

Two-Dimensional Photovoltaics and Two-Dimensional Material Application

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Abstract. As an emerging class of materials, two-dimensional (2D) materials have garnered significant attention in the field of photovoltaics due to their exceptional and unique properties. These materials, characterized by their atomically thin layers, offer promising opportunities for enhancing the efficiency and performance of solar energy conversion. This paper will focus on the principles governing 2D photovoltaic materials, providing an in-depth exploration of their characteristics and their applications in various types of photovoltaic devices. By examining the common features of these materials, the paper aims to offer readers a comprehensive understanding of what 2D materials are and how they can be effectively utilized in solar technology. Furthermore, the paper will also delve into the methods used for preparing and characterizing different types of 2D materials, offering insights into the cutting-edge techniques employed in the field. Additionally, the discussion will extend to the future research directions and potential applications of 2D materials in photovoltaics, encouraging readers to consider the broad scope of their impact. Through this exploration, the paper seeks to provide both scientific insights and practical knowledge for researchers and industry professionals interested in the rapidly growing field of 2D photovoltaics.

Keywords: Two-dimensional (2D) materials, photovoltaics, properties, fabrication, solar cells.

1. Introduction

Although solar energy, as a renewable and sustainable resource, provides us with a lot of convenience and abundant energy in contemporary society, it also faces a series of problems and challenges. Nadarajah Kannan, Divagar Vakeesan illustrates some possible problems and challenges in the paper 'Solar energy for future world' in detail, the only listed part of the views and content. First of all, solar photovoltaic technology is very demanding, industrial costs are expensive and at the same time require advanced manufacturing and installation technology. Second, the performance of solar panels pays great attention to changes in environmental factors, especially the three elements of sunshine intensity, cloud cover and wind speed, in other words, the efficiency of solar power generation directly depends on these three elements. In addition, although the majority of consumers think that solar power or solar cells are green and pollution-free, in fact, solar cells or solar panels are mostly made of some chemicals that are toxic to the environment. Not only is it difficult to degrade, but even after degradation, some substances harmful to the environment may be generated, which is undoubtedly a major difficulty for manufacturers and distributors of solar power industry [1].

However, at the same time, a new type of recyclable material, 2D materials, has emerged in the world. 2D photovoltaics, derived from the application of 2D materials, are beginning to make a name for themselves in the field of energy production and are gradually being accepted by more people. Lin Wang, Kah-Wee Ang put forward valuable points in their paper. Despite the fact that the photovoltaic efficiency of 2D crystal-based photovoltaic devices is currently relatively low, or that the technical level of 2D photovoltaic power generation is far lower than that of traditional solar cells, this is mainly due to the problem of their thickness not being solved, which has caused a limitation in light absorption [2]. However, the inherent advantages of 2D materials are actually very suitable for manufacturing the next generation of photovoltaic devices. For example, transparency, flexibility, light weight, high absorption rate, etc., which are not possessed by traditional solar power generation materials.

2. The basic principle of two-dimensional(2D) photovoltaics

Before getting to know the basic principle of 2D photovoltaics, it is important to clarify what two-dimensional(2D) materials are and their basic properties. A 2D material is characterized by a sheet-like form that has a thickness of just a few nanometers, typically around 1 to 2 atoms. In this structure, electrons are able to move freely within the 2D plane.

2.1. Properties of 2D materials

2D materials possess some remarkable properties, it mainly manifests in the 3 prospects of Mechanical, Electrical, and Optical. For the mechanical properties, graphene, the most well-known 2D material, possesses the highest tensile strength and modulus found in nature. Investigations into graphene's mechanical characteristics have been conducted extensively. The initial comprehensive experimental analysis of its elastic modulus and force was performed using an atomic force microscope (AFM). Graphene demonstrates nonlinear elasticity and brittle failure. Findings indicate that its Young's modulus is approximately 1.0 TPa, while the third-order elastic stiffness measures - 2.0 TPa. It experiences catastrophic fracture at an intrinsic strength of 130 GPa, which stands as the highest recorded value among real-world materials. Other researchers still utilized AFM to assess the elastic constants of graphene layers ranging from one to five layers thick. Research on graphene nanoflakes under 10 nm thickness reveals that their elastic constants fluctuate between 1 and 5 Nm^{-1} . Mechanical tests on graphene illustrate that it undergoes nonlinear elastic deformation when subjected to tensile stress until reaching its inherent strength, followed by strain softening prior to breaking apart. In contrast to bulk materials, 2D structures can endure higher mechanical strains due to their unique atomic configurations. Additionally, the reduced thickness of these materials often results from local strains induced by manipulation methods such as poking or folding them like paper; reports suggest that graphene can tolerate up to a structural damage level of 25% without fracturing [3]. Certain Electronic, optical, and mechanical properties of 2D materials is shown in figure 1.

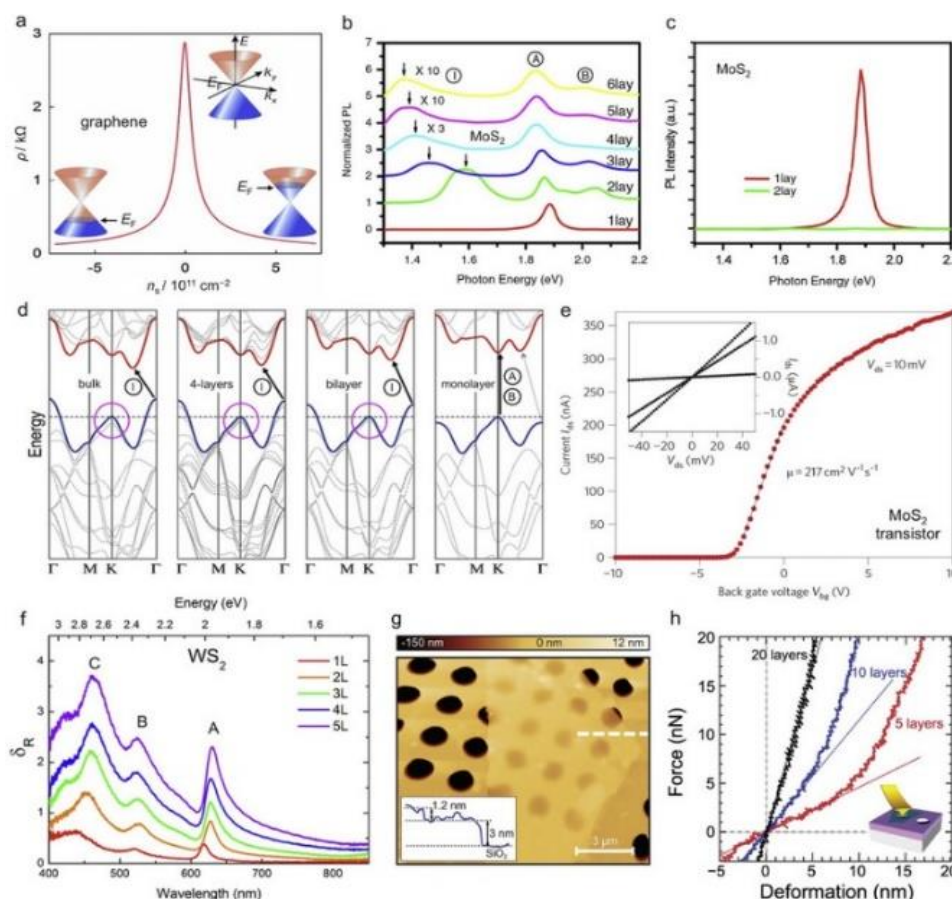


Figure 1. Certain Electronic, optical, and mechanical properties of 2D materials

Also, in the aspect of electrical properties, graphene serves as an illustrative example when discussing electrical properties. Its single-atom thickness means that all carbon atoms are entirely exposed to the environment, distinguishing it from bulk materials. The electrical characteristics of this one-atom-thick graphene are particularly sensitive to foreign particles that may adhere to its surface. Consequently, modifying the chemical composition of graphene's surface enables us to manipulate various factors such as doping type, carrier concentration, bandgap, and work function. These attributes position graphene as a competitive functional material in semiconductor technology compared to traditional bulk materials.

In contrast, altering the electrical properties of bulk materials necessitates a uniform distribution of foreign atoms not just on their surfaces but also throughout their volume. To cater to diverse applications effectively, it is essential to create heterogeneous interfaces with tunable electrical properties; this can enhance functionality and improve device performance while allowing for greater flexibility in device design. Thus, employing straightforward chemical techniques to engineer the electrical properties of graphene presents a promising alternative for developing high-performance electronic and optoelectronic devices suitable for real-world applications [4].

Besides, in the optical area, Kumbhakar P, Chowde Gowda C, and colleagues clearly mention in their research that graphene is a leading material in the realm of 2D substances [5]. The interactions between light and this material result in remarkable optical characteristics that influence areas such as optoelectronics, nanoelectronics, and nonlinear optics. The Graphene's linear absorption feature is shown in figure 2.

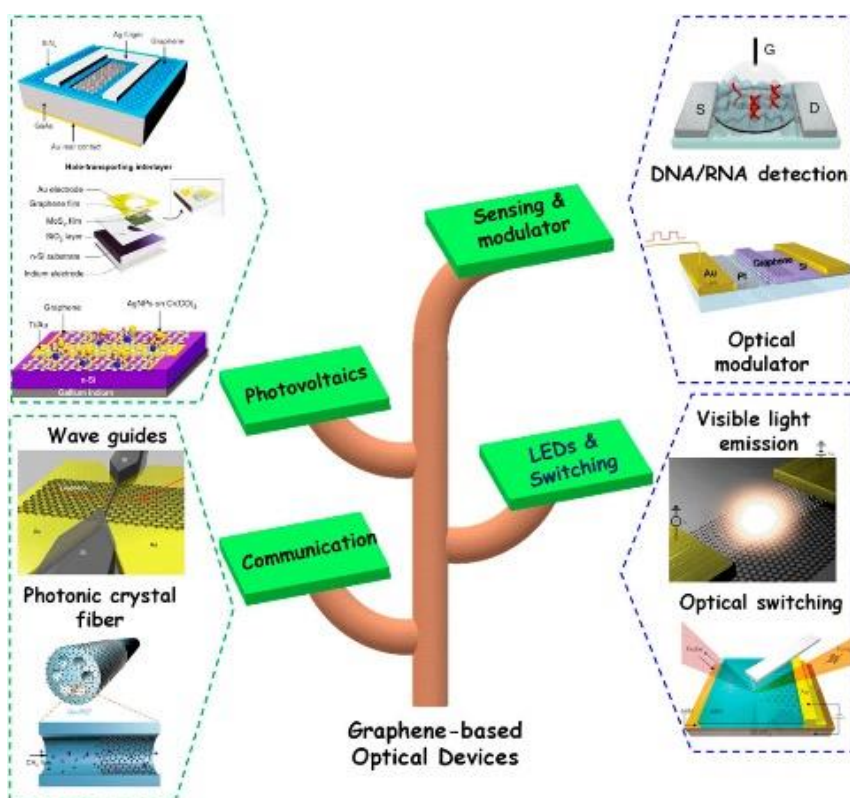


Figure 2. Graphene's linear absorption feature

The figure illustrates that graphene's linear absorption features a band centered around 260 nm, attributed to the $\pi-\pi^*$ transition of sp^2 hybridized carbon atoms. Notably, graphene does not produce any visible fluorescence. Numerous studies have previously explored its potential applications in ultrafast optical switches, solar cells, optical modulators, plasma devices, transparent LEDs, low-voltage displays, rapid optical communication systems, and advanced photodetectors within the ultraviolet spectrum. Researchers believe that graphene's UV absorption properties could be highly beneficial for solid-state lighting technologies. Recently, there has been growing interest in optical switches as alternatives to traditional electrical ones. Nomi et al. significantly improved nonlinear

absorption in graphene by integrating plasma waveguides and successfully developed an ultrafast optical switch linked to a conventional waveguide.

In parallel, significant findings have emerged from recent investigations into black phosphorus (BP). This material exhibits high mobility and possesses a direct bandgap that changes with thickness. The optical and electrical characteristics of multilayer BP films can be adjusted through periodic stress application. Its tunability surpasses that of transition metal dichalcogenides (TMDs), achievable via low-temperature periodic stress modulation for quantum confinement effects. Consequently, BP is poised for extensive use across various domains such as photovoltaics and optoelectronics [5].

2.2. The principle of application of two-dimensional materials in photovoltaic devices

The atomic thickness of 2D materials just talked about before provides a natural benefit by achieving an exceptionally high surface-to-volume ratio. This elevated ratio facilitates notable enhancements in light absorption and interface quality, improving the material's interaction with light and increasing solar energy absorption. Enhancing contact between various layers or materials can boost charge transport while minimizing recombination losses, among other advantages. A group of researchers from Korea examined the distinctions between vertically aligned 2D crystals and those grown horizontally, focusing primarily on production efficiency. Unlike horizontally growing 2D semiconductor crystals that can be formed on any substrate, vertically aligned variants may prove more effective for applications where the final device's surface area is crucial—such as in hydrogen generation reactions, lithium-ion batteries, and chemical sensors—since they allow for preferential exposure of high-activity edge sites over the substrate surface. Notably, the sensitivity of chemical resistance sensors correlates directly with active surface area because their sensing mechanism relies on variations in carrier concentration and/or mobility due to adsorbed analyte molecules at the active surface. Consequently, various types of 2D structural materials have emerged as promising candidates for high-sensitivity chemical sensors owing to their remarkably high surface-to-volume ratios. Their application is expected to expand significantly in everyday life moving forward [6].

Generally, the use of 2D materials in solar energy devices leverages their distinctive characteristics to improve multiple facets of solar energy conversion, such as light absorption, charge separation, and flexibility. Ongoing research and development focus on addressing existing challenges and maximizing the potential of these materials for future solar technologies.

2.3. Application of two-dimensional material heterostructures in photovoltaics

Two-dimensional(2D) stacked crystals, commonly referred to as 2D heterostructures, have emerged as a highly desirable structure over the past few decades. Their varied chemical and physical characteristics have piqued the interest of numerous researchers, leading to new avenues of investigation. This has also promoted the development of 2D heterostructures exhibiting intriguing thermal, optical, and electrical properties. The layers of two-dimensional materials that interact through weak van der Waals forces can be separated to create isolated atomic layers. These individual layers can then be rearranged into both horizontally and vertically aligned heterostructures.

This text above provides a conceptual overview of heterostructures made from two-dimensional materials. The following section will cover the methods for growth and specific applications related to these heterostructures. Besides the conventional indirect techniques used for growing two-dimensional crystals, modern vapor deposition technologies are opening up new possibilities for directly creating two-dimensional heterostructures, thus offering more opportunities within the semiconductor sector. This advancement has led to various applications including high-efficiency LEDs, photodetectors, neuromorphic devices, and lasers. Typically, two-dimensional heterostructures are formed by integrating multiple semiconductors that create a distinct electronic band structure at their interfaces. Materials sharing similar elemental properties—like carbon-based substances (g-C₃N₄ and graphene) or transition metal dichalcogenides (TMDs) such as MoS₂ and WS₂—can be combined effectively. A well-defined classification system based on recent

developments may assist researchers in anticipating future areas of study: The properties of single-layer, double-layer, and multilayer graphene differ significantly. By layering 2D semiconductors with graphene in these structures, researchers aim to leverage the strengths of both materials for use in electronic devices. In comparison to p-n junctions, p-i-n configurations, and series solar cells, Schottky barrier solar cells feature simpler designs and manufacturing processes; they only require establishing a metal-semiconductor junction that generates an internal electric field within the depleted region of the semiconductor. Recently observed impressive photon absorption capabilities have been noted in 2D semiconductors just a few atomic layers thick. For Schottky barrier solar cells to perform optimally, key factors include having a strong electric field at the metal/semiconductor interface along with defect-free surfaces (to prevent free electron energy level pinning), effective photon absorption mechanisms, and efficient carrier transport systems. Generally speaking, layered 2D semiconductors possess self-terminating atomic planes without dangling bonds on their surfaces which contributes to forming high-quality interfaces while minimizing interface traps [7].

3. Common two-dimensional photovoltaic materials: Graphene, WS₂, black phosphorus, MoS₂

This section will discuss three typical two-dimensional materials, focusing on their structures and properties. First, graphene consists of a single layer of carbon atoms arranged in a hexagonal pattern. Serving as the fundamental building block for other carbon allotropes such as graphite and carbon nanotubes, graphene does not have an intrinsic bandgap; however, its exceptional electrical conductivity and mechanical strength render it valuable in hybrid photovoltaic systems as well as components within composite materials aimed at enhancing performance. The figure 3 below shows the Graphene structures in different dimensions.

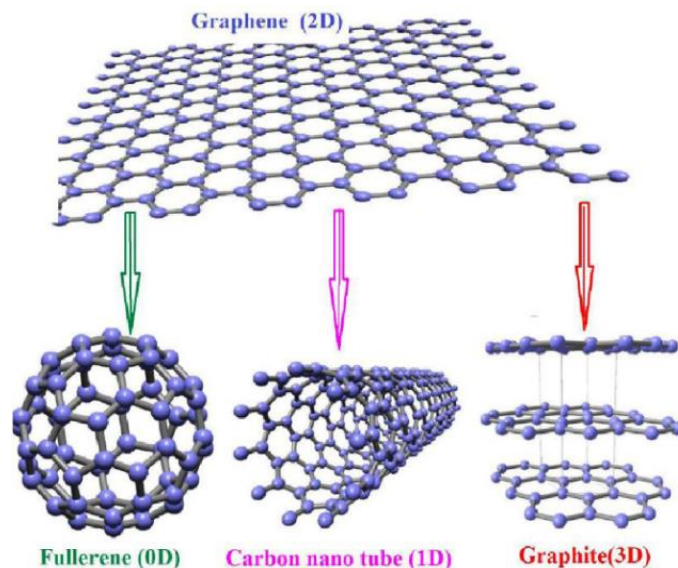


Figure 3. Graphene Structure

Next, WS₂ (Tungsten Disulfide) shares similarities with MoS₂ but has tungsten atoms instead of molybdenum within its layered structure. Like MoS₂, WS₂ also presents a direct bandgap when in monolayer form, offering strong light absorption and favorable electronic properties. This material shows promise for use in flexible and lightweight solar devices.

Additionally, black phosphorus represents another 2D material with a layered configuration where phosphorus atoms create a puckered honeycomb lattice. Regarding its properties, black phosphorus possesses a tunable direct bandgap that changes depending on the number of layers present; this versatility makes it suitable for various optical and electronic applications. It is well-known for having high carrier mobility along with anisotropic characteristics.

Lastly, MoS₂ (Molybdenum Disulfide) is a transition metal dichalcogenide (TMD) characterized by its layered architecture. It features molybdenum atoms situated between two layers of sulfur atoms. In terms of properties, MoS₂ exhibits a direct bandgap in its monolayer form, which enhances both light absorption and electronic characteristics. It is recognized for its high carrier mobility and stability, making it ideal for photovoltaic applications.

4. Methods of Preparation and Characterization of Two-Dimensional Materials

4.1. Preparation of Two-Dimensional Materials

It is a common method to prepare heterojunction photodetectors by wet transfer of two-dimensional material to semiconductor substrate. In the process of wet transfer to prepare the heterojunction, different preparation process details have a significant effect on the properties of the heterojunction formed by two-dimensional materials and semiconductors. Taking the typical two-dimensional material graphene (Gr) as an example, a series of identical Gr/Si heterojunction photodetectors were prepared by wet transfer. The Industrial flow chart shows in figure 4 below.

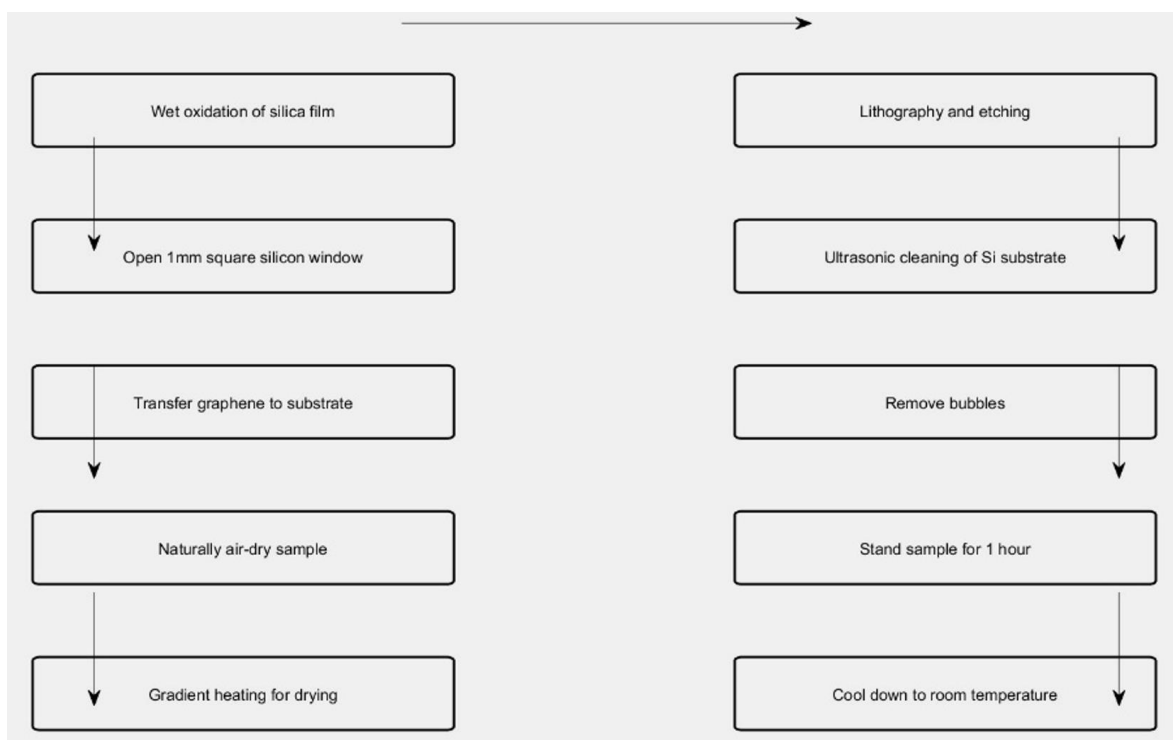


Figure 4. The wet transfer preparation of identical Gr/Si heterojunction photodetectors

(1) A 3000-angstrom silica film was wet-oxidized on a low resistivity N-type zoned silicon substrate with <100> crystal orientation and epitaxial N-type epitaxial layer of 50-micron thickness (resistivity of about 16 ohm-cm). Through lithography and etching techniques, a 1 mm square silicon window is opened on the silica thin film to expose the silicon substrate to form a van der Waals heterojunction with graphene.

(2) Gr transfer to substrate. First, the Si substrate is ultrasonic cleaned to prepare for Gr. The Gr used in this paper is ACS (Advanced Chemical Supply Company) one-step transfer Gr, which transfers the Gr to the substrate with silicon window without spinning PMMA again. During the transfer process, to minimize the formation of lower bubbles during the Gr floating in the water, use a slide to gradually remove the bubbles until the bubbles can hardly be observed. The substrate was tilted into the water, and Gr was slowly lifted up so that Gr was in the middle of the substrate. At this time, the transferred sample was naturally air-dried, and the sample was placed on the filter paper and covered with a petri dish to prevent dust from falling into the substrate. The substrate was left standing for 1h.

(3) Drying of heterojunction sample. The sample was placed on the preheated hot plate, and gradient heating was adopted to avoid excessive evaporation during heating, which would cause Gr to be broken by bubbles. After the whole drying process was completed, the sample was cooled to room temperature naturally, a certain amount of acetone was poured into a clean petri dish, the sample was soaked in acetone to remove glue, the hot plate was preheated at 45 °C, the acetone was heated for 2 h, and the PMMA was accelerated to dissolve, the acetone was replaced and soaked for 12 h, and another clean petri dish was used to cover the sample to reduce acetone volatilizing and avoid dust entering. After the degluing process, the acetone solution remaining on the surface of the sample was cleaned with anhydrous ethanol, the ethanol was blown dry with the ear wash ball, the sample was placed on the filter paper, covered with the petri dish and left to evaporate completely, and the sample was placed on the preheated hot plate for constant temperature (50 °C) drying.

(4) Graphene selective etching, used to isolate different heterojunction devices, while etching most of the non-photosensitive areas of graphene. The PMMA point is placed on the Gr layer above the silicon oxide window to protect the local Gr. In order to avoid the adhesion of PMMA between points, place it on the preheated hot plate at 60 °C in advance and add hot glue, which not only accelerates the solidification of PMMA, but also ensures the uniformity of PMMA dispensing. After the whole dispensing process was completed, the hot plate was heated to 85 °C, the PMMA was solidified for 15 min, and the sample was placed into the chamber of the oxygen plasma cleaning machine for oxygen plasma dry etching. The RF power was 70 W, the oxygen flow rate was 40 mL/min, and the etching time was 2.5 min. Then, the sample after etching is degummed. The degumming procedure here is the same as that after transfer drying. However, due to the large thickness of PMMA layer, the process of heating acetone in water bath takes a little longer. After the degumming step is completed, the sample is dried at 170 °C for 40 min.

(5) Annealing. Finally, the whole sample was annealed and placed in the CVD annealing furnace for annealing treatment. It is protected by Ar atmosphere and annealed at 400 °C for 2 h. On the one hand, the annealing treatment is to further remove the PMMA on the surface of Gr before transfer and the PMMA during etching. On the other hand, the volatile impurities remaining during the solution transfer process will also be removed due to the annealing in CVD, and the residual water in the interlayer will also be removed. Gr/ Silicon heterojunction can be obtained through the above preparation process.

4.2. Characterization of Two-Dimensional Materials

Characterizing graphene/silicon heterojunction photodetectors involves a variety of techniques to assess their performance, material quality, and device functionality. Here are the key characterization methods:

For the Spectral Response Measurement in the concentration of Optical Characterization, it can help determine the photodetector's response to different wavelengths of light. This helps in understanding the wavelength range over which the device is sensitive. Also, Quantum Efficiency Measurement helps measure the external quantum efficiency (EQE) or internal quantum efficiency (IQE) to evaluate how effectively the device converts incident photons into electrical signals.

Secondly, Current-Voltage (I-V) Characteristics on Electrical Characterization, it related to assess the current response of the photodetector under various applied voltages. This provides information about the dark current, photogenerated current, and overall electrical behavior. Besides, Dark Current and Noise Measurement will help measure the dark current (current in the absence of light) and noise characteristics to determine the noise equivalent power (NEP) and sensitivity of the photodetector.

Regarding spectroscopic techniques, it is important to mention Raman Spectroscopy and X-ray Photoelectron Spectroscopy (XPS). Raman Spectroscopy serves to assess the quality and layer count of graphene. The resulting Raman spectra reveal information about the D, G, and 2D peaks, which reflect the structural and electronic characteristics of graphene. On the other hand, X-ray Photoelectron Spectroscopy (XPS) is utilized to examine the chemical composition and electronic

states of elements present at the surface of the heterojunction, offering valuable insights into the interface chemistry between graphene and silicon.

5. Application of 2D Materials in Various Types of Photovoltaic Devices

5.1. Thin Film Battery

Due to their thin nature, 2D materials contribute to the flexibility and lightweight characteristics of thin film batteries. Also, it can be engineered to improve the stability and longevity of thin film batteries by enhancing the chemical and mechanical stability of the electrodes and electrolytes.

The adaptability of two-dimensional materials is particularly advantageous for applications in flexible electronics and wearable technology. Research conducted by some Chinese scholars has delved into this topic. Unlike conventional batteries that rely on traditional coating techniques and metal current collectors, the electrode materials in these systems can detach from the current collectors due to repeated bending. In contrast, the atomic-scale thickness of two-dimensional materials promotes mechanical flexibility, while their nanostructured design ensures effective contact with other electrode components. This makes them especially suitable for future wearable battery designs. The variety of synthesis methods and innovative electrode configurations, along with improved performance under repetitive deformation, represent significant advancements in this field. Numerous studies have reported on flexible, bendable, and even foldable batteries utilizing two-dimensional materials; these achievements are primarily realized through diverse electrode arrangements or material nanostructures that enhance both electrochemical and mechanical properties. Recent developments in wearable batteries—including lithium-ion, sodium-ion, aluminum-ion batteries as well as various lithium-sulfur types—serve as excellent illustrations of this progress [8].

5.2. Heterojunction Battery

Rechargeable batteries, often referred to as secondary batteries, are designed to be recharged by reversing the current flow. Common types of these batteries include lithium-sulfur, metal-ion, and metal-air variants. Research indicates that heterojunction structures formed from two-dimensional materials offer several benefits such as improved charge transport dynamics, rapid ion diffusion pathways, suitable adhesion for metal ions, a large specific surface area, and enhanced electrochemical performance. These characteristics make them promising candidates for next-generation rechargeable battery electrodes [9]. The figure 5 shows the heterostructures in Vertical and Lateral.

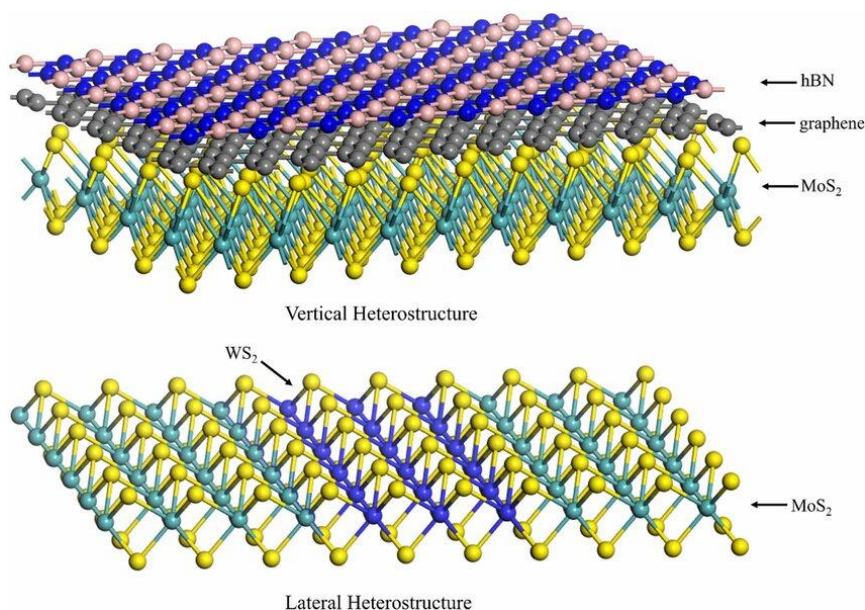


Figure 5. Vertical heterostructures and Lateral heterostructures

5.3. Multi-junction Battery

Multi-junction solar cells, which hold great promise for the future, have demonstrated both high theoretical and experimental efficiencies. These efficiencies are anticipated to exceed the Shockley-Queisser limit, positioning them as significant players in the photovoltaic sector. The underlying principle of these cells is relatively straightforward: by arranging two or more solar cells either in series or parallel configurations, lattice thermalization losses can be minimized, leading to enhanced energy conversion efficiency. Conventional multi-junction solar cells consist of various subcells with different bandgaps made from multiple semiconductor materials, resulting in engineering and manufacturing complexities. However, incorporating single-layer two-dimensional (2D) materials—particularly transition metal dichalcogenides like MoS₂, MoSe₂, WS₂, and WSe₂—into photodetection and photovoltaic applications reveals unique properties. Consequently, it becomes feasible to create a piezoelectric photovoltaic multi-junction cell using a singular 2D material by applying varying strains across identical subcells composed of that material. This approach not only boosts conversion efficiency but also simplifies intricate engineering requirements. Thus, it can be concluded that multi-junction solar cells possess substantial potential for practical applications [10].

6. Conclusion

In the field of solar energy, two-dimensional (2D) materials are emerging as promising candidates to enhance photovoltaic device efficiency while reducing production costs. Their unique single-layer thickness and high surface area contribute to superior electrical and optical properties, such as high electron mobility and broad light absorption. These materials, including MoS₂, WS₂, black phosphorus, and graphene, show significant potential in photovoltaic applications due to their ability to improve light absorption, electron-hole pair generation, and separation processes.

Techniques like chemical vapor deposition and liquid-phase exfoliation are commonly used to synthesize 2D materials, while methods like Raman spectroscopy and transmission electron microscopy help characterize their structures. Despite these advancements, challenges remain in employing 2D materials, particularly in the development of transparent conductive electrodes (TCEs). Integrating solution-processed graphene with metal nanowires, carbon nanotubes, or microgrid structures could offer a path forward, although the high costs of these materials limit their large-scale adoption.

Looking ahead, integrating multidimensional materials, such as combining 2D with organic compounds or nanomaterials, could improve photoelectric conversion efficiency and device performance. Researchers are also focusing on developing biodegradable and eco-friendly materials to minimize environmental impact. While obstacles remain, advancements in 2D photovoltaic technology hold great promise for creating more efficient and sustainable solar energy solutions.

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