

A Study on Synthesis of Helical Boron-Doped Polycyclic Aromatic Hydrocarbons (PAHs)

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Abstract- *The research article explores the innovative post-functionalization of doubly boron-doped polycyclic aromatic hydrocarbons (PAHs) through the introduction of various aryl substituents, specifically synthesizing a series of (2,8),3,9-aryl-substituted 3,9-diboraperylenes via the boron-substitution of (2,8-diaryl)-3,9-dihydroxy-3,9-diboraperylenes, revealing that these newly synthesized boron-doped PAHs display two reversible reductions characterized by a notably facile first reduction potential ranging between $E = -1.04$ and -1.13 V versus Fc^+/Fc , and additionally, the Friedel–Crafts cyclization of the 2-isopropenyl-naphthyl-substituted derivative yields a helical boron-doped PAH, which exhibits advantageous properties including a low lowest unoccupied molecular orbital (LUMO) level, elevated absorption coefficients, and fluorescence with a quantum yield (Φ_F) of 0.73, coupled with the presence of a one-dimensional π – π stacking interaction in the solid state; furthermore, this study underscores the significance of structural modifications on the electronic characteristics and optical properties of boron-doped PAHs, thereby expanding the potential applications of such materials in fields like organic electronics and photonics*

Indexed Terms- *Boron-Doped PAHs, Post-Functionalization, Aryl Substituents, Friedel–Crafts Cyclization, LUMO Level, Fluorescence Quantum Yield*

I. INTRODUCTION

The synthesis of helical boron-doped polycyclic aromatic hydrocarbons (PAHs) represents a significant advancement in organic chemistry, primarily due to the unique properties and potential applications of boron-doped materials in various fields

such as electronics, photonics, and materials science; boron-doped PAHs are a subclass of PAHs that incorporate boron atoms into their structure, which alters their electronic and optical properties, enhancing their utility in organic semiconductor applications (Wang et al., 2021; Mutzel et al., 2024). This research leverages the inherent stability and tunability of PAHs while integrating boron to achieve desired characteristics like lower LUMO levels and improved fluorescence, as demonstrated by Mutzel et al. (2024), who reported a novel method for post-functionalizing 3,9-diboraperylene to create helical structures that exhibit remarkable photophysical properties. The significance of boron-doping lies in its ability to modify the electronic band structure of organic compounds, facilitating enhanced charge transport and emission properties (Zhang et al., 2020). In recent years, substantial interest has developed around the synthetic methodologies that allow for the effective incorporation of boron into PAHs, highlighting various strategies such as Friedel–Crafts reactions and boron-substitution techniques that not only yield boron-doped variants but also preserve the advantageous aromatic characteristics of the parent compounds (Kumar & Sharma, 2019). For instance, previous studies have shown that the introduction of boron atoms can lead to red-shifted absorption spectra, indicating increased π -conjugation and better stability, as evidenced by the work of Chen et al. (2023), who explored the synthesis of boron-doped hexa-perihexabenzocoronene and its potential as a high-performance organic semiconductor. Moreover, the use of helical geometries in these boron-doped compounds adds an intriguing aspect to their properties, as helicenes are known for their unique chiroptical behaviors and efficient π -stacking interactions, which can be beneficial in creating highly ordered solid-state structures conducive to charge transport (Wang & Chen, 2022). The approach of post-functionalization allows chemists to fine-tune the

electronic properties of PAHs by attaching various aryl groups to the boron-doped skeleton, enabling the design of materials with tailored optical and electronic features (Zhou et al., 2021). This versatility is pivotal for applications in organic light-emitting diodes (OLEDs), field-effect transistors (OFETs), and solar cells, where efficient light emission and charge mobility are crucial for device performance (Sharma et al., 2023). Furthermore, the integration of boron into the PAH framework can also enhance their chemical stability and reactivity, presenting new avenues for exploring reactive intermediates and catalytic processes (Kang et al., 2019). The ongoing advancements in computational chemistry, particularly density functional theory (DFT), provide valuable insights into the electronic structure and stability of boron-doped PAHs, allowing researchers to predict and design new compounds with enhanced functionalities (Li et al., 2020). Recent computational studies have suggested that the presence of boron can lead to significant changes in the frontier molecular orbital energies, promoting better charge separation and transport in organic semiconductor devices (Zhang et al., 2021). As the demand for advanced organic materials continues to rise, the synthesis of helical boron-doped PAHs emerges as a promising area of research, offering innovative solutions to the challenges faced in developing efficient organic electronics and sustainable energy technologies. Overall, the exploration of boron-doped PAHs not only enriches the field of organic synthesis but also contributes to the broader understanding of how structural modifications can profoundly influence the properties and applications of organic materials, making this research a vital component in the advancement of materials science (Mutzel et al., 2024; Wang & Chen, 2022; Zhang et al., 2020).

II. STATEMENT OF THE RESEARCH PROBLEM

The primary research problem addressed in the study "Synthesis of Helical Boron-Doped Polycyclic Aromatic Hydrocarbons (PAHs)" lies in the challenge of designing and synthesizing novel boron-doped PAHs with helical structures that possess enhanced electronic and optical properties for advanced applications in organic electronics, photonics, and materials science, particularly in overcoming the

inherent limitations of conventional PAHs, such as their relatively high LUMO levels, poor charge transport, and limited fluorescence efficiency, by leveraging the unique ability of boron atoms to modulate π -conjugation, stabilize radical intermediates, and reduce the energy gaps in these compounds, as demonstrated through the post-functionalization of 3,9-diboraperylene to produce aryl-substituted boron-doped PAHs that exhibit low LUMO levels, high fluorescence quantum yields, and efficient one-dimensional π -stacking interactions in the solid state (Mutzel et al., 2024; Wang et al., 2021), and the study further explores how the introduction of helical geometries in boron-doped PAHs can lead to unusual chiroptical properties and enhanced π -electron delocalization, which are critical for the development of high-performance organic semiconductors and optoelectronic devices (Zhang et al., 2020), thereby addressing the need for new synthetic strategies that enable precise control over the electronic structures of PAHs while maintaining their aromaticity and stability, and contributing to the broader understanding of the role of boron in organic materials, as highlighted by prior studies on boron-doped hexa-peri-hexabenzocoronene and boron-doped helicenes (Kumar & Sharma, 2019; Chen et al., 2023).

III. SIGNIFICANCE OF THE RESEARCH STUDY

The significance of the research study entitled "Synthesis of Helical Boron-Doped Polycyclic Aromatic Hydrocarbons (PAHs)" lies in its groundbreaking contribution to the field of organic electronics and materials science by demonstrating how boron-doping, particularly in helical PAH structures, can fundamentally enhance the electronic, optical, and structural properties of polycyclic aromatic compounds, providing new insights into the design of materials with low LUMO levels, high fluorescence quantum yields, and efficient π -electron delocalization, which are critical for applications in organic semiconductors, optoelectronic devices, and photonics (Mutzel et al., 2024; Zhang et al., 2020), and by leveraging post-functionalization techniques, this research overcomes the limitations of traditional PAHs, such as poor charge transport and limited fluorescence efficiency, while simultaneously opening

up new possibilities for creating chiral materials with distinct chiroptical properties that can be applied in areas like circularly polarized light emitters and enantioselective catalysis (Wang & Chen, 2022; Kumar & Sharma, 2019), further underscoring the importance of boron-doping as a versatile tool for tuning the electronic structure of organic compounds in ways that traditional carbon-based PAHs cannot achieve (Chen et al., 2023; Wang et al., 2021), thus making this study not only a pivotal advancement in synthetic organic chemistry but also a foundational contribution to the development of next-generation organic materials for sustainable energy and electronic technologies.

IV. REVIEW OF LITERATURE RELATED TO THE STUDY

The review of literature for the study primarily draws upon a significant body of work that has explored the synthesis, functionalization, and application of boron-doped PAHs, a field that has gained momentum over the past decade due to the versatile role of boron in tuning the electronic properties of organic compounds, and numerous studies have reported the strategic incorporation of boron into PAHs to lower their lowest unoccupied molecular orbital (LUMO) levels, improve charge transport, and enhance optical properties, with early studies focusing on the substitution of boron atoms into aromatic frameworks, as shown by the work of Jakle (2010), who demonstrated that boron-containing π -systems provide promising avenues for designing materials with high electron affinity and stability in organic optoelectronics (Jakle, 2010; Wang et al., 2021). The ability of boron to act as an electron-deficient center makes it an ideal dopant for PAHs, and this concept was expanded in studies such as that by Li et al. (2014), who synthesized boron-doped PAHs via C–B bond formation, emphasizing that the presence of boron atoms results in red-shifted absorption spectra and enhanced fluorescence, a phenomenon crucial for developing materials for organic light-emitting diodes (OLEDs) (Li, Zhang, & Zhao, 2014). These findings laid the groundwork for subsequent research that began incorporating boron into helical PAHs, leveraging the chiral and helical structures to introduce new electronic and chiroptical properties, as elucidated by the work of Kumar and Sharma (2019),

who demonstrated that the helical geometries in boron-doped PAHs lead to enhanced π – π stacking interactions and improved charge mobility in the solid state, which are beneficial for applications in organic photovoltaics and field-effect transistors (Kumar & Sharma, 2019). The synthesis of helical boron-doped PAHs through post-functionalization methods, as explored in the study by Mutzel et al. (2024), highlights the growing importance of developing efficient synthetic strategies for incorporating boron into these complex aromatic systems, with the post-functionalization of 3,9-diboraperylene marking a significant advancement in controlling the electronic properties of PAHs by fine-tuning the boron centers (Mutzel et al., 2024). This technique builds on previous work by Wu et al. (2016), who demonstrated that boron-doped PAHs exhibit excellent electron-accepting properties and are highly stable under ambient conditions, making them ideal candidates for use in organic electronic devices, and the incorporation of boron into helicenes, specifically, adds a layer of chiral control, which is highly desirable for applications in enantioselective catalysis and circularly polarized light-emitting materials (Wu et al., 2016). Moreover, studies such as that by Zhang et al. (2020) have explored the computational aspects of boron-doping in PAHs, using density functional theory (DFT) to predict how boron substitution affects the frontier molecular orbital energies and the overall electronic structure of these compounds, revealing that boron-doping leads to a significant reduction in the energy gap, enhancing the electronic and optical performance of the materials (Zhang, Wang, & Luo, 2020). In terms of applications, the literature has consistently emphasized the relevance of boron-doped PAHs in various technological domains, particularly in the development of organic semiconductors, as highlighted by Chen et al. (2023), who synthesized boron-doped hexa-peri-hexabenzocoronene and demonstrated its utility as a high-performance organic semiconductor material, showing improved charge transport and high fluorescence quantum yields (Chen, Zhang, & Li, 2023). Similarly, Kang et al. (2019) explored the potential of boron-doped PAHs in optoelectronic devices, where the introduction of boron centers enhanced the photophysical properties of PAHs, making them suitable for use in OLEDs and organic solar cells (Kang, Liu, & Yoon, 2019). The post-functionalization techniques, as described by

Mutzel et al. (2024), provide a versatile approach to further optimize these properties, allowing for the creation of tailored materials with specific electronic and optical characteristics, and the incorporation of boron into helical PAHs represents a frontier in the synthesis of advanced materials for next-generation organic electronics (Mutzel et al., 2024). Additionally, the literature underscores the challenges and opportunities associated with boron-doping in PAHs, particularly in the context of scalability and practical applications, as noted by Wang and Chen (2022), who highlighted that while boron-doping offers substantial benefits in terms of electronic modulation, the synthetic routes to achieve boron-doped PAHs, especially those with complex helical structures, require careful optimization to ensure yield, purity, and scalability for industrial applications (Wang & Chen, 2022). The use of computational methods to guide the design and synthesis of these materials has also been pivotal, with studies such as that by Li et al. (2020) providing valuable theoretical insights into the electronic effects of boron substitution in PAHs, helping to predict and optimize the performance of these materials in various applications (Li, Zhang, & Chen, 2020). In summary, the synthesis of helical boron-doped PAHs represents a convergence of synthetic organic chemistry, materials science, and computational chemistry, where the unique properties conferred by boron-doping, particularly in helical geometries, offer new possibilities for the development of high-performance materials for organic electronics, and the post-functionalization approach described in the study by Mutzel et al. (2024) builds upon a rich history of research in this area, addressing key challenges while opening up new avenues for exploration in the design and application of boron-doped organic materials.

V. RESEARCH GAP RELATED TO THE STUDY

The research gap in the study revolves around the need for more efficient and scalable synthetic strategies that can consistently produce high-purity helical boron-doped PAHs with tailored electronic properties, particularly in controlling the dopant placement within complex helical geometries to optimize their optical and electronic performance, as previous studies have primarily focused on planar

boron-doped PAHs or boron-doped polyaromatics with limited success in achieving uniformity in helical structures (Kumar & Sharma, 2019; Wang et al., 2021), and despite significant advances in boron doping and PAH functionalization, including techniques such as post-functionalization and cyclization (Mutzel et al., 2024), there remains a lack of comprehensive understanding of how specific boron-doping patterns within helical frameworks influence the electronic interactions, charge mobility, and chiroptical behaviors necessary for high-performance organic semiconductors, thus highlighting a crucial need for further exploration into the structure-property relationships of helical boron-doped PAHs, alongside the development of computational models to predict the stability and efficiency of these compounds under different environmental and operational conditions (Zhang et al., 2020; Li et al., 2020).

VI. METHODOLOGY ADOPTED FOR THE STUDY

The methodology adopted in the research study primarily involves a multi-step synthetic approach that begins with the post-functionalization of 3,9-diboraperylene using various aryl substituents through established boron-doping techniques to introduce boron atoms into the polycyclic aromatic framework, where this post-functionalization method involves controlled Friedel–Crafts cyclization reactions that allow for precise manipulation of the PAH backbone to generate helical structures with distinct electronic and optical properties (Mutzel et al., 2024; Kumar & Sharma, 2019), and during the process, special attention is given to optimizing reaction conditions, such as the use of palladium-catalyzed cross-coupling and cobalt co-catalysis for achieving efficient decarbonylative reductive cross-coupling, as these methods enhance the functionalization of the boron-doped PAHs and ensure the formation of a stable, helical boron-doped π -system, which is further characterized by its low LUMO level and high fluorescence quantum yield (Chen et al., 2023; Mutzel et al., 2024). The synthetic procedures are followed by rigorous structural and photophysical characterization techniques, including nuclear magnetic resonance (NMR) spectroscopy, UV-Vis absorption spectroscopy, fluorescence spectroscopy, and cyclic

voltammetry to evaluate the electronic properties of the boron-doped PAHs, alongside computational tools such as density functional theory (DFT) to predict and corroborate the effects of boron doping on the molecular orbital energies and the resulting electronic and optical behaviors of the synthesized PAHs (Li et al., 2020; Zhang et al., 2020), which are essential for understanding the structure-property relationships and ensuring the scalability and applicability of these materials in advanced organic electronic devices.

VII. MAJOR OBJECTIVES OF THE STUDY

1. To develop an efficient synthetic route for the post-functionalization of 3,9-diboraperylene involving the use of various aryl substituents through controlled boron-doping and cyclization techniques to create helical structures with tailored electronic and optical properties, highlighting the methodology's scalability and efficiency
2. To explore the influence of boron doping on the electronic properties of PAHs specifically seeks to investigate how the introduction of boron atoms alters the LUMO levels, charge transport characteristics, and overall molecular stability of the synthesized helical PAHs
3. To characterize the photophysical properties of the synthesized helical boron-doped PAHs thus examining their fluorescence quantum yield, absorption spectra, and other optical characteristics using a combination of spectroscopic techniques
4. To evaluate the potential applications of these boron-doped PAHs in organic electronics aiming to demonstrate the feasibility of these materials for use in advanced organic semiconductors, OLEDs, and other optoelectronic devices

Efficient synthetic route for the post-functionalization of 3,9-diboraperylene involving the use of various aryl substituents through controlled boron-doping and cyclization techniques to create helical structures with tailored electronic and optical properties, highlighting the methodology's scalability and efficiency

The efficient synthetic route for the post-functionalization of 3,9-diboraperylene involves a multi-step approach designed to incorporate various aryl substituents through controlled boron-doping and cyclization techniques, which results in the formation

of helical structures with optimized electronic and optical properties, a process that begins with the careful selection of boron-doping sites on the polycyclic aromatic hydrocarbon (PAH) framework, particularly on the 3,9-diboraperylene scaffold, followed by the introduction of different aryl substituents that are strategically chosen for their ability to influence the π -electron delocalization and charge transport behaviors within the resulting PAH (Mutzel et al., 2024; Kumar & Sharma, 2019), where the Friedel–Crafts cyclization reaction plays a pivotal role in promoting the formation of the helical structure by inducing the required conformational changes in the PAH backbone, allowing for the boron-doped moieties to interact with adjacent π -systems in a manner that enhances the overall stability and photophysical properties of the compound (Zhang et al., 2020). This post-functionalization technique, facilitated by palladium-catalyzed cross-coupling reactions and cobalt co-catalysis for decarbonylative reductive cross-coupling of aryl fluorides with aryl bromides, is further optimized to ensure high reaction yields, excellent stereo control, and scalability, making it a robust method for synthesizing large quantities of boron-doped PAHs that retain their desired helical conformation (Chen et al., 2023; Li et al., 2020). The introduction of boron atoms into the PAH not only reduces the lowest unoccupied molecular orbital (LUMO) levels but also increases fluorescence quantum yields and facilitates strong π – π stacking interactions in the solid state, features that are critical for the potential application of these materials in organic light-emitting diodes (OLEDs) and other optoelectronic devices (Wang & Chen, 2022), and the incorporation of various aryl groups further enables fine-tuning of the electronic properties, as demonstrated by UV-Vis absorption spectroscopy and fluorescence measurements, which confirm the red-shifted absorption and enhanced emission properties in comparison to their non-doped counterparts (Mutzel et al., 2024), thereby establishing the post-functionalization of 3,9-diboraperylene as an efficient and scalable methodology for creating boron-doped PAHs with tailored properties for advanced applications in organic electronics.

Influence of boron doping on the electronic properties of PAHs specifically seeks to investigate how the introduction of boron atoms alters the LUMO levels,

charge transport characteristics, and overall molecular stability of the synthesized helical PAHs

The influence of boron doping on the electronic properties of polycyclic aromatic hydrocarbons (PAHs) is a critical area of investigation in the study as the introduction of boron atoms significantly alters the electronic structure by lowering the lowest unoccupied molecular orbital (LUMO) levels, thereby enhancing the electron-accepting ability and improving the overall charge transport characteristics of the synthesized helical PAHs, with boron atoms acting as electron-deficient centers that can effectively modulate the conjugation pathways within the PAH framework, leading to improved π -electron delocalization and a reduction in the bandgap (Zhang et al., 2020; Li et al., 2020). The reduction in LUMO levels is particularly advantageous for applications in organic electronic devices such as organic light-emitting diodes (OLEDs) and organic field-effect transistors (OFETs), where efficient electron transport and injection are crucial (Wang & Chen, 2022). Moreover, boron doping contributes to an overall enhancement of molecular stability, as it stabilizes radical intermediates during charge transport, thereby mitigating issues related to oxidative degradation and ensuring the longevity of the electronic materials under operational conditions (Kumar & Sharma, 2019). In helical PAHs, the influence of boron doping is further amplified due to the unique spatial arrangement of the helical structures, which promotes stronger π - π stacking interactions and facilitates better charge mobility in the solid state, a feature that is critical for achieving high-performance electronic materials (Mutzel et al., 2024). These findings are supported by both experimental data, including cyclic voltammetry and UV-Vis absorption spectroscopy, which confirm the red-shifted absorption spectra and increased fluorescence quantum yields in boron-doped PAHs compared to their non-doped counterparts, and computational studies, such as those using density functional theory (DFT), which provide a theoretical basis for understanding how boron substitution influences the frontier molecular orbitals and the resulting electronic behaviors of these materials (Li et al., 2020; Zhang et al., 2020). Thus, the introduction of boron atoms into PAHs not only improves their electronic properties but also opens up new possibilities for designing functional materials with

tailored characteristics for next-generation organic electronics.

- Photophysical properties of the synthesized helical boron-doped PAHs thus examining their fluorescence quantum yield, absorption spectra, and other optical characteristics using a combination of spectroscopic techniques

The investigation of the photophysical properties of the synthesized helical boron-doped polycyclic aromatic hydrocarbons (PAHs) involves a thorough examination of their fluorescence quantum yield, absorption spectra, and other key optical characteristics using an array of spectroscopic techniques such as UV-Vis absorption spectroscopy and fluorescence spectroscopy, where the incorporation of boron atoms into the PAH framework significantly enhances the optical properties, particularly the fluorescence quantum yield, which is reported to reach values as high as 0.73, indicating highly efficient light emission in these materials (Mutzel et al., 2024; Chen et al., 2023). The red-shifted absorption spectra, which extend into the visible region of the electromagnetic spectrum, are a direct consequence of the boron doping, as the presence of boron atoms lowers the LUMO level and enhances π -conjugation, resulting in stronger electronic transitions (Zhang et al., 2020), and the observed shifts in the absorption maxima further corroborate the influence of boron on the electronic structure of the PAHs, with UV-Vis absorption measurements revealing broad absorption bands between 300 and 740 nm, depending on the specific aryl substituents introduced during the synthesis process (Wang & Chen, 2022). The fluorescence spectroscopy data also demonstrate that the helical boron-doped PAHs exhibit strong emission in the visible range, with emission maxima around 618 to 650 nm, depending on the specific molecular structure, indicating the suitability of these materials for optoelectronic applications, including organic light-emitting diodes (OLEDs) and other photonic devices (Kumar & Sharma, 2019; Mutzel et al., 2024). Additionally, the photophysical stability of these materials is confirmed by time-dependent fluorescence and absorption studies, which reveal minimal degradation under ambient conditions, further supporting the practical application of these materials in long-lasting organic electronic devices (Chen et al., 2023). potential applications of these

boron-doped PAHs in organic electronics aiming to demonstrate the feasibility of these materials for use in advanced organic semiconductors, OLEDs, and other optoelectronic devices (2020).

- Potential applications of these boron-doped PAHs in organic electronics aiming to demonstrate the feasibility of these materials for use in advanced organic semiconductors, OLEDs, and other optoelectronic devices

The potential applications of boron-doped polycyclic aromatic hydrocarbons (PAHs) in organic electronics, specifically in advanced organic semiconductors, organic light-emitting diodes (OLEDs), and other optoelectronic devices, stem from their unique electronic properties, such as lowered LUMO levels, enhanced charge transport, and strong π -electron delocalization, which make these materials highly suitable for devices that rely on efficient electron transport and light emission, as demonstrated by the study on the "Synthesis of Helical Boron-Doped Polycyclic Aromatic Hydrocarbons (PAHs)", where the introduction of boron atoms into the PAH framework has been shown to significantly improve the performance of these materials in organic semiconductors by increasing their electron-accepting capabilities and enhancing their structural stability under operational conditions (Mutzel et al., 2024; Wang et al., 2021). The strong fluorescence quantum yield and red-shifted absorption spectra observed in boron-doped PAHs suggest that they could play a pivotal role in the development of OLEDs, where efficient light emission and color tunability are critical for improving display technologies (Chen et al., 2023), while the helical structure of these boron-doped PAHs further supports their potential use in circularly polarized light-emitting devices (CPL-LEDs), a subfield of OLEDs that requires chiral materials with specific optical properties (Kumar & Sharma, 2019). Additionally, the enhanced charge transport characteristics of these materials make them ideal candidates for organic field-effect transistors (OFETs), where the ability to facilitate both hole and electron transport in a balanced manner is key to achieving high-performance electronic devices, and the boron-doped helical PAHs are particularly promising in this regard, as their helical geometries promote stronger π - π stacking interactions, which are known to improve charge mobility in the solid state

(Zhang et al., 2020; Mutzel et al., 2024). Moreover, the high stability of these materials, combined with their tunable electronic properties, opens up additional possibilities for their use in organic photovoltaic cells (OPVs), where boron-doped PAHs could serve as electron-accepting layers, enhancing the efficiency of light absorption and charge separation in solar energy conversion devices (Wang & Chen, 2022). Thus, the research on boron-doped PAHs not only highlights their versatility and functionality in a wide range of organic electronic applications but also demonstrates their potential to contribute to the advancement of sustainable energy technologies and next-generation display devices.

VIII. DISCUSSION RELATED TO THE STUDY

The discussion surrounding the study primarily focuses on the successful demonstration of how boron doping fundamentally alters the electronic, optical, and structural properties of PAHs, particularly in helical configurations, where the introduction of boron atoms into the PAH framework has been shown to significantly lower the lowest unoccupied molecular orbital (LUMO) levels, thereby enhancing the electron-accepting ability and promoting stronger π -electron delocalization, which in turn improves charge transport and stability, making these materials highly promising for various applications in organic electronics (Mutzel et al., 2024; Wang et al., 2021). This study highlights the versatility of boron atoms in modulating the photophysical properties of PAHs, as evidenced by the high fluorescence quantum yield (up to 0.73) and red-shifted absorption spectra, which are indicative of enhanced π -conjugation and strong electronic transitions, making the synthesized helical boron-doped PAHs particularly suitable for applications in organic light-emitting diodes (OLEDs) and organic semiconductors (Chen et al., 2023). Moreover, the helical structure of these boron-doped PAHs introduces unique chiroptical properties, which could be explored further for applications in circularly polarized light-emitting devices (CPL-LEDs) and enantioselective catalysis, as the helical geometries promote efficient π - π stacking interactions and stabilize the electronic structure of the materials under operational conditions (Kumar & Sharma, 2019). The study also discusses the scalability of the synthetic methodology, emphasizing the effectiveness of post-

functionalization and cyclization techniques in producing these materials in high yields while maintaining their structural and electronic integrity, which is crucial for advancing their use in commercial organic electronic devices (Zhang et al., 2020). Furthermore, the research highlights the role of computational modeling, particularly density functional theory (DFT) calculations, in predicting the electronic behaviors and guiding the synthesis of these materials, allowing for a deeper understanding of the structure-property relationships that govern their performance in optoelectronic applications (Li et al., 2020; Wang & Chen, 2022). Overall, the study provides compelling evidence that boron-doped PAHs, especially in their helical form, represent a significant advancement in the field of organic electronics, offering new opportunities for the development of efficient and durable organic semiconductors, OLEDs, and other optoelectronic devices.

IX. CHEMICAL REACTIONS RELATED TO THE STUDY

The synthesis of helical boron-doped polycyclic aromatic hydrocarbons (PAHs) involves several key chemical reactions designed to incorporate boron atoms into the PAH framework through a combination of post-functionalization and cyclization techniques, where the initial step involves the functionalization of 3,9-diboraperylene via boron substitution using aryl substituents, which is achieved through a palladium-catalyzed cross-coupling reaction between aryl fluorides and aryl bromides, a process that facilitates the introduction of boron atoms at specific positions in the PAH structure, thereby creating the necessary sites for subsequent cyclization (Mützel et al., 2024; Kumar & Sharma, 2019). In this reaction, palladium catalysts such as Pd(PPh₃)₄ are employed alongside SPhos ligands to promote the decarbonylative reductive cross-coupling, ensuring efficient formation of C(sp²)-C(sp²) bonds between the aryl moieties and the PAH backbone (Li et al., 2020). Once the boron atoms are integrated into the PAH framework, the Friedel-Crafts cyclization reaction is initiated to induce the helical structure, with this step typically involving a Lewis acid catalyst, such as FeCl₃, which facilitates the cyclization of the aryl-substituted 3,9-diboraperylene, leading to the formation of the final

helical boron-doped PAH (Wang & Chen, 2022). The successful creation of the helical geometry is confirmed through various characterization techniques such as nuclear magnetic resonance (NMR) spectroscopy and X-ray crystallography, which verify the structural integrity and proper positioning of the boron atoms within the PAH (Chen et al., 2023). In addition to these key reactions, the optical and electronic properties of the synthesized boron-doped PAHs are examined through spectroscopic methods, including UV-Vis absorption and fluorescence spectroscopy, revealing significant red-shifts in the absorption spectra and enhanced fluorescence quantum yields as a result of the boron doping (Zhang et al., 2020). Furthermore, density functional theory (DFT) calculations are employed to predict and analyze the effects of boron substitution on the frontier molecular orbitals, demonstrating that the presence of boron atoms lowers the LUMO level and improves electron-accepting properties (Li et al., 2020), thereby enhancing the potential application of these materials in organic electronics, particularly in organic light-emitting diodes (OLEDs) and organic semiconductors (Mützel et al., 2024; Wang & Chen, 2022).

CONCLUSION

The synthesis of helical boron-doped polycyclic aromatic hydrocarbons (PAHs) involves several key chemical reactions designed to incorporate boron atoms into the PAH framework through a combination of post-functionalization and cyclization techniques, where the initial step involves the functionalization of 3,9-diboraperylene via boron substitution using aryl substituents, which is achieved through a palladium-catalyzed cross-coupling reaction between aryl fluorides and aryl bromides, a process that facilitates the introduction of boron atoms at specific positions in the PAH structure, thereby creating the necessary sites for subsequent cyclization (Mützel et al., 2024; Kumar & Sharma, 2019). In this reaction, palladium catalysts such as Pd (PPh₃) are employed alongside SPhos ligands to promote the decarbonylative reductive cross-coupling, ensuring efficient formation of C(sp²)-C(sp²) bonds between the aryl moieties and the PAH backbone (Li et al., 2020). Once the boron atoms are integrated into the PAH framework, the Friedel-Crafts cyclization reaction is initiated to induce the helical structure, with this step typically involving a

Lewis acid catalyst, such as FeCl₃, which facilitates the cyclization of the aryl-substituted 3,9-diboraperylene, leading to the formation of the final helical boron-doped PAH (Wang & Chen, 2022). The successful creation of the helical geometry is confirmed through various characterization techniques such as nuclear magnetic resonance (NMR) spectroscopy and X-ray crystallography, which verify the structural integrity and proper positioning of the boron atoms within the PAH (Chen et al., 2023). In addition to these key reactions, the optical and electronic properties of the synthesized boron-doped PAHs are examined through spectroscopic methods, including UV-Vis absorption and fluorescence spectroscopy, revealing significant red-shifts in the absorption spectra and enhanced fluorescence quantum yields as a result of the boron doping (Zhang et al., 2020). Furthermore, density functional theory (DFT) calculations are employed to predict and analyze the effects of boron substitution on the frontier molecular orbitals, demonstrating that the presence of boron atoms lowers the LUMO level and improves electron-accepting properties (Li et al., 2020), thereby enhancing the potential application of these materials in organic electronics, particularly in organic light-emitting diodes (OLEDs) and organic semiconductors (Mutzel et al., 2024; Wang & Chen, 2022).

Scope for further research and limitations of the study
The scope for further research in the study lies in exploring the broader application of boron-doped PAHs across various organic electronic devices, including organic photovoltaics, organic field-effect transistors (OFETs), and circularly polarized light-emitting devices (CPL-LEDs), by examining how different doping patterns and aryl substitutions affect their charge mobility, stability, and optical properties, while future work could also focus on fine-tuning the synthesis process to allow for more precise control over the positioning of boron atoms within the helical PAH structures to achieve even more efficient electronic and photonic properties, as well as investigating the scalability of the synthetic methods for industrial-scale production of these materials; additionally, further computational and experimental studies could be conducted to predict and optimize the performance of boron-doped PAHs under various environmental conditions, and to explore new functionalization strategies that incorporate different

heteroatoms or metal catalysts to expand the versatility of these materials for use in a wider range of optoelectronic applications, thus creating new possibilities for energy-efficient devices. However, the limitations of this study include the complexity and cost associated with the synthesis of helical boron-doped PAHs, as well as the challenges in achieving consistent and reproducible structural configurations during large-scale production, while another limitation is the relatively limited understanding of the long-term stability and degradation pathways of these materials in real-world operating conditions, especially under exposure to heat, light, and environmental stressors, which may hinder their practical application in commercial organic electronics, highlighting the need for further research to address these challenges and enhance the applicability of boron-doped PAHs in future electronic technologies.

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