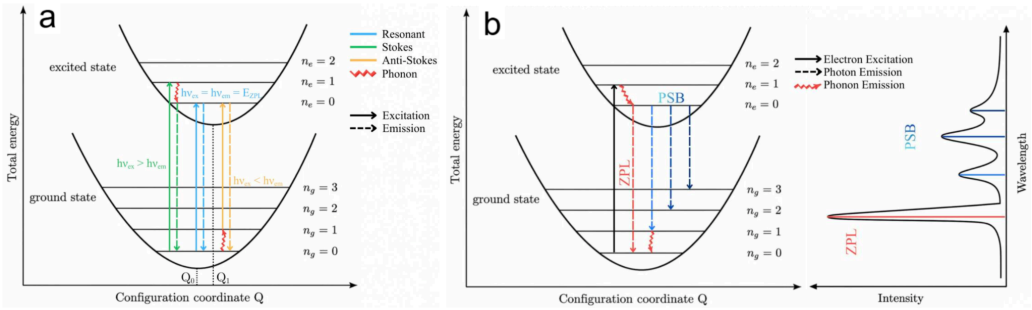

Figure 5. (a) Configuration coordinate diagram (CCD) of the three excitation schemes: resonant, Stokes, and anti-Stokes; (b) absorption-emission in a CCD and the corresponding emission spectrum

4.2. Spin-related functionalities beyond single-photon emission

h-BN is attractive not only for hosting bright SPEs, but also for hosting optically addressable spin defects. Unlike conventional SPEs, a spin-active SPE acts as a spin–photon interface that combines optical addressability, efficient optical transition, and robust spin coherence. This is highly valuable for quantum applications, where the spin stores and accumulates information, while the photon carries it over long distances. Spin coherence determines how well the spin preserves information.

DOI: 10.54254/2753-8818/2026.33629

Longer coherence allows more time for spin to preserve or accumulate phase, thus improving memory performance and sensitivity in quantum applications.

The working principle of a spin-photon interface is the optical manipulation of spin states via spin-dependent excitation and decay pathways. Spin-selective intersystem crossing produces spin-dependent fluorescences, which enables optical spin initialization and readout, turning a passive emitter into a spin-active device. Optically detected magnetic resonance (ODMR), the primary tool for probing and controlling such system, exploits the spin-dependent optical behavior by applying microwave radiation resonant with the spin splitting, which drives Rabi oscillation between spin sublevels to alter photoluminescence, allowing the spin transition to be read out optically. In the h-BN, defects can sit only a few atomic layers from the surface and probe nearby magnetic fields with high spatial resolution. Room-temperature ODMR has been observed in both boron-vacancy-related and carbon-related single defects, showing that h-BN can host optically addressable spins rather than merely bright emitters.

Among known h-BN defects, V_B^- is the best-established spin defect. It exhibits a ground-state spin triplet with zero-field splitting near 3.45 GHz between $m_s = 0$ and $m_s = \pm 1$ spin sublevels and room-temperature ODMR, but its inherent low quantum efficiency (~6-12%) as a result of broad phonon-assisted emission at ~800 nm limits its brightness and sensitivity [16,17]. On the other hand, carbon-related defects are gaining increasing research attention because they offer visible, efficient single-photon emission and spin addressability. Coherent spin control of carbon-related SPEs in h-BN, identified to be a spin-triplet ground-state manifold, has been achieved under ambient conditions, yet the true identities of the quantum emitters in h-BN remains elusive, with most assignments based on indirect spectroscopy and first-principles investigation rather than atomistic identification [18].

5. Device integration and design considerations

Unlike conventional 3D defect hosts, h-BN can be exfoliated, transferred, stacked, patterned, and integrated with other 2D materials and photonic structures. This makes h-BN attractive as a material with optically and spin-active defects that can also be embedded into hybrid device architectures. The relevance of h-BN to device integration was first established in the broader 2D materials community as an atomically flat, chemically stable, low-disorder substrate for graphene devices, and has subsequently become a central component in vdW heterostructures involving graphene, transition-metal dichalcogenides (TMDs) and other 2D crystals.

In that sense, h-BN demands a more integrated view of material engineering. An emitter with excellent photoluminescence in an isolated flake is not automatically device-ready. Desirable defects must also be identifiable, reproducible, spectrally stable and tunable if necessary, and compatible with the surrounding environment. Device design requires bridging atomic defect physics with photonic mode engineering, electrical control, and architecture integration rather than treating these as separate problems. Device relevance therefore becomes the key metric.

5.1. Demonstrated applications and device integration

A direct application of single-photon emitters is quantum photonics, where non-classical light emitted by SPEs is essential for quantum key distribution, photonic quantum computing, and integrated quantum optics. h-BN emitters operating at room temperature can be exceptionally bright and integrable into nanophotonic structures. In monolithic integration, h-BN is directly patterned into optical structures such as waveguides and cavities, so that emitters coexist with the photonic

DOI: 10.54254/2753-8818/2026.33629

mode, enhancing quality factor, coupling efficiency, and photon collection. In hybrid integration, h-BN provides active SPEs and other more mature photonic platforms provide waveguides, resonators or cavities, with SPEs maintaining high single-photon purity after encapsulation and nanofabrication. Another device application is quantum sensing. The 2D nature of h-BN allows defects to be placed atomically close to the target environment while being optically accessible, serving as a local probe that reads out magnetic field, strain, or temperature via photoluminescence. Already demonstrated in V_B^- centres, it is now being used for quantitative magnetic imaging of vdW ferromagnets such as Fe_3GeTe_2 and strain sensing in h-BN flakes [19,20]. More recent work shows that carbon-related spin defects can act as multi-axis nanoscale magnetic sensors for vectorial quantum magnetometry [21].

Optical excitation alone is for laboratory demonstrations, but scalable quantum technologies require control over emission intensity, wavelength, charge state, and switching behaviours. The graphene/h-BN heterostructure with graphene as an atomically thin electrode and h-BN as the host for SPEs has demonstrated stark tuning of SPEs, reversibly activation and bias modulation, suggesting that many emitters in h-BN may exist in optically dark states and become active only under suitable electrostatic conditions. Therefore, the optical behaviour of h-BN defects depends not only on atomic structure, but also on charge environment, local electric field and heterostructure geometry.

5.2. Design challenges in device fabrication and integration

Despite rapid progress made, the practical application of h-BN emitters is still limited by two levels of challenges: at the emitter-level, the microscopic identity, reproducibility and optical stability, and at the device-level, coupling to photonic architectures. It is necessary to separate the challenges into two levels since solving one does not automatically solve the other: a defect performing well in an isolated flake is not necessarily device-ready, and a sophisticated platform cannot compensate for an unidentified or unstable emitter.

At the emitter-level, the key challenges are identification, reproducibility, and stability. h-BN can host many candidate defects with similar photoluminescence signatures, making atomic assignment difficult for optical spectra alone. A combination of growth control, post-growth engineering, computational screening and spectroscopy is often required. Therefore, many SPEs are discovered only statistically, but in integrated devices, one must control not only the defect identity, but also the position, emission, charge state and spin functionality. Significant progress has been made. However, full control of the exact defect species and device-relevant properties remains incomplete. In addition, practical devices require SPEs to be stable under fabrication, illumination, electrical bias, and cycling. Instabilities such as blinking, bleaching, spectral diffusion and charge-state switching remain performance-limiting issues, especially for integrated photonics where a cavity or waveguide may enhance emission of a defect only if it remains spectrally stable and well aligned with the optical mode.

At the device level, the key challenges are optical coupling, fabrication compatibility, control, and scalability. Emitters must be spatially close to optical mode maxima and spectrally close to the photonic mode to ensure efficient coupling, and must survive transfer, lithography, annealing, metallization or encapsulation, all of which can introduce strain, surface damage, charge traps or local disorder, and cause spectral diffusion, broaden the linewidth, destabilize the charge state or quench emission. In addition, practical devices may require wavelength tuning, charge states stabilization or optical output modulation, yet electrical or strain control can introduce additional noise and stability if not well applied. Ultimately, a scalable platform demands spatially controlled,

DOI: 10.54254/2753-8818/2026.33629

spectrally matched, stable emitters that are compatible with the photonic architecture as well as the full fabrication workflow, which remains limited.

5.3. Design rules, trade-offs and future research directions

A useful design framework for h-BN defect devices should start from the structure–property relationship. At the structure level, important variables include defect species, charge state, local symmetry, layer thickness, strain field, nearby impurities, dielectric environment and proximity to surfaces. These govern optical metrics such as ZPL energy, Debye–Waller factor, linewidth, brightness, lifetime, polarization, spectral diffusion and photostability, and spin properties such as spin multiplicity, zero-field splitting, ODMR contrast, coherence time, and hyperfine coupling. At the device level, these microscopic properties must be matched to the intended function and be consistent during operation.

Quantum photonics favor bright, stable single-photon emission with high SP purity, a narrow linewidth, a large ZPL fraction, or Debye–Waller factor, and a predictable dipole orientation. Quantum sensing instead prioritizes strong spin-dependent photoluminescence, large ODMR contrast, long coherence time and strong coupling to the external field of interest over optical indistinguishability. For electrically tunable devices, stable charge-state control and resistance to quenching near graphene or metal electrodes become crucial. There is no best h-BN defect – different device functions necessitate different optimal defects, as summarized in Table 1.

Table 1. Indicative target metrics for h-BN quantum emitters in representative quantum applications: $g^{(2)}(0)$ denotes multiphoton suppression, M denotes photon indistinguishability, CE is the collection efficiency, RR is the repetition rate, <n> is the mean photon number per pulse, OT is the preferred operating temperature, and T2 is the spin coherence time

Application	$g^{(2)}(0)$	M	CE	RR (GHz)	<n>	OT	T_2 (ms)
Quantum key distribution	<0.1	-	>0.5	>0.1	≈1	RT	-
Optical quantum computing	<0.01	>0.99	>0.9	1	≈1	-	-
Spin-photon interface	<0.1	>0.8	>0.3	>0.1	≈1	RT	>0.1
Quantum radiometry	<0.01	-	>0.99	>0.9	≈1	RT	-
Imaging	-	-	>0.5	-	-	RT	-
Quantum sensing	-	-	>0.5	-	-	RT	>0.01

Design trade-offs are fundamental. To illustrate, thin h-BN flakes maximize surface proximity, making integration with other 2D materials easier, but on the other hand, expose defects more to surface adsorbates, charge noise and environmental fluctuations; by contrast, thicker h-BN flakes improve optical stability and reduce noise, but may weaken near-field sensing. Another example is, high-energy irradiation can create emitters at chosen locations, but may introduce undesirable damage and secondary defects; growth-based doping can improve scalability, but may produce a distribution unless growth chemistry is strictly controlled. The comprehensive engineering trade-offs are summarized in Table 2. The practical challenge is not to maximize every property simultaneously, but to identify the optimal compromise for target applications.

DOI: 10.54254/2753-8818/2026.33629

Table 2. Qualitative engineering trade-off chart for h-BN quantum defect platforms. Device design is governed not by a single optimization axis, but a network of coupled engineering trade-offs

Engineering parameter		Gain	Sacrifice	Trade-off	Applications
Host thickness	Thin h-BN flake	Surface proximity, coupling, vdW hybrid integration	Photostability, charge-state stability	Sensitivity vs Stability	Quantum sensing, hybrid vdW device integration
	Thick h-BN flake	Bulk isolation, optical stability	Surface proximity, sensing resolution		Stable SPEs, cavity -coupled photonics
Defect creation	Deterministic	Site control, scalable pattern	Scalability, extra damage	Precision vs Throughput	Deterministic arrays, targeted defect type
	Growth-based	Scalability, wafer- level compatibility	Site precision		Large-area manufacturing
Local strain field	More strain	Activation, tuning, localization	Mechanical and spectral instability	Tunability vs Uniformity	Cavity matching, targeted defect type
	Less strain	Spectral uniformity	Tunability		Uniform SPEs
Photonic environment	Strong cavity coupling	Brightness, CE enhancement	Spatial, spectral & dipole alignment, ease of fabrication	Brightness vs complexity	On-chip quantum photonics
	Weak cavity coupling	Simple fabrication, less mismatch	Brightness		Standalone SPEs, passive photonics
Electrical control	Strong contact coupling	Charge-state control, Stark tuning, modulation	Charge noise, screening, quenching	Control vs Disturbance	Tunable quantum emitters for opto-electronic devices

DOI: 10.54254/2753-8818/2026.33629

Table 2. (continued)

	Weak contact coupling	Isolation, better optical stability	Active control, tunability		Passive photonic devices
Device architecture	Hybrid	Mature external platform	Alignment issue, complex interface	Maturity vs Unity	Practical integrated devices
	Monolithic	Material simplicity, compact integration	Less mature fabrication		Proof-of-concept devices
Operation condition	Room temperature	Practical deployment	Coherence and indistinguishability	Practicality vs Performance	Room temperature sensing
	Cryogenic temperature	Coherence and indistinguishability	Practical deployment		Quantum network, advanced photonics

A forward-looking h-BN platform should be designed around an experimental–computational workflow. First, synthesis and engineering methods should be selected according to the target defect. First-principles calculations should then be used to screen candidate structures for key properties such as formation energy, optical transition energies, spin multiplicity, and strain or electric-field response. Correlative characterization should link atomic structure to measured optical or spin behaviors via photoluminescence, ODMR and Raman mapping. Device testing should be performed early since an emitter that performs well in an isolated flake may behave differently after transfer, encapsulation, and nanofabrication.

This reflects a broad shift from emitter discovery to defect design. Reliable progress requires building defect databases that connect atomic structure, synthesis condition, optical spectrum, spin signature and device performance. An ideal h-BN platform with single-photon emission and coherent spin control would satisfy four criteria: deterministic identification and creation, reproducible optical and spin properties, tunable and stable charge state and emission energy, and compatible photonic integration. In practice, the best h-BN quantum defect is not simply the brightest emitter or with the longest-coherence spin, but the one that can be deliberately engineered, stabilized and coupled to a device.

6. Conclusion

This review has shown that progress in h-BN quantum emitters depends on multiple levels of understanding, from host electronic structure and defect physics to synthesis and processing, to device integration and optimization. First-principles studies have revealed a broad family of intrinsic and extrinsic defects that can generate localized states, spin manifolds and optical transitions. However, theoretical richness also underscores the central issue: the microscopic identities of many

DOI: 10.54254/2753-8818/2026.33629

experimentally observed emitters remain uncertain. It is important not only to catalogue possible defects, but to determine which defects are experimentally reproducible and application-relevant, and how they can be stabilized and optimized. Defect formation is found to be highly sensitive to synthesis and processing history. But despite this expanding engineering toolbox, reproducibility and defect specificity remain incomplete.

From a functional standpoint, h-BN defect centers exhibit bright single-photon emission, high quantum efficiency, tunable optical response, and in selected cases, optically addressable spin states. Room-temperature ODMR and coherent control extends its role beyond a simple SPE host. From a structural standpoint, the 2D vdW structure of h-BN allows intimate coupling to photonic architectures, electrical components, and vdW heterostructures, while also enabling near-surface sensing with high spatial resolution. The design rule is that integrated quantum applications require bright emitters that are position-controlled, spectrally stable, electrically or mechanically tunable, and nanostructure-compatible.

Overall, h-BN possesses a distinctive and constantly evolving position in quantum materials. It may not yet match diamond NV centers in spin coherence or III–V quantum dots in optical indistinguishability, but it offers a rare combination of room-temperature emission and spin addressability, surface sensitivity, and heterostructure compatibility as a versatile 2D material platform. The future impact of h-BN quantum technology therefore depends on closing the gap between atomic-scale defect physics and scalable device implementation, which demands not only better quantum emitters, but better design rules.

References

[1] Blum, V., Gehrke, R., Hanke, F., Havu, P., Havu, V., Ren, X., Reuter, K., & Scheffler, M. (2009). Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 180(11), 2175–2196. https: //doi.org/10.1016/j.cpc.2009.06.022

[2] Weston, L., Wickramaratne, D., Mackoit, M., Alkauskas, A., & Van de Walle, C. G. (2020). Native point defects and impurities in hexagonal boron nitride. Physical Review B, 102(9). https: //doi.org/10.1103/physrevb.102.099903

[3] Huang, P., Grzeszczyk, M., Vaklinova, K., Watanabe, K., Taniguchi, T., Novoselov, K. S., & Koperski, M. (2022). Carbon and vacancy centers in hexagonal boron nitride. Physical Review B, 106(1). https: //doi.org/10.1103/physrevb.106.014107

[4] Maciaszek, M., & Baur, B. (2026). CBVB-nH complexes as prevalent defects in metal-organic vapor-phase epitaxy-grown hexagonal boron nitride. Npj 2D Materials and Applications. https: //doi.org/10.1038/s41699-026-00675-4

[5] Li, S., & Gali, A. (2022). Bistable carbon-vacancy defects in h-BN. Frontiers in Quantum Science and Technology, 1. https: //doi.org/10.3389/frqst.2022.1007756

[6] Mu, Z., Cai, H., Chen, D., Kenny, J., Jiang, Z., Ru, S., Lyu, X., Koh, T. S., Liu, X., Igor Aharonovich, & Gao, W. (2022). Excited-State Optically Detected Magnetic Resonance of Spin Defects in Hexagonal Boron Nitride. Physical Review Letters, 128(21), 216402–216402. https: //doi.org/10.1103/physrevlett.128.216402

[7] Maciaszek, M., Lukas Razinkovas, & Audrius Alkauskas. (2022). Thermodynamics of carbon point defects in hexagonal boron nitride. Physical Review Materials, 6(1). https: //doi.org/10.1103/physrevmaterials.6.014005

[8] Malik, M. W., Ullah, S., Wang, B., Jaddi, S., Zeng, Y., & Raskin, J.-P. (2023). Oxygen activated CVD growth of large-area multilayer h-BN on polycrystalline copper foils. Journal of Crystal Growth, 606, 127088. https: //doi.org/10.1016/j.jcrysgro.2023.127088

[9] Lu, G., Wu, T., Yuan, Q., Wang, H., Wang, H., Ding, F., Xie, X., & Jiang, M. (2015). Synthesis of large single-crystal hexagonal boron nitride grains on Cu–Ni alloy. Nature Communications, 6(1). https: //doi.org/10.1038/ncomms7160

[10] Liu, H., Mendelson, N., Abidi, I. H., Li, S., Liu, Z., Cai, Y., Zhang, K., You, J., Mohsen Tamtaji, Wong, H., Ding, Y., Chen, G., Igor Aharonovich, & Luo, Z. (2022). Rational Control on Quantum Emitter Formation in Carbon-

DOI: 10.54254/2753-8818/2026.33629

Doped Monolayer Hexagonal Boron Nitride. ACS Applied Materials & Interfaces, 14(2), 3189–3198. https: //doi.org/10.1021/acsami.1c21781

[11] Tang, T. W., Ritika Ritika, Mohsen Tamtaji, Liu, H., Hu, Y., Liu, Z., Galligan, P. R., Xu, M., Shen, J., Wang, J., You, J., Li, Y., Chen, G., Igor Aharonovich, & Luo, Z. (2025). Structured-Defect Engineering of Hexagonal Boron Nitride for Identified Visible Single-Photon Emitters. ACS Nano. https: //doi.org/10.1021/acsnano.4c11413

[12] Wu, Y.-T., Guo, X., Jing, P.-T., Liu, G.-L., Cheng, Z., Xu, J.-L., Bao, Y., Xu, H., Zhang, L.-G., Zhan, D., Yan, J.-X., Liu, L., & Shen, D.-Z. (2025). Site-Controlled Carbon Implantation for Quantum Emitter Engineering in Hexagonal Boron Nitride. ACS Applied Materials & Interfaces, 17(47), 64864–64874. https: //doi.org/10.1021/acsami.5c16791

[13] Yang, T., Huang, P., Qiu, Z., Han, Y., Guan, D., Lyu, P., Su, J., Novoselov, K. S., Fang, H., & Lu, J. (2026). Atomic-Scale Engineering and Strain Modulation of Quantum Defects in Hexagonal Boron Nitride. ACS Nano, 20(13), 10594–10604. https: //doi.org/10.1021/acsnano.5c22322

[14] Mashnoon Alam Sakib, Triplett, B., Harris, W., Hussain, N., Senichev, A., Melika Momenzadeh, Bocanegra, J., Polina Vabishchevich, Wu, R., Boltasseva, A., Shalaev, V. M., & Shcherbakov, M. R. (2024). Purcell-Induced Bright Single Photon Emitters in Hexagonal Boron Nitride. Nano Letters, 24(40), 12390–12397. https: //doi.org/10.1021/acs.nanolett.4c02581

[15] Xu, Q., Gao, B., Zhao, L., Lv, G., Yang, J., & Li, X. (2025). Enhanced Performance of Single-Photon Emitter Hosted in Hexagonal Boron Nitride via Two-Photon Excitation. ACS Photonics, 12(4), 2178–2186. https: //doi.org/10.1021/acsphotonics.5c00105

[16] Scholten, S. C., Singh, P., Healey, A. J., Robertson, I. O., Haim, G., Tan, C., Broadway, D. A., Wang, L., Abe, H., Ohshima, T., Kianinia, M., Reineck, P., Aharonovich, I., & Tetienne, J.-P. (2024). Multi-species optically addressable spin defects in a van der Waals material. Nature Communications, 15(1). https: //doi.org/10.1038/s41467-024-51129-8

[17] Li, X., Scully, R. A., Shayan, K., Luo, Y., & Strauf, S. (2019). Near-Unity Light Collection Efficiency from Quantum Emitters in Boron Nitride by Coupling to Metallo-Dielectric Antennas. ACS Nano, 13(6), 6992–6997. https: //doi.org/10.1021/acsnano.9b01996

[18] Stern, H. L., M. Gilardoni, C., Gu, Q., Eizagirre Barker, S., Powell, O. F. J., Deng, X., Fraser, S. A., Follet, L., Li, C., Ramsay, A. J., Tan, H. H., Aharonovich, I., & Atatüre, M. (2024). A quantum coherent spin in hexagonal boron nitride at ambient conditions. Nature Materials, 23(10), 1379–1385. https: //doi.org/10.1038/s41563-024-01887-z

[19] Huang, M., Zhou, J., Chen, D., Lu, H., Nathan, Li, S., Alghamdi, M. A., Djugba, D., Shi, J., Wang, H., & Du, C. (2022). Wide field imaging of van der Waals ferromagnet Fe3GeTe2 by spin defects in hexagonal boron nitride. Nature Communications, 13(1). https: //doi.org/10.1038/s41467-022-33016-2

[20] Lyu, X., Tan, Q., Wu, L., Zhang, C., Zhang, Z., Mu, Z., Zúñiga-Pérez, J., Cai, H., & Gao, W. (2022). Strain Quantum Sensing with Spin Defects in Hexagonal Boron Nitride. Nano Letters, 22(16), 6553–6559. https: //doi.org/10.1021/acs.nanolett.2c01722

[21] Gilardoni, C. M., Barker, S. E., Curtin, C. L., Fraser, S. A., Powell, O. F. J., Lewis, D. K., Deng, X., Ramsay, A. J., Adhikari, S., Li, C., Igor Aharonovich, Tan, H. H., Mete Atatüre, & Stern, H. L. (2025). A single spin in hexagonal boron nitride for vectorial quantum magnetometry. Nature Communications, 16(1), 4947–4947. https: //doi.org/10.1038/s41467-025-59642-0