

THE EFFECT OF TEMPERATURE ON THE EMISSION PROPERTIES OF BORON NITRIDE: EXPERIMENTAL AND DFT ANALYSIS

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Abstract. Hexagonal boron nitride (h-BN) is a wide-bandgap semiconductor with structural and electronic characteristics that make it a promising material for diverse technological applications. In this work, the electronic and optical properties of pristine and multilayered h-BN nanosheets were systematically investigated using density functional theory (DFT) simulations. The findings provide valuable insights into the fundamental properties of h-BN nanosheets and their potential for applications in electronics, photonics, and energy storage devices. The 2.2 eV emission observed in BN material occurs as a result of localized states associated with defects, and these emission lines become more intense and sharper with decreasing temperature. The fact that the energy position (2.2 eV) remains constant at both temperatures indicates that the emission is associated with specific defect states and that the energy position of these states does not change with temperature. The correlated color temperature (CCT) and color rendering index (CRI) were determined based on the specific color coordinates obtained from the emission spectra of this compound using the Color Calculator software developed by OSRAM SYLVANIA.

Keywords: Hexagonal boron nitride, nanosheets, emission, color temperature.

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1 Introduction

Boron nitride (BN) is a wide-bandgap semiconductor with a hexagonal crystal structure, which is closely related to graphite. In its bulk form, BN exists in several polymorphs, including hexagonal boron nitride (h-BN), cubic boron nitride (c-BN), and wurtzite boron nitride (w-BN), each of which exhibits distinct properties (Hidalgo et al., 2013; Wentorf et al., 1980; Akashi et al., 1986; Solozhenko et al., 1999). The hexagonal form, h-BN, is the most well-known and studied, consisting of alternating boron and nitrogen atoms arranged in a honeycomb lattice (Fukamachi et al., 2023). This structure is similar to graphite, with layers held together by weak van der Waals forces, allowing for easy exfoliation into two-dimensional (2D) nanosheets. These 2D nanosheets exhibit unique properties that differ significantly from the bulk material, making them a subject of intense interest in materials science (Ismayilova, 2025). Further studies have also highlighted the significance of such 2D nanosheets (Ismayilova et al., 2024).

Earlier research has also contributed to the understanding of these materials (Roy et al.,

2021; Asadullayeva et al., 2022). Corso et al. (2004) and Novoselov et al. (2005) successfully synthesized hexagonal boron nitride (h-BN), a structure resembling graphene. This material exhibits excellent electrical insulating properties and remarkable thermal conductivity (Novoselov et al., 2005).

In its bulk form, h-BN is an electrical insulator with a wide band gap (~ 5.9 eV) (Fan et al., 2022), making it a promising candidate for applications in neutron detectors (Watanabe et al., 2004; Golberg et al., 2010; Ahmed et al., 2016; Jahangirli et al., 2025), ultraviolet light emitters (Watanabe et al., 2009; Jiang & Lin, 2017), single-photon emitters (Tran et al., 2016; Liu et al., 2022), nano photonics (Taylor, 1955; Caldwell et al., 5). The stability and inertness of h-BN also make it an ideal material for use in extreme environments, including high-temperature and high-radiation conditions (Gonzalez *et al.*, 2018). In contrast to graphene, which is highly conductive, the insulating nature of BN is attributed to the presence of a significant band gap, making it ideal for use as a substrate in graphene-based devices, where electrical isolation is needed (Dean et al., 2010).

When exfoliated into nanosheets, the properties of BN undergo significant changes, particularly in terms of surface area, electronic structure, and mechanical behavior. These 2D BN nanosheets maintain the hexagonal lattice structure of their bulk counterpart but exhibit enhanced properties due to their reduced dimensionality. The wide bandgap of bulk BN is preserved in the nanosheet form, but their electronic properties can be tuned by doping, functionalization, or applying external strain (Topsakal et al., 2009), Elaheh et al., 2025. Additionally, BN nanosheets exhibit high mechanical strength, excellent thermal conductivity, and high chemical stability, making them promising materials for applications in composite materials, sensors, and energy storage devices (Vanmathi et al., 2024). Beyond two-dimensional systems, comparable advances have also been reported for three-dimensional boron nitride and related nanostructured materials (Asadullayeva et al., 2025). These 3D structures, including porous frameworks, bulk nanocomposites, and hierarchical assemblies, have demonstrated excellent stability, tunable porosity, and enhanced functional performance. Their unique structural characteristics enable applications in catalysis, adsorption, energy storage, and electronic devices, extending the versatility of BN-based materials beyond their 2D forms (Mehrabova et al., 2024; Asadullayeva et al., 2024; Tagiyev et al., 2015; Ismayilova et al., 2024; Naghiyev et al., 2022).

From a theoretical perspective, Density Functional Theory (DFT) has been extensively applied to study the properties of BN nanosheets at the atomic scale. DFT calculations provide valuable insights into the electronic structure, charge distribution, optical properties, and the effects of various modifications such as doping, defects, or functionalization. For example, DFT studies have shown that doping BN nanosheets with different elements can modify their electronic properties, allowing for the tuning of the bandgap or the introduction of magnetism (Debashis et al., 2021). Investigation carried out by Debashis et al., (2021) reveal that, the V-Ir and W-Fe co-doped h-BN nanosheets (h-BNNS) exhibit strong half-metallic behavior in the ferromagnetic (FM) state, while the Ti-Ni and Ta-Ru co-doped h-BNNS display diluted magnetic semiconducting behavior, making these TM-TM pair co-doped h-BNNS promising candidates for spintronic applications. Similarly, applying strain to BN nanosheets can lead to changes in their electronic band structure, making them suitable for various applications in flexible electronics (Liu et al., 2022).

DFT also plays a crucial role in understanding the interactions of BN nanosheets with other materials. This includes studies on their interaction with molecules for use in gas sensing, or their integration with other 2D materials to create heterostructures with enhanced properties. The ability to model these interactions at the atomic level allows for the design and optimization of BN nanosheets for specific technological applications.

As BN nanosheets continue to show promise in various fields, DFT remains an essential tool for exploring their fundamental properties and guiding experimental efforts in the design of advanced nanomaterials. The continued study of BN nanosheets via DFT simulations will enable

the tailoring of these materials for cutting-edge applications in electronics, catalysis, and energy storage. The optical properties of BN can be controlled through defect engineering and doping, making it a promising material for various laser systems, light-emitting diodes, and quantum technologies. This makes BN suitable for applications in low-temperature quantum optics, photonic devices, optical sensors, and bioimaging technologies. In addition, this study also reveals the possibilities of controlling the emission properties of BN through defect engineering.

2 Research methods

2.1 Experimental method

Photoluminescence (PL) measurements were carried out using a PL/PLE/Raman spectrometer device manufactured in Japan. The emission of the samples was studied using lasers with different wavelengths: 532 nm (Nd- YAG) and 785 nm. Photoluminescence from the sample was scattered by a grating (100 g/mm-1) monochromator MS 5207 I and MS 3704 I (SOL Instruments, Inc), detected by a CCD multiplier DU 491A-1.7.

2.2 DFT method

To explore the effects of substitutional doping on the electronic properties of boron nitride (BN) nanosheets, we performed theoretical simulations using Density Functional Theory (DFT), as implemented in the Quantum Atomistix ToolKit (QuantumATK) software package. The exchange-correlation interactions were approximated using the generalized gradient approximation (GGA), with the Perdew-Burke-Ernzerhof (PBE) functional for the parameterization. To describe the electron-ion interactions, norm-conserving pseudopotentials from the PseudoDojo library were employed. The hybrid Heyd-Scuseria-Ernzerhof (HSE06) functional was utilized for accurate electronic structure calculations.

The Monkhorst-Pack method was applied for k-point grid sampling, with a grid of $11 \times 11 \times 1$ used for structural optimizations and $16 \times 16 \times 1$ for property calculations. A plane-wave energy cutoff of 500 eV was set to ensure convergence of the calculations. Both the pristine and doped nanosheets were fully optimized until the forces on each atom were reduced to below 0.005 eV/Å and the total energy change between iterations was less than 10^{-3} eV.

3 Result and discussion

3.1 Experimental results

Fig. 10 shows the emission spectra of BN material obtained at different temperatures. The main objective of the study is to study the temperature dependence of BN emission properties and to evaluate the significance of the obtained results in optoelectronic applications of the material. In the study, the emission spectra of boron nitride (BN) material were measured at room temperature (300 K) and low temperature (77 K). A laser beam with a wavelength of 325 nm was used for excitation and the emitted light was recorded with high sensitivity. The spectra were recorded in the energy range of 1.9 eV to 2.4 eV.

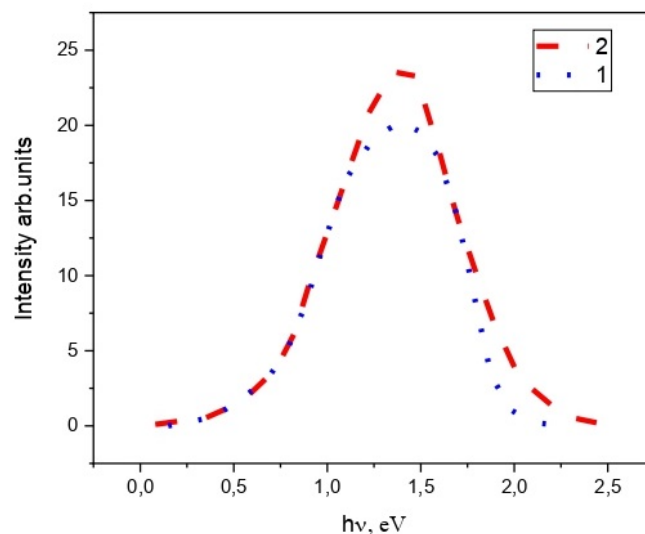


Figure 1: Emission spectra of the BN crystal at $T = 300$ K (1) and 77 K (2).

The studied spectra show that at both temperatures the main photoluminescence peak is located at an energy level of approximately 2.2 eV. This peak is associated with intrinsic defects or the formation of localized energy states in the BN material. The maximum intensity in the spectrum obtained at room temperature is lower than at low temperatures. This is due to the effect of thermal activation: at high temperatures, non-radiative recombination processes are enhanced. As a result, the photoluminescence efficiency decreases. The width of the spectrum is wider, which indicates that the energy levels are more exposed to thermal dispersion. In the spectrum obtained at low temperatures, the photoluminescence intensity increases significantly and the half-width of the spectrum takes a narrower form. This observation is explained by the weakening of non-radiative processes and the more stable trapping of electrons in localized defect states. Under these conditions, the emission line becomes narrower and the stability of the energy levels increases. The constant peak energy position (2.2 eV) at both temperatures indicates that the emission is associated with specific defect states and the energy position of these states does not change with temperature. This is an important indicator of the stable optical properties of the material. The results of this study show that the photoluminescence intensity and spectral properties of the BN material are significantly dependent on temperature.

The chromaticity coordinates of the BN (CIE) compound study in this work. The correlated color temperature (CCT) and color rendering index (CRI) were determined based on the specific color coordinates obtained from the photoluminescence (PL) spectra of this compound using the Color Calculator software developed by OSRAM SYLVANIA. Furthermore, the chromaticity coordinates ($x = 0.3374$, $y = 0.3941$) corresponding to the CCT of BN were calculated using McCamy's equation, where $n = (x - 0.3320)/(y - 0.1858)$.

The calculated CCT was approximately 7068 K. This undoped phosphor exhibits emission that is close to red light. It was found that the CCT value calculated using McCamy's equation coincides with the result obtained from the Color Calculator. The CRI value for pure BN obtained from the Color Calculator was 71 . According to the current literature, these findings suggest that pure BN is a promising candidate for applications in display technologies, general illumination, and red light-emitting diode (LED) devices.

3.2 DFT results

To construct the BN nanosheet from the bulk structure, at first step we built and analyzed bulk hexagonal boron nitride (h-BN) structure. The bulk structure was first optimized to ensure that the lattice parameters were in agreement with experimental data and previous theoretical results $a = 2.503\text{\AA}$, $b = 6.661\text{\AA}$. Using the ATK interface, the primitive cell of h-BN was created, and the system was fully relaxed.

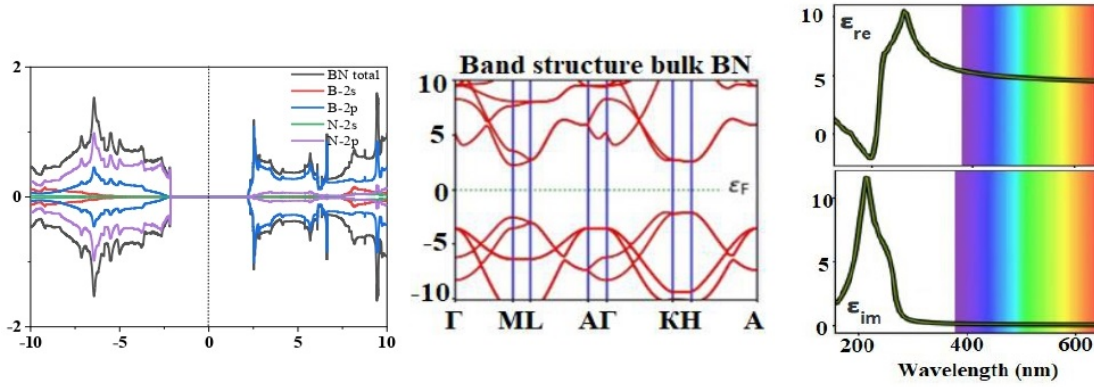


Figure 2: Calculated band structure, DOS, real and imaginary part of dielectric function for bulk BN structure.

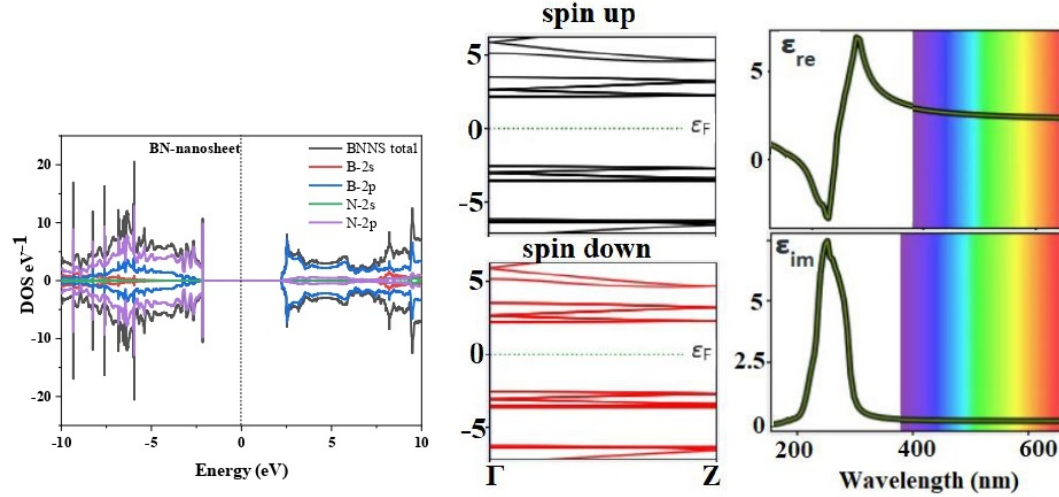


Figure 3: Calculated band structure, DOS, real and imaginary part of dielectric function for nanosheet BN structure.

To obtain the 2D nanosheet, we cleaved the bulk structure along the (001) plane, which is perpendicular to the c-axis, to obtain the desired 2D sheet. To avoid interactions between periodic images in the simulation, a vacuum layer of at least $20\text{\AA}$ was introduced in the direction perpendicular to the nanosheet. The final nanosheet structure was further analyzed for its electronic properties, including the band structure, density of states and optic properties to ensure accurate representation of its characteristics. Based on spin-unrestricted calculations, Fig. 3 displays the corresponding band structures, DOS and dielectric functions for the BNNS. In the case of pure nanosheet, spin up and spin down bands absolutely symmetrical, thereby not

contributing to spin polarization. The band structure clearly demonstrates that BNNS exhibits a semiconducting behavior characterized by a wide fundamental band gap of 4.90 eV, which deviates by approximately 1.8 % from bulk structure.

Using the screened hybrid functional Heyd–Scuseria Ernzerhof approximation and the generalized gradient approximation, the band structures corresponding to $n = 2, 4$ and 8 layer BN are shown in Fig. 4. It is demonstrated that the four systems are semi-conductors, with direct band gap at the M-point.

Consider that the band structures for the HSE and GGA approximations have a very similar shape around the Fermi level, where the direct gap is situated at the M-point in the valence band maximum (VBM) and conduction band minimum in the Brillouin zone. Additionally, there is a modest increase in the band gap favoring HSE over GGA. Additionally, one concludes that the band gap energy gradually decreases as the number of layers increases from $n = 2$ to $n = 8$, without changing the direct band gap shape of the forbidden gap. The band gap are 4.85 eV for 2 layer, 4.73 eV for 4 layer and 4.61 eV for 8 layer structure.

As shown in Fig. 5, the dielectric constant $\varepsilon(0)$ is approximately 4.85 and gradually increases toward the mid-UV region. In the deep UV region, $\varepsilon_1(\omega)$ decreases within the energy range of 4.55 eV to 5.99 eV. The highest peak value of $\varepsilon_1(\omega)$, around 3.67, is observed at 5.47 eV in the extreme UV region. The optoelectronic characteristics of 2D hexagonal layered BN materials with $\eta = 2, 4$ and 8 are examined in this section. It is investigated how the number of layers affects the band structures and crystalline characteristics of layered BN. Numerous optical characteristics are examined, including the complex dielectric function, the absorption coefficient, conductivity, reflectivity, refraction index, extinction coefficient, and EELs.

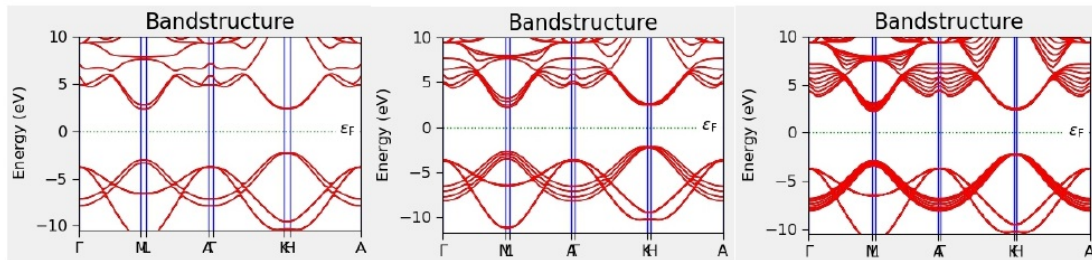


Figure 4: Band structure calculation of 2, 4 and 8 layered BN structure.

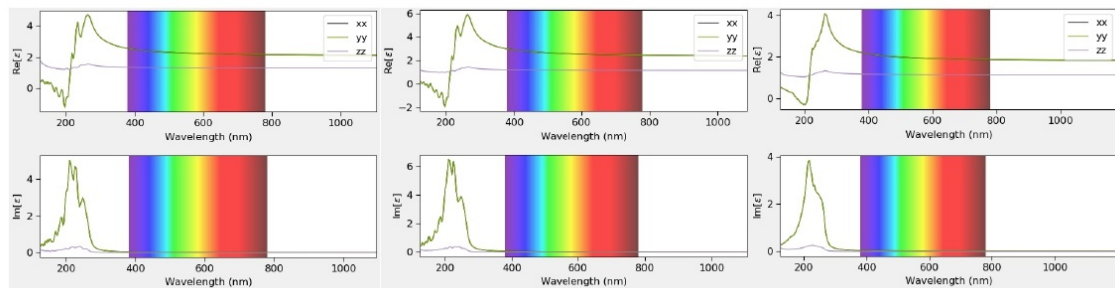


Figure 5: Calculated real and imaginary part of dielectric function of 2, 4 and 8 layered BN structure.

4 Conclusion

The photoluminescence observed in BN material with a maximum energy of 2.2 eV occurs as a result of localized states associated with defects, and the intensity of these emission lines increases sharply with decreasing temperature. At low temperatures, the half-width of the spectrum narrows and the position of the energy maximum does not change. The calculated CCT was approximately 7068 K. This undoped phosphor exhibits emission that is close to red light. It was found that the CCT value calculated using McCamy's equation coincides with the result obtained from the Color Calculator. These properties indicate that BN material has significant potential for new generation optoelectronic devices and quantum technologies. In this study, we comprehensively analyzed the electronic and optical properties of hexagonal boron nitride nanosheets using first-principles DFT calculations. The results confirmed that h-BN retains a wide direct band gap across different layer configurations, with a slight reduction in band gap energy as the number of layers increases from two to eight. The dielectric and optical responses were also found to evolve with increasing layer thickness, underscoring the potential for tuning the material's properties for specific applications. Overall, this work highlights the promise of h-BN nanosheets as versatile two-dimensional materials suitable for semiconducting and optoelectronic devices. The insights gained from these simulations can inform the design of next-generation components leveraging the unique characteristics of boron nitride nanostructures.

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