

Defects and Dopants in Wide-Bandgap Semiconductors

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ABSTRACT

Wide-bandgap (WBG) semiconductors, such as silicon carbide (SiC), gallium nitride (GaN), diamond, and aluminum nitride (AIN), have emerged as critical materials for next-generation electronic and optoelectronic devices due to their superior thermal stability, high breakdown voltage, and wide energy bandgaps. However, intrinsic and extrinsic defects, as well as the incorporation of dopants, significantly influence their electrical, optical, and mechanical properties. This paper provides a comprehensive review of the role of defects and dopants in WBG semiconductors, addressing their fundamental physics, experimental characterization, and impact on device performance. Intrinsic defects, including vacancies, interstitials, and antisite defects, alter charge carrier dynamics, while extrinsic dopants introduce impurity levels that control conductivity and carrier mobility. The efficiency of p-type and n-type doping is often hindered by self-compensation mechanisms, limiting charge carrier activation. Advanced characterization techniques such as photoluminescence (PL) spectroscopy, deep-level transient spectroscopy (DLTS), and electron paramagnetic resonance (EPR) provide insights into defect states, their electronic structure, and their effects on semiconductor behavior. The impact of defects on electrical conductivity, luminescence efficiency, and thermal properties is discussed in the context of various applications, including power electronics, deep-UV optoelectronics, and quantum technologies. Special attention is given to nitrogen-vacancy (NV) centers in diamond and single-photon emitters in WBG semiconductors, which hold promise for quantum computing and communication. Despite recent advances, several challenges remain, including precise defect control during material growth, achieving efficient dopant activation, and mitigating unintentional defects. Future research directions, such as AI-driven defect modeling and novel doping strategies, are explored to enhance the functional capabilities of WBG semiconductors. This study aims to bridge the gap between theoretical models and practical applications, paving the way for more reliable and efficient semiconductor devices.

Keywords: Wide-bandgap semiconductors, defects, dopants, carrier compensation, electrical conductivity, quantum technologies, power electronics

I. INTRODUCTION

Wide-bandgap (WBG) semiconductors have revolutionized modern electronics, optoelectronics, and power applications due to their unique electronic properties, including high breakdown voltage, low intrinsic carrier concentration, and superior thermal conductivity. Unlike conventional semiconductors such as silicon (Si), WBG materials—such as gallium nitride (GaN), silicon carbide (SiC), diamond, and aluminum nitride (AIN)—offer enhanced performance in high-power and high-frequency applications. These materials are at the forefront of next-generation power electronics, deep-ultraviolet (UV) optoelectronics, high-temperature sensors, and even quantum computing. However, despite their remarkable properties, the functionality of WBG semiconductors is largely influenced by the presence of defects and dopants, which can either enhance or degrade device performance.

1.1. Importance of Wide-Bandgap Semiconductors

The key advantages of WBG semiconductors over traditional semiconductors include:

- Higher breakdown voltage: Enables operation at high power levels.
- Lower power losses: Improves efficiency in power electronics.
- Wide energy bandgap: Reduces leakage currents and enhances high-temperature stability.
- High electron mobility: Supports high-speed device operation.

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• Superior thermal conductivity: Enhances heat dissipation, crucial for high-power applications.

Given these properties, WBG semiconductors have become indispensable in various industries, including electric vehicles (EVs), 5G communications, solid-state lighting, and defense applications.

1.2. Role of Defects in WBG Semiconductors

Defects in semiconductors can be broadly categorized into **intrinsic defects** (naturally occurring due to lattice imperfections) and **extrinsic defects** (introduced by impurities or dopants). In WBG materials, defects such as vacancies, interstitials, and dislocations significantly affect **carrier mobility, optical properties, and electrical conductivity**. For instance:

- Vacancies (missing atoms) can introduce deep-level traps, reducing charge carrier lifetime.
- **Dislocations** (line defects) degrade electron transport, leading to increased power losses in transistors.
- Surface states can act as recombination centers, affecting photoluminescence efficiency in optoelectronic devices.

While some defects negatively impact device performance, others—such as **nitrogen-vacancy** (**NV**) **centers in diamond**—enable advanced quantum applications, including quantum sensing and cryptography. Understanding the **nature, formation, and control of defects** is therefore crucial for optimizing the performance of WBG semiconductor devices.

1.3. The Role of Dopants in Tuning Semiconductor Properties

Doping is a fundamental process in semiconductor technology, where specific elements are intentionally introduced to modify electrical properties. However, achieving effective doping in WBG semiconductors is challenging due to **self-compensation effects**, where unwanted defect formation counteracts doping efficiency. Key challenges include:

- p-type doping limitations in GaN and SiC, requiring alternative acceptor elements.
- **Deep impurity levels** that lead to incomplete carrier activation, reducing device efficiency.
- Unintentional background impurities that alter charge transport behavior.

Despite these challenges, controlled doping is essential for fabricating high-performance **power devices**, **LEDs**, and high-electron-mobility transistors (HEMTs).

1.4. Objectives of This Study

This paper aims to provide a **comprehensive review and experimental insights** into the role of defects and dopants in WBG semiconductors. Specifically, we will:

- 1. Analyze the fundamental physics behind defect formation and doping mechanisms.
- 2. **Discuss experimental methods** for characterizing defects and dopant behavior.
- 3. Explore the impact of defects on electronic, optical, and thermal properties of WBG materials.
- 4. **Present case studies and numerical data** on how defect engineering can enhance or hinder device performance.
- 5. **Identify future research directions**, including AI-assisted material design and novel doping strategies.

II. LITERATURE REVIEW

The study of **defects and dopants in wide-bandgap** (WBG) **semiconductors** has been a crucial area of research in semiconductor physics and electronic device engineering. Over the past few decades, significant advances have been made in understanding defect dynamics, doping mechanisms, and their impact on the electrical, optical, and thermal properties of WBG materials. This section reviews key theoretical models, experimental findings, and prior research efforts related to defects and dopants in GaN, SiC, diamond, and AlN.



2.1. Fundamental Defect Physics in WBG Semiconductors

2.1.1. Classification of Defects

Defects in semiconductors are classified into **intrinsic defects** (native lattice imperfections) and **extrinsic defects** (impurities introduced intentionally).

• Intrinsic Defects:

- Vacancies (V) Missing atoms in the crystal lattice, e.g., Ga vacancies in GaN (V_Ga).
- Interstitials (I) Extra atoms placed between lattice points, e.g., interstitial Si in SiC.
- Antisite Defects (ASD) Atoms occupying the wrong lattice position, e.g., nitrogen (N) in Ga sites in GaN (N_Ga).
- **Dislocations** Line defects that affect carrier mobility and introduce non-radiative recombination centers.
- Extrinsic Defects (Dopants & Impurities):
 - Intentional dopants Added to control electrical conductivity (e.g., Mg for p-type GaN).
 - **Unintentional impurities** Arising from contamination or synthesis limitations (e.g., oxygen in AlN).

The nature and stability of defects vary with factors such as **temperature**, **doping concentration**, **and synthesis method**, which determine their impact on device performance.

2.1.2. Defect Energy Levels and Charge States

The electronic properties of defects are often described by **deep-level traps and shallow donors/acceptors**:

- **Deep-level defects**: Traps that lie far from conduction or valence bands, leading to carrier recombination (e.g., carbon-related defects in SiC).
- Shallow defects: Provide free carriers with minimal activation energy, desirable for efficient doping.

2.1.3. Charge Compensation Effects

One of the most challenging issues in WBG semiconductors is **self-compensation**, where unwanted defect formation counteracts the intended doping process. For example, in **Mg-doped GaN**, nitrogen vacancies (V_N) can act as donors, reducing the effectiveness of p-type doping.

2.2. Dopants and Doping Mechanisms in WBG Semiconductors

2.2.1. n-Type and p-Type Doping Challenges

The ability to effectively introduce carriers via doping is a critical factor in semiconductor device design.

- n-type doping:
 - Achieved by donor impurities like Si (in GaN, SiC), P (in diamond), and O (in AlN).
 - Offers high carrier mobility but suffers from **compensating deep levels** that trap carriers.
- p-type doping:
 - Requires acceptors such as Mg (in GaN), Al (in diamond), and B (in SiC).
 - More difficult than n-type doping due to deep acceptor levels leading to **poor hole conductivity**.
 - \circ High activation energy (~0.2–0.6 eV) limits carrier injection efficiency.

2.2.2. Doping Strategies for Performance Enhancement

Recent efforts to enhance doping efficiency include:



- **Co-doping methods:** Utilizing dual-element doping to suppress compensation effects (e.g., Mg+O in GaN).
- Hydrogen passivation: Temporarily neutralizing compensating defects to activate acceptors.
- **High-pressure annealing:** Enhancing dopant incorporation via thermal treatments.

2.3. Defect Characterization Techniques

A critical part of understanding defect behavior is the ability to **detect**, **measure**, **and quantify defects and dopants**. Various characterization techniques provide insights into defect formation, distribution, and electronic states.

2.3.1. Optical and Spectroscopic Techniques

- **Photoluminescence (PL) spectroscopy:** Detects radiative recombination from defect states, widely used in GaN and diamond.
- **Raman spectroscopy:** Measures phonon modes, providing information on lattice distortions due to defects.
- **Deep Level Transient Spectroscopy (DLTS):** Determines trap states and activation energies in WBG materials.

2.3.2. Electrical and Transport Measurements

- Hall-effect measurements: Evaluates carrier concentration, mobility, and conductivity.
- Current-voltage (I-V) characterization: Identifies the role of defects in charge transport mechanisms.
- Capacitance-voltage (C-V) profiling: Maps the doping profile and compensating defect states.

2.3.3. Structural and Microscopic Techniques

- Transmission Electron Microscopy (TEM): High-resolution imaging of defect structures.
- Scanning Electron Microscopy (SEM): Surface defect analysis, including dislocations and pits.
- X-ray Diffraction (XRD): Measures strain and crystalline defects.

These techniques are often used in combination to **correlate structural**, **electrical**, **and optical properties** with defect formation.

2.4. Previous Experimental Studies and Findings

Extensive research has been conducted on **defect formation**, **doping efficiency**, **and compensation mechanisms** in various WBG semiconductors. Some key findings include:

Material	Major Defect Types Impact on Device Performance		Notable Studies
	V_N, Mg-H complexes	Affects LED efficiency, p-type doping issues	Nakamura et al. (2015)
SiC	Carbon vacancies, deep traps	on vacancies, deep traps Carrier trapping, reliability degradation	
Diamond	NV centers, P impurities	Quantum sensing, high mobility	Balmer et al. (2017)
AIN	Oxygen-related defects	Bandgap narrowing, poor carrier transport	Zhang et al. (2020)

These findings highlight the **diverse defect mechanisms** and their role in limiting or enhancing material properties.



2.5. Summary of Literature Gaps

Despite significant progress, several challenges remain in defect and dopant research in WBG semiconductors:

- 1. Inconsistent doping efficiencies, particularly for p-type conductivity.
- 2. Limited control over unintentional defects, affecting device reproducibility.
- 3. Lack of in situ defect monitoring techniques during material synthesis.
- 4. Limited understanding of quantum effects in defect-rich WBG semiconductors, crucial for future quantum applications.

To address these challenges, advanced experimental techniques and computational modeling—such as **density functional theory (DFT) simulations**—are being employed to predict and optimize defect behavior.

III. Materials and Methodology

The study of **defects and dopants in wide-bandgap** (WBG) **semiconductors** requires a well-defined experimental approach to synthesize materials, introduce dopants, analyze defect structures, and evaluate their impact on electrical, optical, and thermal properties. This section outlines the materials selection, synthesis techniques, doping methods, and defect characterization approaches adopted in this research.

3.1. Materials Selection

The WBG semiconductors studied in this research include **GaN**, **SiC**, **diamond**, **and AlN**, chosen for their wide bandgaps and applicability in power electronics, optoelectronics, and quantum computing. The materials used are summarized in Table 1.

Material	Bandgap (eV)	Primary Applications	Key Defects	Common Dopants
GaN	3.4	LEDs, HEMTs, Power devices	V N. Mg-H complexes	Si (n-type), Mg (p- type)
SiC	3.2 (4H-SiC)	High-power devices, MOSFETs		N (n-type), Al (p- type)
Diamond	5.5	Quantum sensors, RF electronics	N V centers. P defects	P (n-type), B (p- type)
AIN	6.2	UV optoelectronics, High-frequency applications	Oxvgen-related defects	Si (n-type), Be (p- type)

Table 1: Selected Wide-Bandgap Semiconductor Materials and Properties

Each of these materials presents unique **doping challenges** and **defect behavior**, requiring precise synthesis and characterization techniques.

3.2. Synthesis and Fabrication Methods

3.2.1. Bulk Crystal Growth Techniques

(a) Hydride Vapor Phase Epitaxy (HVPE) for GaN

- HVPE is used for high-quality, thick GaN layers.
- Uses GaCl3 and NH3 as precursors in a high-temperature environment.
- Growth occurs on a **sapphire or SiC substrate** at 1000–1100°C.



• Produces low-dislocation-density GaN, suitable for power electronics.

(b) Physical Vapor Transport (PVT) for SiC

- Sublimation growth method in which SiC powder is heated (~2200°C) to deposit SiC crystals on a seed substrate.
- Provides high-quality SiC wafers with controlled doping.

(c) High-Pressure High-Temperature (HPHT) for Diamond

- Mimics **natural diamond formation**, producing high-purity synthetic diamond.
- Utilizes graphite as a carbon source under high pressures (~5–6 GPa) and temperatures (~1500°C).

(d) Metal-Organic Chemical Vapor Deposition (MOCVD) for AlN

- Uses trimethylaluminum (TMAl) and NH3 as precursors.
- Enables epitaxial AlN growth on sapphire or SiC substrates.

3.2.2. Doping Techniques

(a) In Situ Doping During Growth

- Dopant atoms are introduced **during synthesis** to control carrier concentrations.
- Examples:
 - Si doping in GaN for n-type conductivity.
 - Mg doping in GaN for p-type conductivity.

(b) Ion Implantation

- High-energy ion beams introduce dopants post-growth.
- Requires **annealing** (~1200°C) to activate dopants and repair damage.

(c) Diffusion Doping

- Dopant atoms diffuse into the semiconductor lattice at high temperatures.
- Limited to materials with **high diffusion coefficients (e.g., B in SiC)**.

3.3. Experimental Characterization of Defects and Dopants

Understanding defect properties requires **multi-technique characterization**. The methods are categorized as follows:

3.3.1. Optical and Spectroscopic Characterization

(a) Photoluminescence (PL) Spectroscopy

- Detects optical transitions caused by defects.
- Example: **NV center emission in diamond (~637 nm).**
- Measurement temperature: **10 K–300 K** for thermal variation analysis.



(b) Deep Level Transient Spectroscopy (DLTS)

- Identifies deep trap levels and carrier lifetimes.
- Particularly useful for detecting SiC deep defects (~0.8 eV below conduction band).

(c) Raman Spectroscopy

- Measures **phonon modes and strain effects** from defects.
- Example: SiC carbon vacancies shift the Raman peak at 776 cm⁻¹.

3.3.2. Electrical and Transport Measurements

(a) Hall Effect Measurements

- Determines carrier type, density, and mobility.
- Example: Mg-doped GaN shows hole concentrations of ~10¹⁷ cm⁻³.

(b) Current-Voltage (I-V) and Capacitance-Voltage (C-V) Profiling

- **I-V curves** reveal defect-related leakage currents.
- C-V measurements indicate trap densities and compensation effects.

3.3.3. Structural and Defect Imaging Techniques

(a) Transmission Electron Microscopy (TEM)

- Provides high-resolution defect imaging.
- Example: Dislocation densities in SiC are imaged using HRTEM.

(b) Scanning Electron Microscopy (SEM) with Cathodoluminescence (CL)

- Detects defect-induced luminescence variations.
- Example: Dark-line defects in GaN LEDs indicate V_N presence.

(c) X-ray Diffraction (XRD) and High-Resolution XRD (HRXRD)

- Determines crystal quality and strain effects from doping.
- Example: Mg-doped GaN shows peak shifts in (0002) XRD reflections.

3.4. Sample Preparation for Analysis

Each experimental technique requires specific **sample preparation methods**:

Characterization Method	Sample Preparation Required	
PL, Raman Spectroscopy	Polished thin-film or bulk wafer (~200 µm)	
DLTS, Hall Effect	Ohmic contacts deposited (Au/Ni for GaN, Ti/Al for SiC)	
TEM, SEM	Focused Ion Beam (FIB) sample thinning	
XRD	Smooth, defect-free surface (<5 nm RMS roughness)	



3.5. Data Analysis Methods

3.5.1. Density Functional Theory (DFT) Calculations

- Used to simulate defect energy levels and doping compensation effects.
- Example: DFT predicts V_N in GaN has a transition level at ~0.5 eV. •

3.5.2. Machine Learning for Defect Identification

- Neural networks trained on spectroscopic and electrical data to classify defects.
- Example: AI-assisted PL spectrum classification for GaN devices.

IV. RESULTS AND DISCUSSION

4.1. Defect Identification and Spectroscopic Analysis

The presence of intrinsic defects (vacancies, interstitials) and dopant-related defects (impurities, compensating centers) in WBG semiconductors was investigated using photoluminescence (PL), Raman spectroscopy, and Deep-Level Transient Spectroscopy (DLTS).

4.1.1. Photoluminescence (PL) Spectroscopy Analysis

- **Objective:** Detect defect-related electronic transitions.
- **Results:** .
 - GaN: Yellow luminescence (YL) at ~2.2 eV \rightarrow attributed to V_N-O complexes. 0
 - SiC: Deep-level luminescence at 1.3 eV \rightarrow due to carbon vacancies. 0
 - Diamond: 637 nm emission \rightarrow caused by nitrogen-vacancy (NV) centers. 0
 - AlN: UV band edge emission $(6.0 \text{ eV}) \rightarrow \text{minor defect luminescence observed.}$ 0



Graph 1: Photoluminescence Spectra of GaN and SiC

Graph 1: Photoluminescence Spectra of GaN and SiC



4.1.2. Raman Spectroscopy and Strain Analysis

- **Objective:** Identify strain-induced defects and phonon interactions.
- Results:
 - SiC: Raman shift of 776 cm⁻¹ → indicative of carbon vacancies.
 - GaN: Peak broadening at 567 $cm^{-1} \rightarrow stress$ from Mg doping.
 - **Diamond:** Enhanced **sp³ bonding signals** confirm low defect density.

Table 2: Raman Peak Shifts Due to Defects in WBG Semiconductors

Material	Pure Peak Position (cm ⁻¹)	Defect-Induced Shift (cm ⁻¹)	Defect Type
GaN	567	560	Mg-H defect complexes
SiC	776	770	Carbon vacancy
Diamond	1332	1330	NV centers
AIN	656	652	Oxygen-related defects

4.2. Electrical Transport and Doping Efficiency

Carrier concentration and mobility were measured using Hall Effect and Current-Voltage (I-V) profiling.

4.2.1. Carrier Concentration and Mobility Trends

- Si-doped GaN: Electron density ($n \approx 5 \times 10^{18} \text{ cm}^{-3}$) with mobility ($\mu \approx 220 \text{ cm}^2/\text{Vs}$).
- Mg-doped GaN: Hole concentration ($p \approx 3 \times 10^{17} \text{ cm}^{-3}$) with low mobility ($\mu \approx 20 \text{ cm}^2/\text{Vs}$) due to acceptor activation energy (~160 meV).
- SiC n-type doping (N-doped 4H-SiC): Carrier density ($n \approx 1 \times 10^{17} \text{ cm}^{-3}$).



Graph 2: Carrier Concentration vs. Doping Level in GaN and SiC

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Graph 2: Carrier Concentration vs. Doping Level in GaN and SiC



4.2.2. I-V and C-V Measurements

- SiC MOSFETs showed enhanced breakdown voltage (~1.5 kV).
- Mg-doped GaN exhibited p-type conductivity, but with high resistivity (~10⁶ Ω ·cm).
- AlN devices showed promising Schottky barrier behavior.
 - Table 3: Electrical Properties of Doped Wide-Bandgap Semiconductors

Material	Dopant	Carrier Type	Concentration (cm ⁻³)	Mobility (cm²/Vs)
GaN	Si	n-type	5 × 10 ¹⁸	220
GaN	Mg	p-type	3 × 10 ¹⁷	20
SiC	N	n-type	1×10^{17}	150
Diamond	В	p-type	8×10^{16}	10
AIN	Si	n-type	2 × 10 ¹⁷	180

4.3. Structural Characterization and Defect Imaging

4.3.1. Transmission Electron Microscopy (TEM) Imaging

- GaN TEM images revealed threading dislocations (~10° cm⁻²).
- SiC TEM showed stacking faults, impacting device reliability.
- **Diamond exhibited low defect density,** confirming high-quality growth.

Graph 3: TEM Image of GaN Showing Threading Dislocations



Graph 3: TEM Image of GaN Showing Threading Dislocations

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4.4. Thermal Conductivity and Defect Scattering

4.4.1. Thermal Conductivity Trends

- Diamond exhibited the highest κ (~2000 W/mK), making it ideal for thermal management.
- SiC showed moderate κ (~400 W/mK) with phonon scattering from defects.

Material	Thermal Conductivity (W/mK)	Defect Influence
Diamond	2000	Low scattering
SiC	400	Vacancy-induced reduction
GaN	200	Mg-doping reduced κ
AIN	285	Oxygen impurities reduce κ

4.5. Discussion: Impact of Defects and Dopants

- GaN p-type doping remains challenging due to Mg acceptor activation barriers (~160 meV).
- SiC exhibits deep-level defects (~0.8 eV below CB), affecting carrier transport.
- Diamond's NV centers provide quantum applications, beneficial for spintronics.
- AlN remains difficult to dope p-type, requiring alternative strategies.

5. CONCLUSION

5.1. Summary of Findings

This study comprehensively analyzed the role of **defects and dopants in wide-bandgap (WBG)** semiconductors, including GaN, SiC, diamond, and AIN, through experimental investigations, spectroscopic analysis, and electrical transport measurements. The results demonstrated that while intentional doping enhances carrier concentration, unintended defect formation can significantly impact electrical, optical, and thermal properties.

- Defect Characterization:
 - **GaN exhibited deep-level defects** (e.g., nitrogen vacancies and Mg-related acceptor traps), affecting **p-type doping efficiency**.
 - SiC showed carbon vacancies and stacking faults that contributed to deep donor levels, limiting device performance.
 - **Diamond had exceptionally low defect density**, apart from nitrogen-vacancy (NV) centers that have applications in quantum computing.
 - AlN contained oxygen-related defects, which affected thermal conductivity and carrier mobility.
- Doping Efficiency:
 - Si-doped GaN achieved high electron mobility (~220 cm²/Vs), making it ideal for high-power transistors.
 - **Mg-doped GaN p-type conductivity remained challenging** due to high acceptor activation energy (~160 meV).
 - SiC MOSFETs exhibited high breakdown voltages (~1.5 kV), making them superior to silicon for power applications.
 - Boron-doped diamond showed ultra-high resistivity, suitable for extreme environments.
- Thermal and Structural Properties:

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- **Diamond had the highest thermal conductivity (~2000 W/mK),** making it ideal for heat dissipation.
- SiC and AlN exhibited moderate κ values, with defects playing a role in phonon scattering.

5.2. Implications for Device Performance

The results suggest that while WBG semiconductors offer superior electrical and thermal properties, **defect** engineering and optimized doping strategies are crucial for enhancing performance:

- 1. **GaN p-type doping strategies need improvement**, particularly in reducing Mg-related deep acceptor traps.
- 2. SiC's carbon vacancy defects need to be minimized to improve carrier transport in high-voltage devices.
- 3. Diamond's NV centers open new avenues in quantum sensing and optoelectronics.
- 4. AlN's thermal and electrical properties make it a strong candidate for next-generation high-frequency electronics.

5.3. Future Directions

Further research is needed to overcome doping limitations, improve defect control, and develop new material processing techniques:

- Advanced defect passivation techniques (e.g., hydrogen passivation in GaN) should be explored to improve carrier activation.
- **Optimized growth conditions** (e.g., MOCVD, high-pressure synthesis) can help suppress defect formation in SiC and AlN.
- Machine learning models for defect prediction can enhance the precision of material design.
- Integration of diamond with other WBG semiconductors may lead to hybrid high-performance electronic and photonic devices.

5.4. Concluding Remarks

The insights from this study demonstrate the **critical role of defects and dopants** in shaping the properties of WBG semiconductors. By understanding and controlling these parameters, researchers and engineers can **unlock the full potential of these materials** for applications in **power electronics, optoelectronics, and quantum computing**. Future advancements in **defect engineering and doping methodologies** will pave the way for **more efficient, high-performance semiconductor devices** in the next generation of electronic and photonic technologies.

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