Simen Owen Academic Proceedings Series

Vol. 3 2026

Review **Open Access**

Electronic Coupling Effects of 2D Material Heterostructures and Their Applications in Flexible Optoelectronic Devices

Yueyang Cong [1,*]

[1] Dongying No.1 High School, Dongying, Shandong, China
* Correspondence: Yueyang Cong, Dongying No.1 High School, Dongying, Shandong, China

Abstract: In the post-Moore era, flexible optoelectronic devices are rapidly advancing towards wearable and portable applications, placing higher demands on material optoelectronic performance and mechanical flexibility. Single 2D materials have inherent limitations, graphene lacks a bandgap, limiting photoelectric conversion efficiency; transition metal dichalcogenides (TMDs) like MoS_2 have low carrier mobility; and black phosphorus is prone to oxidation, affecting long-term stability. These challenges are difficult to address through single material modification. 2D material heterostructures, formed through interlayer composite structures, leverage electronic coupling effects to enhance performance synergistically, providing an effective solution to overcome these limitations. This paper reviews common construction methods for typical 2D heterostructures, such as graphene-based, TMDs-based, and black phosphorus-based structures, including van der Waals stacking, covalent bonding, and solution assembly. It focuses on the mechanisms of interlayer charge transfer, exciton transfer, and orbital hybridization, and discusses how layer number control, strain application, and interface modification influence these coupling effects. Additionally, this work surveys the application of these heterostructures in flexible photodetectors, flexible light-emitting diodes (LEDs), and flexible solar cells, comparing their photoelectric response speed, energy conversion efficiency, and bending stability. Finally, challenges such as interlayer delamination, environmental instability, and difficulties in large-scale fabrication are discussed, with future directions in interface engineering and multifunctional heterostructure integration proposed for enhancing practical applications.

Keywords: 2D heterostructures; electronic coupling effects; flexible optoelectronic devices; charge transfer; interface engineering

Received: 15 December 2025
Revised: 31 January 2026
Accepted: 11 February 2026
Published: 18 February 2026

1. Introduction

Flexible optoelectronic devices, with their light weight, flexibility, and ability to conform to the human body or curved surfaces, have shown broad application prospects in fields such as smart wearables, portable sensors, and flexible displays [1]. The core of improving their performance lies in the selection and optimization of functional materials. Due to their atomic-level thickness, excellent electronic transport properties, and good mechanical flexibility, 2D materials have become key candidates for flexible optoelectronic devices, and related research has become a hot topic in the field of electrical and electronic engineering [2].

However, the performance defects of single 2D materials limit their use in high-end flexible devices: Graphene, while exhibiting excellent conductivity and thermal conductivity, has a zero bandgap, making it difficult to function in optoelectronic conversion and switching devices; TMDs have tunable bandgaps but suffer from low carrier mobility and insufficient conductivity; black phosphorus, as a direct bandgap material, exhibits excellent optoelectronic response, but is easily oxidized in air, severely affecting the device's lifespan [3]. To overcome these limitations, researchers have turned to 2D heterostructures, where different 2D materials are combined to exploit interlayer electronic coupling effects, achieving a "1+1>2" performance enhancement.

In recent years, significant progress has been made in the research of 2D heterostructures. In terms of construction methods, van der Waals stacking technology has become the main approach for fabricating high-quality heterostructures due to its ability to precisely control the interlayer arrangement, while solution assembly and covalent functionalization methods offer potential for large-scale fabrication [4]. Regarding electronic coupling mechanisms, studies have found differences in coupling types across various heterostructures: For example, graphene-TMDs heterostructures mainly enhance device conductivity and optoelectronic response through charge transfer coupling, while heterostructures formed between black phosphorus and WSe_2 show significant exciton transfer coupling, enhancing luminescent efficiency [5]. Covalently bonded heterostructures improve interlayer binding strength and electronic transport stability via orbital hybridization coupling. These coupling effects can be regulated by adjusting material layer numbers, applying mechanical strain, and modifying interface functional groups, providing flexible pathways for device performance optimization [6].

In flexible optoelectronic applications, heterostructures have demonstrated unique advantages: Flexible photodetectors based on graphene/MoS_2 heterostructures show several times the response speed compared to single MoS_2 devices; flexible LEDs made from black phosphorus/WSe_2 heterostructures maintain stable light emission after repeated bending; and heterostructures of MXene and graphene used in flexible photovoltaic devices significantly improve energy conversion efficiency [7]. However, existing studies still have notable gaps: Most research focuses on coupling mechanisms and device performance under ideal conditions, with insufficient exploration of how mechanical deformation in flexible scenarios (such as bending and stretching) affects electronic coupling effects [8]. Interlayer interface compatibility remains a major issue, with long-term use prone to delamination, affecting device stability. In large-scale fabrication, ensuring consistency of heterostructures remains challenging, limiting their engineering application.

Based on these issues, this paper systematically reviews the construction methods, electronic coupling mechanisms, and applications of 2D heterostructures in flexible optoelectronic devices, clarifying the intrinsic relationship between "structural design-coupling regulation-performance optimization." It summarizes the core challenges in current research and proposed solutions, providing valuable insights for the development and practical application of flexible optoelectronic devices in the field of electrical and electronic engineering.

2. Construction and Structural Characteristics of 2D Heterostructures

2D heterostructures are materials formed by stacking different 2D materials together, allowing the combination of their individual strengths and overcoming their inherent limitations. Various methods have been developed to construct high-quality 2D heterostructures, each with its own benefits and challenges.

2.1. Construction Methods

Van der Waals Stacking is the most common technique for creating 2D heterostructures. This method utilizes weak van der Waals forces between adjacent layers, allowing materials with different crystal structures and properties to be stacked without altering their intrinsic features. It is particularly advantageous for combining materials like graphene and transition metal dichalcogenides (TMDs), enhancing their electronic and optoelectronic properties [9]. For instance, graphene/TMDs heterostructures are widely used in flexible photodetectors, benefiting from the complementary properties of each material.

Covalent Bonding involves chemically bonding two 2D materials at their interface. This results in stronger interlayer interactions than van der Waals stacking, which enhances the mechanical and electronic stability of the heterostructure. The covalent bonding technique allows better control over electronic coupling, making it suitable for applications that demand robust interlayer interaction, such as graphene-hBN heterostructures [10]. However, this method is more complex, as it requires activation of the material surfaces before bonding can occur.

Solution Assembly is a scalable approach that disperses 2D materials in a solvent before depositing them onto a substrate. This method is particularly useful for large-scale production of heterostructures, such as graphene/MoS_2, where multiple layers are stacked to optimize performance. Solution-based methods are cost-effective and can be easily adapted for mass production, making them ideal for creating high-quality 2D heterostructures in flexible electronics.

2.2. Structural Characteristics

The structural properties of 2D heterostructures are crucial for determining their performance in optoelectronic devices. Important factors include the number of layers, interlayer interactions, and the application of strain.

Layer Number Control plays a significant role in the electronic properties of 2D heterostructures. For instance, materials like MoS_2 exhibit a tunable bandgap that shifts from indirect to direct as the number of layers decreases. This tunability allows for precise control over the optoelectronic properties, which is beneficial for applications such as photodetectors and light-emitting diodes (LEDs).

Interlayer Interactions refer to the type of bond or force between the layers of the heterostructure. Van der Waals stacking offers flexibility, making it suitable for flexible electronics, while covalent bonding enhances the mechanical strength and electronic stability of the heterostructure [11]. These interactions influence the electronic, thermal, and mechanical properties, which are key to device performance.

Strain Engineering involves applying mechanical strain to 2D heterostructures to tune their electronic properties. By stretching or compressing the layers, strain engineering can modify carrier mobility, bandgap, and interlayer coupling. This technique is particularly useful for optimizing flexible devices, as it enables enhancement of the electronic properties under bending or stretching, which are common in flexible optoelectronic applications.

3. Types and Mechanisms of Electronic Coupling in 2D Heterostructures

2D heterostructures, formed by stacking different 2D materials, exhibit unique electronic properties from interlayer interactions. These coupling effects significantly enhance optoelectronic device performance by combining the strengths of individual materials. The type and nature of coupling vary depending on the materials and construction methods, making it crucial to understand these mechanisms for optimization.

3.1. Charge Transfer Coupling

Charge transfer is a prominent coupling mechanism in 2D heterostructures, occurring when electrons or holes move between adjacent layers due to differences in electronic structures. For instance, in graphene/MoS_2 heterostructures, graphene donates electrons to MoS_2, modulating carrier concentration and enhancing conductivity and optoelectronic properties [12]. This charge transfer boosts performance in devices like flexible photodetectors by improving carrier mobility, resulting in faster response times and better sensitivity. By choosing materials with complementary electronic properties, charge transfer can be tailored to optimize device performance.

3.2. Exciton Transfer Coupling

Exciton transfer is another important coupling mechanism that enhances the optical properties of 2D heterostructures. Excitons, bound pairs of electrons and holes, are formed when light excites electrons in semiconductors. In heterostructures like black phosphorus/WSe_2, excitons generated in black phosphorus transfer to WSe_2, where they recombine and emit light. This transfer improves luminescence efficiency, making the heterostructures ideal for flexible LEDs. By controlling exciton transfer, the emission efficiency and wavelength of flexible LEDs can be optimized.

3.3. Orbital Hybridization Coupling

Orbital hybridization occurs when electron orbitals from adjacent layers overlap, enhancing the interlayer interaction and electronic stability. This coupling is particularly significant in covalently bonded heterostructures, such as graphene/h-BN, where orbital interactions between carbon and nitrogen atoms strengthen the material's stability and improve charge transport. Orbital hybridization is crucial in designing stable, high-performance flexible devices, as it ensures strong interlayer interactions, enhancing device reliability and functionality, especially under mechanical stress [13].

3.4. Strain-Induced Coupling

Strain engineering modifies the interlayer coupling by applying mechanical strain to 2D heterostructures, tuning electronic properties such as carrier mobility, bandgap, and conductivity. This coupling can induce new electronic states, such as band gap shifts, beneficial for enhancing device performance. For example, applying tensile strain to graphene/TMD heterostructures can shift the bandgap of TMDs, improving their photodetector performance. Strain-induced coupling is particularly useful in flexible electronics, as it enhances performance under deformation, optimizing devices for real-world applications.

Collectively, the diverse electronic coupling mechanisms in 2D heterostructures can be categorized and correlated with their physical origins, representative material systems, and functional impacts, as summarized in Table 1.

Table 1. Summary of Electronic Coupling Mechanisms in 2D Heterostructures.

Coupling Type	Physical Origin	Typical Material Systems	Key Influencing Factors	Primary Device Impact
Charge Transfer Coupling	Band alignment-driven carrier migration across interface	Graphene/MoS_2, Graphene/WS_2, MXene/TMDs	Work function difference, interlayer distance, doping	Enhanced photoresponse speed, improved conductivity
Exciton Transfer Coupling	Interlayer diffusion and radiative recombination of excitons	BP/WSe_2, MoS_2/WSe_2, BP/MoS_2	Dielectric environment, layer stacking angle, strain	Increased photoluminescence quantum yield, tunable emission wavelength
Orbital Hybridization Coupling	Overlap and mixing of atomic orbitals at covalent interfaces	Covalently bonded graphene/h-BN, functionalized TMD heterobilayers	Chemical bonding, surface activation, interface functional groups	Improved interlayer mechanical strength, stable charge transport

Strain-Induced Coupling	Mechanical deformation modulating band structure and orbital overlap	Graphene/TMDs on elastomers, wrinkled BP heterostructures	Applied tensile/compressive strain, substrate curvature	Dynamic bandgap tuning, enhanced light absorption, adaptive optoelectronic response

4. Control and Optimization of Electronic Coupling Effects in 2D Heterostructures

The performance of 2D heterostructures in optoelectronic devices depends on how their electronic coupling effects are controlled. Techniques like layer number control, strain engineering, and interface functionalization have been developed to regulate these effects and enhance device performance.

4.1. Layer Number Control

The number of layers in 2D heterostructures plays a significant role in optimizing electronic properties. For materials like MoS_2, the bandgap can shift from indirect to direct as the number of layers decreases, making monolayers suitable for optoelectronic applications. By controlling the number of layers in each material, the interlayer coupling can be tuned to enhance conductivity, charge transfer, and light emission. For example, stacking MoS_2 with graphene in a controlled sequence enhances charge transfer, improving the device's photodetector performance.

4.2. Strain Engineering

Strain engineering modifies the electronic properties of 2D heterostructures by applying mechanical strain, which influences the interlayer coupling, bandgap, and carrier mobility. Strain can be induced by stretching the material or using substrates that introduce strain during fabrication. This method is crucial for flexible electronics, where deformation is inevitable. For instance, applying tensile strain to graphene/TMD heterostructures reduces the TMD's bandgap, improving light absorption and photodetection. Strain also enhances carrier mobility and can optimize exciton transfer, benefiting light-emitting devices [14].

4.3. Interface Functionalization

The interface between the layers in 2D heterostructures is key to determining the strength and stability of interlayer interactions. Interface functionalization involves modifying the interface's chemical composition or structure to enhance coupling. Adding functional groups or using surface treatments can improve bonding strength and electronic coupling, leading to better charge transfer and device stability. For example, introducing nitrogen or oxygen-containing groups at the interface can strengthen interactions, enhancing the heterostructure's overall performance, such as increasing optical emission efficiency or improving charge transfer in photodetectors.

4.4. Environmental Control and Stability Enhancement

Environmental factors like humidity and temperature affect the stability of 2D heterostructures. To optimize electronic coupling, it is important to control these factors during fabrication and operation. Techniques such as surface passivation or encapsulation in protective layers can mitigate degradation from oxidation and moisture. These measures help maintain the heterostructure's performance over time, ensuring long-term stability in flexible devices.

5. Research Progress and Performance Comparison of 2D Heterostructure Flexible Photodetectors

Flexible photodetectors based on 2D heterostructures have gained significant attention due to their ability to combine the unique properties of individual 2D materials, enhancing optoelectronic performance. These devices leverage the atomic thickness, high mobility, and mechanical flexibility of 2D materials, making them ideal for applications in wearable electronics, flexible displays, and sensors. Recent advancements in 2D heterostructure photodetectors, including materials like graphene, TMDs, BP, and MXenes, have shown substantial improvements in responsivity, detectivity, and mechanical flexibility.

For example, graphene/MoS_2 heterostructures combine the high conductivity of graphene with the light absorption capabilities of MoS_2, enhancing photoresponse speed and photoelectric conversion efficiency. The charge transfer between layers improves the photodetector's response time, which is critical for high-speed applications. The mechanical flexibility of these heterostructures allows for bending and stretching without significant degradation. In flexible photodetectors, the device maintains high responsivity even under strain, demonstrating excellent mechanical durability.

BP-based heterostructures, combined with TMDs like WSe_2, exhibit strong exciton transfer coupling, boosting photoluminescent efficiency and broadening spectral sensitivity [15]. The direct bandgap of BP improves light absorption, making these heterostructures ideal for visible to near-infrared light detection. MXene/graphene composites show improved energy conversion efficiency in flexible photovoltaic devices, with the MXene layer facilitating charge transfer and the graphene layer enhancing conductivity.

Despite the progress, challenges remain in achieving an ideal balance between responsivity, speed, and mechanical stability. Most research has focused on optimizing one or two properties, but achieving an optimal balance is still a challenge. The interface between layers in 2D heterostructures also plays a critical role in electronic coupling and overall device stability. Additionally, large-scale fabrication of heterostructures with uniform properties is crucial for commercialization.

Table 2 summarizes the performance of typical 2D heterostructure flexible photodetectors, including responsivity, detectivity, response time, and stability under bending. It highlights the significant performance differences between various material combinations.

Table 2. Performance Comparison of 2D Heterostructure Flexible Photodetectors.

Device (Materials)	Responsivity (A/W)	Detectivity (Jones)	Response Time (s)	Bending/Stretching Stability
Graphene/MoS_2 (wrinkled)	~10 to 100	~10^{12}-10^{13}	~10^{-3}-10^{-2}	Tensile strain >100% without degradation
BP/TMD heterostructure	~10-100	~10^{11}-10^{12}	~10^{-4}-10^{-3}	Maintains performance after >1000 bending cycles
MXene/Graphene composite	~100-500	~10^{12}	~10^{-2}	Performance drop <10% after 100 cycles

As shown in Table 2, various material combinations show promising performance in terms of responsivity, detectivity, and mechanical stability. However, further work is required to enhance response time while maintaining mechanical flexibility and durability. The development of techniques for optimizing interlayer coupling and improving large-area uniformity will be essential for advancing flexible photodetector technology.

In conclusion, although significant progress has been made in 2D heterostructure-based flexible photodetectors, challenges remain in balancing responsivity, response time, and stability. Future research will likely focus on improving scalability, addressing interface issues, and enhancing environmental stability to enable widespread application in flexible electronics.

6. Applications of 2D Heterostructures in Flexible Light Emitting and Display Devices

2D heterostructures have shown great promise in flexible light-emitting devices, such as LEDs and flexible displays, due to their tunable electronic and optical properties. These heterostructures combine the strengths of individual 2D materials, enhancing light emission efficiency, spectral range, and mechanical flexibility, all of which are critical for the development of high-performance flexible optoelectronics.

One of the key applications of 2D heterostructures in light-emitting devices is in flexible LEDs. By combining materials like BP with TMDs such as WSe_2 or MoS_2, strong exciton transfer coupling is achieved, which enhances the light-emission efficiency. BP, with its direct bandgap, provides high photoluminescence, while TMDs, with tunable bandgaps, extend the spectral range of emission. This combination results in high-efficiency light emission in flexible, bendable devices. The mechanical flexibility of these heterostructures allows for the creation of bendable or stretchable LED displays, which are crucial for applications in foldable smartphones, wearable technology, and flexible signage.

Additionally, graphene/TMDs heterostructures are widely explored in flexible displays due to their fast charge carrier mobility and high electronic stability, allowing for efficient light emission and high pixel density. These heterostructures enable low-power consumption, rapid switching times, and high optical quality in flexible display applications.

Despite the advancements, challenges remain in enhancing the color purity, efficiency, and lifetime of flexible light-emitting devices. The interface between different 2D materials plays a critical role in controlling the exciton dynamics and charge recombination efficiency. Moreover, the scalability of fabrication methods for large-area flexible displays and maintaining uniformity in device performance are areas requiring further development.

In conclusion, 2D heterostructures are pivotal in advancing flexible light-emitting and display devices, with future research focused on improving efficiency, scalability, and environmental stability.

7. Performance Degradation and Stabilization Techniques in Flexible Conditions for 2D Heterostructures

The mechanical flexibility of 2D heterostructures is one of their most significant advantages for flexible optoelectronic devices. However, the performance of these heterostructures can degrade when subjected to mechanical stress, environmental factors, or prolonged operation. Understanding the mechanisms behind performance degradation and developing stabilization techniques is crucial for ensuring the long-term reliability of flexible devices.

7.1. Performance Degradation Mechanisms

7.1.1. Mechanical Deformation and Strain

In flexible devices, 2D heterostructures are often subject to bending, stretching, or torsional forces. While these materials are inherently flexible, the application of mechanical strain can induce defects, such as cracks or dislocations, particularly at the interfaces between different 2D materials. These defects can disrupt the electronic coupling between layers, leading to reduced carrier mobility and efficiency. The interlayer delamination caused by repeated mechanical deformation can further exacerbate the degradation, weakening the overall performance of the device.

For example, bending a graphene/TMDs heterostructure can cause strain localization, which may lead to changes in the electronic properties of the TMD layer, affecting charge transfer and optical performance. Similarly, tensile strain can cause an increase in carrier scattering, which reduces the photodetector's responsivity and speed.

7.1.2. Environmental Factors

2D materials, especially BP and TMDs, are highly sensitive to environmental conditions, such as humidity, temperature fluctuations, and exposure to oxygen or light. These materials tend to oxidize or degrade under ambient conditions, significantly affecting their stability and performance. For instance, black phosphorus is prone to rapid oxidation when exposed to air, leading to loss of its photonic properties. Likewise, moisture can introduce unwanted adsorbates that interfere with the interface coupling between the 2D layers, causing shifts in the electronic structure and reducing device efficiency.

7.1.3. Interface Instability:

The interfaces between different 2D materials play a critical role in determining the strength and stability of the electronic coupling. However, the interface is often the weakest point in the heterostructure, where defects, poor bonding, or misalignment can occur. Such defects reduce the stability of the heterostructure, particularly under mechanical deformation. As interfaces degrade, the interlayer coupling weakens, leading to reduced performance in optoelectronic devices, such as lower photoresponse and reduced lifetime.

7.2. Stabilization Techniques

7.2.1. Surface Passivation

To combat environmental degradation, surface passivation techniques can be employed to protect 2D heterostructures from exposure to oxygen and moisture. Coating the surfaces of the materials with protective layers, such as atomic layer deposition (ALD) films, graphene oxide, or polymer encapsulation, can significantly enhance the stability of the heterostructure. These coatings act as barriers, preventing oxidation and moisture absorption, which helps to maintain the optoelectronic properties of the materials. For example, passivating BP-based heterostructures with an ultra-thin protective layer can effectively prevent degradation while maintaining their photoluminescent efficiency.

7.2.2. Strain Engineering:

Strain engineering can be used not only to tune the electronic properties of 2D heterostructures but also to mitigate the effects of mechanical deformation. By carefully controlling the application of strain, it is possible to prevent the formation of defects and enhance the stability of the materials. Pre-strained substrates or multi-layer stacking strategies can help distribute the strain evenly across the material, preventing localized strain that could lead to defects. Additionally, dynamic strain adjustment, where strain is applied selectively during device operation, can optimize the coupling effects and minimize performance degradation under bending or stretching conditions.

7.2.3. Interface Engineering:

Optimizing the interfaces between different 2D materials is crucial for enhancing stability and preventing degradation. One approach is interface functionalization, where chemical or physical treatments are applied to the interface to improve bonding strength and minimize defects. Covalent functionalization of the interface can strengthen the interaction between layers and reduce delamination under mechanical stress. Moreover, the use of buffer layers, such as h-BN or $MoSe_2$, can improve interface compatibility, enhancing the overall stability and performance of the heterostructure.

7.2.4. Encapsulation and Encapsulation Materials:

Encapsulation plays a vital role in protecting flexible optoelectronic devices from environmental degradation. Using encapsulation materials, such as silicon oxide, polymer films, or graphene oxide, can shield the heterostructures from moisture, oxygen, and mechanical stresses, ensuring long-term reliability. Advanced encapsulation techniques that maintain flexibility while providing robust protection are critical for the commercialization of flexible devices.

7.3. Stabilization Techniques Flowchart

Figure 1 illustrates the key stabilization techniques used to enhance the performance and durability of 2D heterostructures in flexible devices. These techniques, such as surface passivation, strain engineering, and interface optimization, play a crucial role in improving the stability of the materials under mechanical and environmental stresses.

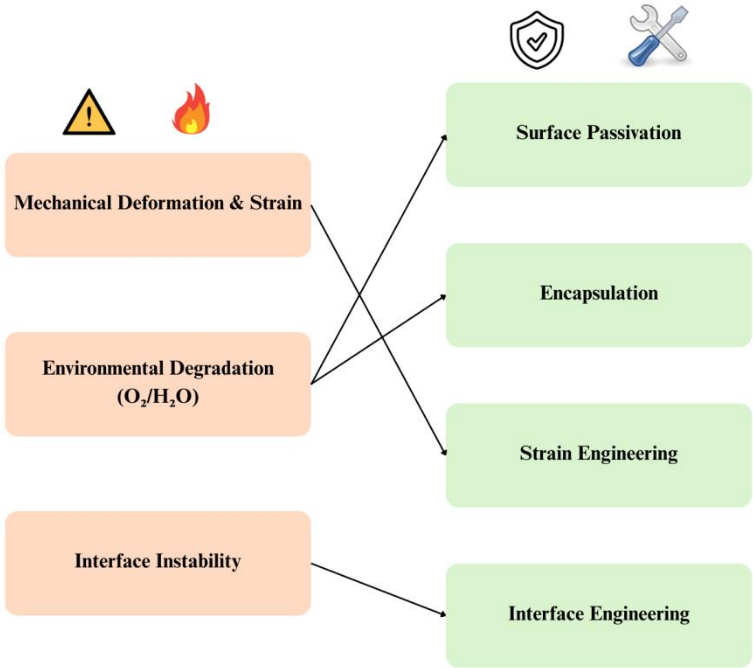

Figure 1. Stabilization Techniques Flowchart for 2D Heterostructures.

8. Engineering Challenges and Future Development Trends of 2D Heterostructures

Despite significant progress in 2D heterostructure research, several engineering challenges hinder their widespread use in commercial optoelectronic devices. Key challenges include scalability, uniformity, stability, and integration of 2D heterostructures into practical devices. Addressing these obstacles will be crucial for realizing the full potential of 2D heterostructures in flexible electronics, sensors, displays, and energy conversion devices.

8.1. Scalability and Large-Scale Fabrication

One of the major obstacles in commercializing 2D heterostructures is producing high-quality, large-area heterostructures in a cost-effective and reproducible manner. Most fabrication methods, such as mechanical exfoliation, chemical vapor deposition (CVD), and solution-based assembly, are suited for laboratory-scale production but face challenges when scaled up. Mechanical exfoliation provides high-quality single layers but is labor-intensive and not scalable for industrial production. CVD can be scaled up but often struggles to produce uniform, large-area films with consistent quality.

To overcome these limitations, researchers are exploring scalable techniques like liquid-phase exfoliation and direct growth, which can be used to produce large-area, high-quality 2D materials. These methods are crucial for ensuring uniformity in large-area heterostructures and are needed for commercial applications in flexible electronics, where uniform performance is required.

8.2. Interface and Layer Alignment

The quality of the interface between the different 2D layers in a heterostructure is critical for device performance. Poor alignment or weak interlayer coupling can degrade the heterostructure's functionality, particularly in optoelectronic devices such as photodetectors or LEDs. Achieving precise alignment and strong interlayer bonding is challenging, and defects at the interface can lead to traps or leakage currents, reducing efficiency.

To address these issues, researchers are developing advanced transfer techniques and interface engineering strategies, such as laser-assisted transfer, wet transfer, and direct growth on flexible substrates. These methods aim to improve layer alignment and interlayer bonding, enhancing device performance. However, controlling these interfaces on a large scale remains a significant challenge.

8.3. Environmental Stability

Many 2D materials, especially black phosphorus and transition metal dichalcogenides (TMDs), are highly sensitive to environmental factors like humidity, temperature, and exposure to oxygen or light. For example, black phosphorus rapidly oxidizes when exposed to air, which significantly degrades its photonic properties. TMDs are also susceptible to surface defects and degradation under ambient conditions, limiting their practical use in flexible optoelectronic devices.

Surface passivation techniques, protective coatings, and encapsulation have been developed to enhance the environmental stability of 2D heterostructures. These methods protect the materials from oxidation and moisture, but ensuring that these protective layers do not interfere with the optoelectronic properties of the devices remains a challenge. Further research is needed to improve the environmental protection of 2D heterostructures, especially for applications requiring long-term stability.

8.4. Future Development Trends

The future development of 2D heterostructures will focus on overcoming the challenges of scalability, interface quality, and environmental stability. Several key trends are likely to shape the future of this field: (1) Advanced Fabrication Techniques: New scalable production methods, such as roll-to-roll processing and laser-assisted growth, will be crucial for large-scale manufacturing of 2D heterostructures. These methods will enable the production of high-quality, uniform materials on flexible substrates, making them suitable for commercial applications. (2) Interface Engineering: Achieving better control over interlayer interactions and layer alignment will be essential for improving the performance and stability of 2D heterostructure devices. Developing new materials or techniques for interface functionalization will help to enhance the coupling between layers and reduce defects. (3) Environmental Protection: Research into self-healing materials and environmentally stable coatings will be key for improving the longevity and reliability of 2D heterostructure-based devices. Materials that can repair themselves or protect the 2D layers from environmental damage will extend the lifetime and performance of flexible optoelectronics. (4) Multifunctional Integration: The integration of multiple functionalities, such as combining sensors, light-emitting components, and energy harvesting elements, into a single 2D heterostructure will enable more compact and efficient systems. Multifunctional devices could lead to innovations like self-powered flexible displays and wearable electronics.

References

1. Z. Wang, and G. Shen, "Flexible optoelectronic sensors: status and prospects," *Materials Chemistry Frontiers*, vol. 7, no. 8, pp. 1496-1519, 2023. doi: 10.1039/d2qm01319c
2. A. K. Katiyar, A. T. Hoang, D. Xu, J. Hong, B. J. Kim, S. Ji, and J. H. Ahn, "2D materials in flexible electronics: recent advances and future prospectives," *Chemical Reviews*, vol. 124, no. 2, pp. 318-419, 2023.
3. D. Maity, D. De, and G. G. Khan, "Black Phosphorus Solution-Phase Preparation and Applications in Energy Conversion," In *Layered Nanomaterials for Solution-Processed Optoelectronics*, 2025, pp. 251-294. doi: 10.1201/9781003509509-10
4. M. Cai, J. Yang, X. Lu, and X. Lu, "Layer-by-layer self-assembly strategies of atomically thin two-dimensional nanomaterials: principles, methods, and functional applications," *ACS Applied Nano Materials*, vol. 7, no. 24, pp. 27940-27959, 2024. doi: 10.1021/acsanm.3c06286
5. H. B. Wang, F. Wang, J. Yang, and M. Fan, "Electric field-induced anisotropy in the electronic properties of blue phosphorus/WSe2 heterojunction," *Materials Today Communications*, vol. 37, p. 107343, 2023.
6. Z. Yi, X. Li, B. Xiao, Q. Jiang, Y. Luo, and J. Yang, "Dual-interface engineering induced by silane coupling agents with different functional groups constructing high-performance flexible perovskite solar cells," *Chemical Engineering Journal*, vol. 469, p. 143790, 2023. doi: 10.1016/j.cej.2023.143790
7. G. Dastgeer, M. W. Zulfiqar, S. Nisar, R. Zulfiqar, M. Imran, S. Panchanan, and Z. Wang, "Emerging role of 2D materials in photovoltaics: efficiency enhancement and future perspectives," *Nano-Micro Letters*, vol. 18, no. 1, p. 32, 2026. doi: 10.1007/s40820-025-01869-z
8. Z. Zhao, H. Fu, R. Tang, B. Zhang, Y. Chen, and J. Jiang, "Failure mechanisms in flexible electronics," *International Journal of Smart and Nano Materials*, vol. 14, no. 4, pp. 510-565, 2023. doi: 10.1080/19475411.2023.2261775
9. R. Dutta, A. Bala, A. Sen, M. R. Spinazze, H. Park, W. Choi, and S. Kim, "Optical enhancement of indirect bandgap 2D transition metal dichalcogenides for multifunctional optoelectronic sensors," *Advanced Materials*, vol. 35, no. 46, p. 2303272, 2023. doi: 10.1002/adma.202303272
10. A. Kumar, D. Solanki, K. Watanabe, T. Taniguchi, A. K. Sood, and A. Das, "Interlayer Phonon Coupling and Enhanced Electron-Phonon Interactions in Doubly Aligned hBN/Graphene/hBN Heterostructures," *ACS nano*, vol. 19, no. 17, pp. 16415-16423, 2025. doi: 10.1021/acsnano.4c17152
11. T. Ding, X. Jiang, J. Quan, R. Wang, M. Li, C. Lan, and M. Zhu, "Recent progress in two-dimensional van der Waals heterojunctions for flexible energy storage applications," *Advanced Composites and Hybrid Materials*, vol. 8, no. 4, p. 324, 2025. doi: 10.1007/s42114-025-01410-1
12. S. Shen, M. F. O. Hameed, C. Zhang, G. Zhu, F. Qin, M. Jiang, and J. Dai, "Tunable Teraherz absorber via strong dual-Tamm plasmon coupling in Graphene-MoS2 based photonic crystals," *Physics Letters A*, 2025. doi: 10.1016/j.physleta.2025.130793
13. D. Wen, R. Yuan, K. Cao, F. Yang, and R. Chen, "Advancements in atomic-scale interface engineering for flexible electronics: enhancing flexibility and durability," *Nanotechnology*, vol. 35, no. 41, p. 412501, 2024. doi: 10.1088/1361-6528/ad64db
14. M. Long, P. Wang, H. Fang, and W. Hu, "Progress, challenges, and opportunities for 2D material based photodetectors," *Advanced Functional Materials*, vol. 29, no. 19, p. 1803807, 2019. doi: 10.1002/adfm.201803807
15. F. Zhao, D. Wang, F. Zhang, B. Cui, Q. Xia, and M. Zhong, "Gate-controlled photoresponse improvement in b-AsP/WSe2 heterostructures with type-I band alignment," *Applied Physics Letters*, vol. 122, no. 15, 2023. doi: 10.1063/5.0144982