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Review

Phase Engineering and Impact of External Stimuli for Phase Tuning in 2D Materials

Shahab Khan*

School of Chemistry and Chemical Engineering, Shaanxi Normal University Xian 710119, China
Department of Chemistry, University of Malakand, Dir Lower Malakand 18800, Pakistan
E-mail: shahabkhan262@snnu.edu.cn

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Abstract: Two-dimensional (2D) materials have captured the imagination of the scientific community for their remarkable properties and potential applications. To further harness the full spectrum of their capabilities, researchers have turned to phase engineering as a powerful tool. Phase engineering involves controlling and manipulating the structural and electronic phases of 2D materials, leading to a wide array of novel and tunable properties. In this comprehensive review, we investigate the exciting world of phase engineering in 2D materials. We start by providing detailed background on the emergence of 2D materials, highlighting their exceptional electronic, mechanical, and optical properties. We then explore the concept of phase engineering, elucidating its principles and significance in tailoring the behavior of 2D materials. Advanced field applications of 2D materials, such as sensing, water desalination, energy storage, and detection were also considered in this review article.

***Keywords*:** 2D Materials, phase engineering, electronic properties, optoelectronics, phase tuning

1. Introduction

The emergence of two-dimensional (2D) materials has sparked a transformative revolution in the field of materials science and engineering. Notable examples of these 2D materials include graphene, transition metal dichalcogenides (TMDs), and black phosphorus, among others. These atomically thin materials exhibit a plethora of extraordinary characteristics, ranging from high carrier mobility and optical transparency to exceptional mechanical strength and thermal conductivity [1]. Their unique properties have ignited a wave of innovation across a multitude of scientific and technological disciplines, including electronics, optoelectronics, energy storage, and beyond. However, the full potential of 2D materials can only be realized through the precise customization of their properties for specific applications. This is where the concept of "phase engineering" comes into play, offering a versatile approach that enables researchers to exert fine control over the phases of 2D materials [2-3]. By manipulating various factors such as atomic arrangement, chemical composition, and external stimuli, researchers can induce phase transitions, resulting in transformative material properties. Phase engineering represents a promising avenue for tailoring 2D materials to meet the demands of specific applications, making them even more versatile and valuable in various fields. In this comprehensive review, we will delve into the dynamic world of phase engineering in 2D materials, exploring the multitude of techniques and strategies employed to modify the phases of these materials. These phase modifications have profound implications for

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electronic and optoelectronic devices, energy storage solutions, and a wide range of emerging technologies [4-5].

One of the most fascinating aspects of phase engineering is its adaptability. Researchers have the flexibility to use various methods, ranging from altering atomic structures and chemical compositions to applying external stimuli, all of which can be fine-tuned to meet specific objectives. This adaptability positions phase engineering as a powerful tool in materials science. Furthermore, this review will not only focus on the current state of phase engineering in 2D materials but also delve into the challenges that researchers face and explore the potential future directions of this field. As the scientific community continues to advance its understanding of phase engineering, the applications of 2D materials in numerous sectors are likely to expand, presenting opportunities for innovations that have the potential to transform industries and impact society. For many years, scientists have been exploring materials with different dimensionalities, including zero-dimensional (0D) quantum dots, one-dimensional (1D) nanowires, and 2D materials such as graphene. These investigations encompass a wide spectrum of applications, driven by the fundamental question of how to effectively manipulate low-dimensional materials through both chemical and physical means. The quest to harness the unique properties of low-dimensional materials has been a critical area of research within the scientific community [6-7].

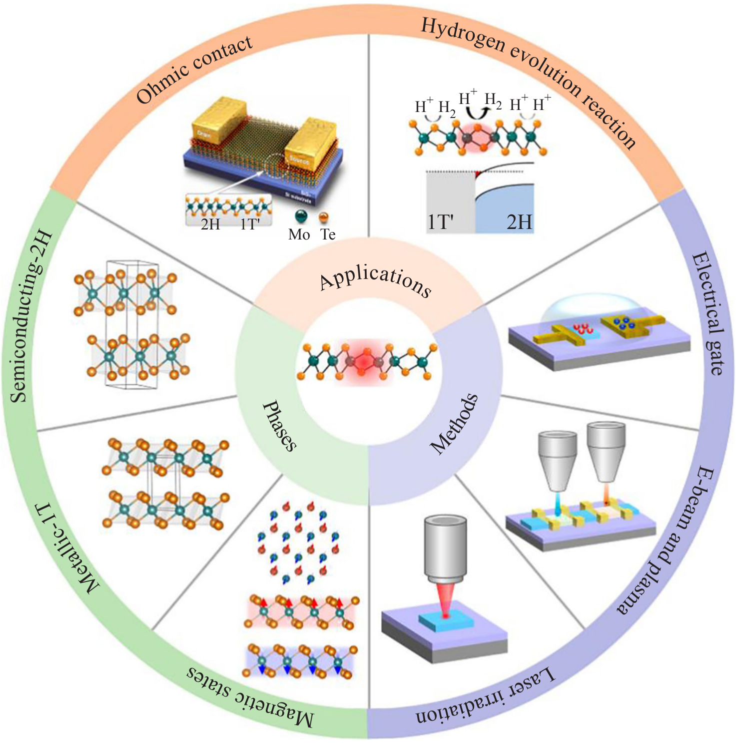

Figure 1. Polymorphic phases and their engineering in 2D materials. Electronic, energy, and optoelectronic devices demonstrate unprecedented operations by phase engineering. *Copyright © 2023 American Chemical Society*

Traditionally, before the rise of 2D layered materials with their polymorphic properties, researchers relied on conventional methods. These included surface treatments, dimension control, and synthesis with varying compositions, which were widely used with emerging materials. These traditional methods have been successful in producing high-performance semiconducting or metallic low-dimensional materials. However, the focus in recent years has shifted towards harnessing the phase tunability and polymorphism of 2D materials, which has garnered significant interest. This shift is primarily driven by the aspiration to develop next-generation electronic and energy devices and to transcend the spatial and technical limitations associated with conventional approaches. In the domain of nanoscale three-dimensional (3D) material fabrication and utilization, the interfaces between different materials play a pivotal role in device design and energy-efficient applications [8]. For instance, the Schottky junction between semiconductors and metals and impedance mismatch in spintronic devices has motivated extensive research into interfaces. What sets 2D materials apart is their unique characteristic of being conceptualized as isolated interfaces with remarkable tunability. These 2D materials, with their van der Waals (vdW) interactions [9-11], offer unprecedented opportunities for engineering. The modification of vdW interactions allows for the manipulation of isolated or layered 2D materials, thus opening up new avenues for applications that revolve around interfaces. This novel approach is not without its challenges, as it demands cutting-edge techniques and a profound understanding of the underlying chemical and physical processes, as depicted in Figure 1 [6]. In essence, the narrative presented in this paragraph highlights the transformative journey of 2D materials and their potential applications through phase engineering. It illustrates how materials science is evolving to meet the demands of modern technology and industry. Phase engineering, which enables precise control over material phases, represents a key driver of innovation in the field of 2D materials, and the ensuing exploration promises new horizons and groundbreaking applications [12-17].

2. Polymorphism in 2D materials

The polymorphism of 2D materials refers to their ability to exist in multiple structural phases or configurations, each with distinct atomic arrangements and properties while maintaining their two-dimensional nature [18]. Polymorphism in 2D materials is a fascinating phenomenon that has garnered significant attention in scientific research. It allows for the tailoring of material properties by transitioning between different structural phases, which can be induced by various external factors, such as strain, temperature, and chemical modifications. The exploration of polymorphism in 2D materials has revealed a wealth of opportunities for designing novel materials with tunable properties. This flexibility is particularly advantageous in applications like electronics, optoelectronics, and energy storage, where the ability to fine-tune the material’s behavior is of paramount importance. The study of polymorphism in 2D materials involves characterizing the different structural phases, understanding the phase transition mechanisms, and exploring the practical implications of such transitions. Researchers are continually uncovering new ways to harness the polymorphic nature of 2D materials to create innovative materials and devices, making it a thriving area of research in the field of materials science [19].

3. Exploring the versatility of phase tuning in 2D materials

Two-dimensional (2D) materials have emerged as a revolutionary class of materials, offering a myriad of extraordinary properties with applications spanning electronics, optoelectronics, and energy storage [20]. One of the key features that make 2D materials so fascinating is their ability to undergo versatile phase tuning, allowing for the tailoring of their properties in a controlled and precise manner. Phase tuning in 2D materials is the process of manipulating their structural and electronic phases to achieve desired characteristics. This involves transitioning between different structural configurations while maintaining their ultrathin, 2D nature. The versatility of phase tuning in these materials has opened up a world of possibilities for researchers and engineers [21]. One of the primary ways to achieve phase tuning in 2D materials is through mechanical strain. By applying strain, such as bending or stretching, to a 2D material, its atomic arrangement can be altered, resulting in changes to its electronic and mechanical properties. This dynamic tunability offers immense potential in the development of flexible and stretchable electronic devices. For example, graphene, one of the most well-known 2D materials, exhibits remarkable electronic properties when subjected to strain, making it suitable for strain-sensitive applications like sensors and flexible electronics. Furthermore, chemical functionalization is another avenue for phase tuning in 2D materials [22]. By introducing specific atoms or molecules to the material’s surface, it is possible to induce structural changes and modify its properties. This approach is particularly valuable for tailoring the chemical reactivity and functionalization of 2D materials. For instance, functionalizing transition metal dichalcogenides (TMDs) can lead to the creation of new semiconducting or catalytic properties, enhancing their performance in electronic and energy-related applications [23]. Beyond strain and chemical functionalization, temperature plays a pivotal role in phase tuning. Many 2D materials exhibit phase transitions at different temperature ranges, which can be harnessed to achieve specific properties. Black phosphorus (Figure 2), for instance, is known for its anisotropic properties that can be controlled by varying the temperature [24-25]. By understanding these transitions, researchers can design materials with tailored electrical and thermal conductivities, opening new horizons for thermal management and thermoelectric applications. In addition to these methods, external fields, such as electrical and optical stimuli, have proven effective in phase tuning. Applying an electric field or irradiating 2D materials with light can lead to significant changes in their electronic structure, enabling the development of unique devices like field-effect transistors and photodetectors.

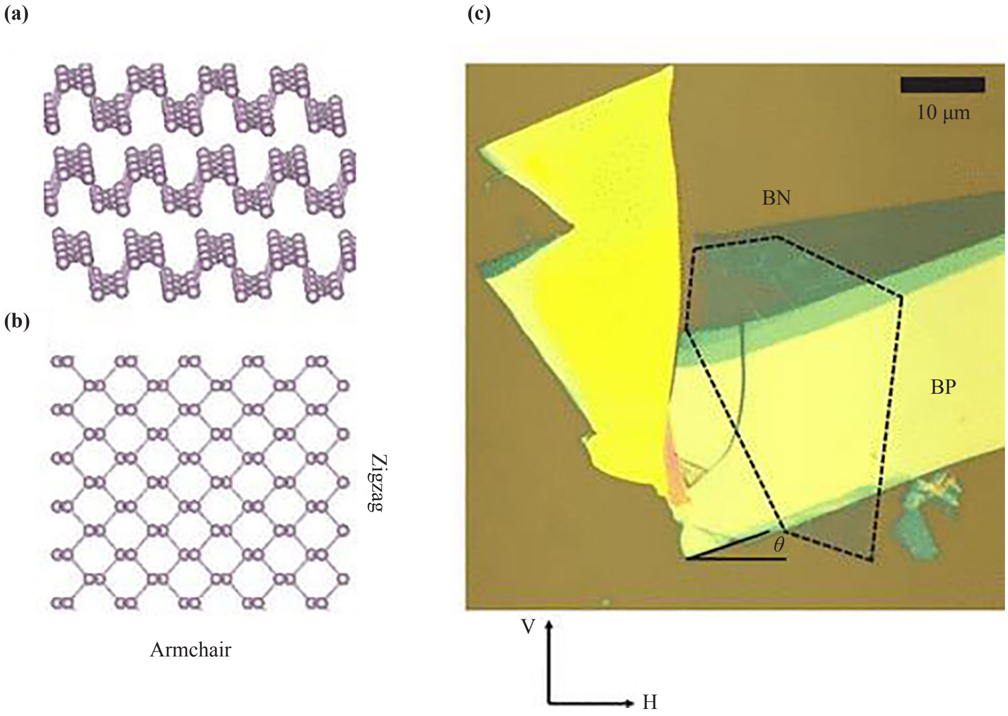

Figure 2. Black phosphorus lattice structure and example picture. (a) Multilayer black phosphorus lattice structure. (b) Top view of a single-layer black phosphorus, with zigzag and armchair orientations. (c) The sample's optical image under study. The dotted line shows that a 4 nm boron nitride (BN) flake partially covers the 16 nm thick black phosphorus (BP) flake. In the lab frame, the directions are designated for the horizontal (H) and vertical (V). H and the flake's long edge make up the angle θ. *Copyright © 2015 American Chemical Society*

The versatile phase tunability of two-dimensional (2D) layered materials stands as a pivotal element for achieving phase interfaces that offer remarkable versatility and potential. Polymorphic 2D materials, in particular, possess a unique feature, such as the absence of vertical dangling bonds between layers. This structural attribute allows for the availability of stable material characteristics even down to atomically thin geometries and across a spectrum of diverse phases [26]. It is this very characteristic that sets polymorphic 2D materials apart from their bulk three-dimensional (3D) counterparts, making them a distinct class of materials with exceptional promise. Within the realm of materials science, the concept of phase engineering in 2D materials has emerged as an area of significant interest and exploration. This concept hinges on the idea that by manipulating various factors, ranging from atomic arrangement to chemical composition and external stimuli researchers can induce them for phase transitions. These transitions, in turn, lead to transformative material properties. In essence, phase engineering opens doors to a multitude of possibilities, enabling precise control over the properties and functionalities of 2D materials. This is not merely an academic pursuit but a practical one with profound implications for diverse applications [27]. The phase tunability of 2D materials is a reflection of their inherently complex nature, encompassing structural variations, quantum states, and electronic/magnetic phases. To fully appreciate the significance of phase engineering in 2D materials, one must delve into the multifaceted factors and parameters that come into play. Among the factors influencing the properties of 2D materials are geometric variables, including lateral dimensions and thickness. These variables exert significant effects on the physical and chemical characteristics of 2D materials. The quantum confinement effect, for instance, comes into play as materials reach nanometer-scale thickness [28]. This effect operates anisotropically along two distinct directions, affecting the properties of the material in a unique manner. The dielectric properties of the media surrounding 2D materials significantly impact their electronic properties. This impact is most evident in the modification of the electronic band structure as a function of material thickness. As the thickness of the 2D material varies, the dielectric media plays a pivotal role in shaping the electronic properties, resulting in a thickness-dependent electronic band structure modulation. This aspect has immense implications for the performance of 2D materials in various applications. Researchers have devoted extensive efforts to understanding the role of atomic edges in 2D materials. These edges have emerged as crucial elements in the local phase engineering of 2D materials. Several studies have focused on finding the lowest energy states that explain phase stability [29]. Such investigations have offered insights into the impact of atomic edges on the properties of 2D materials and their stability. Polymorphic 2D materials exhibit a range of electronic phases, including charge density waves (CDW), superconductivity (SC), Mott insulators, and non-Fermi liquids. The stabilization of these electronic phases is influenced by various factors, such as material thickness, pressure, and magnetic fields. The transition between these strongly correlated electronic states and the stabilization of local phases in response to these factors have significant implications for electronic devices and novel material functionalities. The atomically thin geometry of 2D materials has a profound impact on the interactions between electrons. The electric screening effect, which is often prevalent in bulk materials, is significantly suppressed in 2D materials due to their atomic thinness. This, in turn, leads to the stabilization of versatile electronic phases and introduces the possibility of a thickness-dependent transition between electronic phases. One notable transition occurs between CDW and SC in transition metal dichalcogenides (TMDs), which reveals competing features dependent on material thickness. The competition of different CDW phases at varying thicknesses can be effectively modulated through methods such as ionic gating, temperature adjustments, and control of material thickness. These techniques highlight the adaptability and versatility of phase engineering in 2D materials. 2D magnetic materials represent another dimension of phase engineering with unique magnetic states and interfaces. These materials provide interfaces encompassing a range of phases, such as ferromagnetic metals, antiferromagnetic insulators, and topologically nontrivial antiferromagnetic insulators [30]. In contrast to traditional magnetism observed in three-dimensional (3D) materials, the conceptualization of 2D magnetism revolves around an organized spin arrangement featuring diverse spin dimensionalities across macroscopic length scales. Representative examples of 2D layered magnetic materials, such as Fe_3GeTe_2, $CrGeTe_3$, and $CrBr_3$, exhibit distinct magnetic characteristics. The presence of Ising-type ferromagnets with out-of-plane magnetic anisotropy and in-plane antiferromagnetic spin arrangements underscores the diversity of magnetic phases available in 2D materials [31-32]. The competition among magnetic exchange coupling strengths, magnetic anisotropy (A), and magnetic field (B) governs magnetic phase interfaces in 2D materials. Exotic magnetic phase transitions can be achieved through the modulation of layer thickness, the application of magnetic fields, exposure to light irradiation, electric gating, and the formation of heterostructures with distinct patterns. These diverse tools and techniques highlight the subtle and intricate nature of 2D magnetism. Recent experimental tools have significantly contributed to the understanding of 2D magnetism. Methods like inelastic X-ray scattering, superconducting quantum interference devices, magneto-optic Kerr effect spectroscopy, negatively charged nitrogen-vacancy magnetometers, and SQUID-on-tip microscopy have unveiled the complexities of 2D magnetism and its possible applications. In other words, phase engineering in 2D materials represents a dynamic and multifaceted field with wide-ranging implications for materials science and engineering. It offers a pathway to tailor the properties and functionalities of 2D materials with precision, and this has far-reaching consequences for a multitude of applications. Understanding the interplay of factors such as geometric variables, dielectric media, atomic edges, and electronic phases in 2D materials is crucial for harnessing their full potential. Additionally, the diverse landscape of 2D magnetism adds another layer of complexity and potential applications to the field of phase engineering. With the continued advancement of experimental tools and techniques, the future of phase engineering in 2D materials promises to be even more intriguing and impactful.

4. Phase engineering

For ordinary solid materials, thermodynamic factors like composition, temperature, and pressure have long been important tools in large-scale phase engineering. In the world of two-dimensional (2D) materials, achieving versatile phase interfaces is paramount, and it calls for innovative approaches and the manipulation of polymorphic or multiple states under ambient conditions. Additionally, local phase control through methods like electric gating plays a pivotal role in this endeavor. Temperature, being a fundamental thermodynamic variable, stands as a central player in phase engineering, especially when it comes to tuning the structural and electronic states of materials. Among the most extensively studied materials in this context are the group-6 transition metal dichalcogenides (TMDs), known for their various structural phases, including the hexagonal H, rhombohedral R, and trigonal T phases. These phases are defined by the arrangement of tetrahedra and the stacking orders of layers within the material. Temperature-induced structural phase transitions often occur due to the hybridization of electrons' orbitals in modified lattices, impacting the interlayer stacking order. For instance, molybdenum ditelluride ($MoTe_2$) exhibits orthorhombic (Td) and monoclinic (1T′) phases at different temperatures due to alterations in the stacking order. Temperature control serves as a valuable tool for large-scale phase engineering, with techniques like laser irradiation enabling precise local phase control. Pressure, another significant thermodynamic variable, can exert considerable influence on the lattice constants of TMDs. For example, molybdenum disulfide (MoS_2) transforms into a superconducting state under higher pressures. This transformation is attributed to reduced interlayer spacing and enhanced interlayer coupling, both of which are induced by pressure. Pressure-driven changes can also affect the morphology of the Fermi surface, leading to phenomena like the Lifshitz transition and the emergence of the quantum spin Hall effect. The stoichiometric ratio or chemical composition of TMDs has been explored as a means of phase engineering. For instance, the $Mo_{1-x}WxTe_2$ alloy, which exhibits two distinct states at room temperature, showcases the impact of chemical composition on material properties [33]. Intercalation, a process involving the insertion of ions or molecules into the interlayer spaces of 2D materials, holds significant promise in modifying their electronic, magnetic, and crystal lattice structures. Recent research has focused on achieving versatile phase interfaces, characterized as the "local tuning of phase stability or polymorphs" in 2D materials. Advanced studies delve into aspects such as quantum states, charge density waves (CDW), Mott insulating phases, and superconducting phases [34]. Understanding the role and limitations of intercalation in 2D materials is vital for leveraging unique phase interfaces in various energy and electronic device applications. Intercalated elements play specific roles in inducing structural, electronic, and quantum phase transitions. These roles encompass doping effects, changes in interlayer interactions, atomic plane-sliding, and orbital hybridization. Stabilizing metastable phases and interfaces is crucial for preserving the pristine nature of 2D materials while achieving desired functionalities. Electron-electron and electron-phonon coupling are two interactions that are greatly impacted by intercalation on the strength of the interlayer coupling. Thus, extremely correlated phases, such as CDW and superconducting phases, may be engineered. For example, the concentration of intercalates affects the range of CDW and superconducting phases displayed by intercalated TMDs. Sulfur atomic planes may slide as a result of extra charge transfer caused by intercalated ions between transition metal atoms. A reversible phase transition between metallic and semiconducting (2H) states can be induced by this method. For practical energy storage applications (see Figure 3), graphite intercalation has been thoroughly investigated along with distinct intercalants resulting in superconducting states. Nevertheless, the lack of superconductivity in Li-intercalated graphene implies that successful phase engineering also requires control over other parameters including electron-phonon coupling, phonon-mediated pairing, and electronic donor state creation by intercalation. The advent of quantum states decreased contact resistance, and active catalytic processes have all been made possible by large-scale and local phase engineering. These developments are being investigated further for new optoelectronic, energy, and power devices that are heterophase and vertical. Another use of phase engineering, referred to as the proximity effect, is the fabrication of new material systems by the artificial stacking of atomically thin layers. Through this approach, two-layer effective dielectric constants may be changed, enabling localized and unique phase engineering in polymorphic 2D materials. Charge transfer, diffusion, magnetism induction, superconductivity induction, and other systems are all included in the proximity effect. Doping is a crucial method in the semiconductor industry for managing a material's electrical characteristics. It entails the addition of dopants that support hole or electron transport. Engineering 2D materials are especially well-suited to surface doping, a method that modifies a material's top surface selectively. With 2D materials like graphene and TMDs, a wide range of dopants have been used, including gasses, water, metals, and organics (Figure 4). This method is essential for modifying the electrical characteristics of 2D materials for particular uses, adding to the ever-expanding phase engineering toolset for 2D materials.

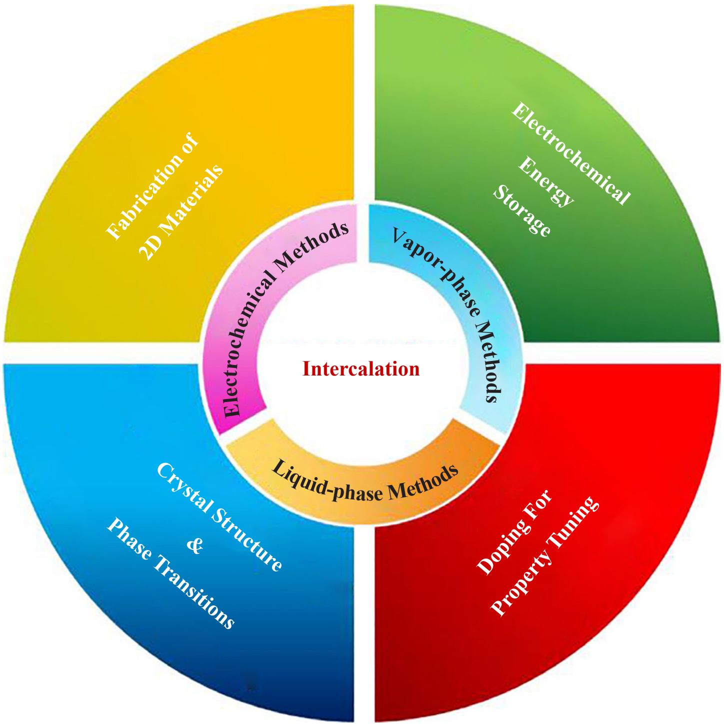

Figure 3. Schematic diagram summarizing different intercalation techniques and applications of intercalation in 2D materials. Recent developments in two-dimensional (2D) materials have resulted in a resurgence of interest in intercalation as an effective method for processing and production. Intercalation is a useful technique for changing the interlayer contacts, doping two-dimensional materials, altering their electronic structure, and even changing them into whole new phases or structures that differ dramatically from one another. Several intercalation techniques and give a thorough overview of the functions and uses of intercalation in optoelectronics, thermoelectrics, catalysis, and next-generation energy storage [34]. Springer Nature© 2023 Springer Nature Limited

Surface charge transfer doping is a technique employed to finely tune the electronic band structure of black phosphorus (BP) by introducing potassium atoms to the top BP layer. This process results in the generation of a vertical electric field, which in turn leads to the modification of the bandgap. The underlying mechanism for this modification is attributed to the giant Stark effect, and it can give rise to a phase transition from the semiconductor state to a band-inverted semimetal state (as visually represented in Figure 5a). Remote modulation doping is an innovative approach in the realm of transition metal dichalcogenides (TMDs) heterostructures. In this context, remote modulation doping is achieved by introducing surface charge doping to the top layer of tungsten diselenide (WSe_2) using PPh_3 [35]. This surface doping process has a profound impact on the doping state of the underlying molybdenum disulfide (MoS_2) layer, resulting in significantly enhanced carrier mobility compared to direct doping methods in MoS_2-based transistors. Direct doping usually leads to Fermi-level pinning, which, in turn, results in the formation of Schottky junctions at metal-semiconductor interfaces. These junctions are associated with substantial contact resistance and a decrease in carrier mobility. In contrast, the remote doping method effectively minimizes surface defects without necessitating chemical bonding, facilitating the achievement of high carrier mobility (as visually depicted in Figure 5b-d). [33] The engineering of 2D materials, particularly the versatile phase tunability of polymorphic 2D materials, plays a critical role in achieving versatile phase interfaces. Unlike their 3D counterparts, polymorphic 2D materials lack vertical dangling bonds between layers [36]. This unique characteristic enables the preservation of stable material properties even in atomically thin geometries and various phases. The weak interlayer interactions within polymorphic 2D materials distinguish them from bulk 3D materials and make them attractive for creating vertical heterophase structures that hold immense potential for innovative devices utilizing subnanometer-scale material phase engineering.

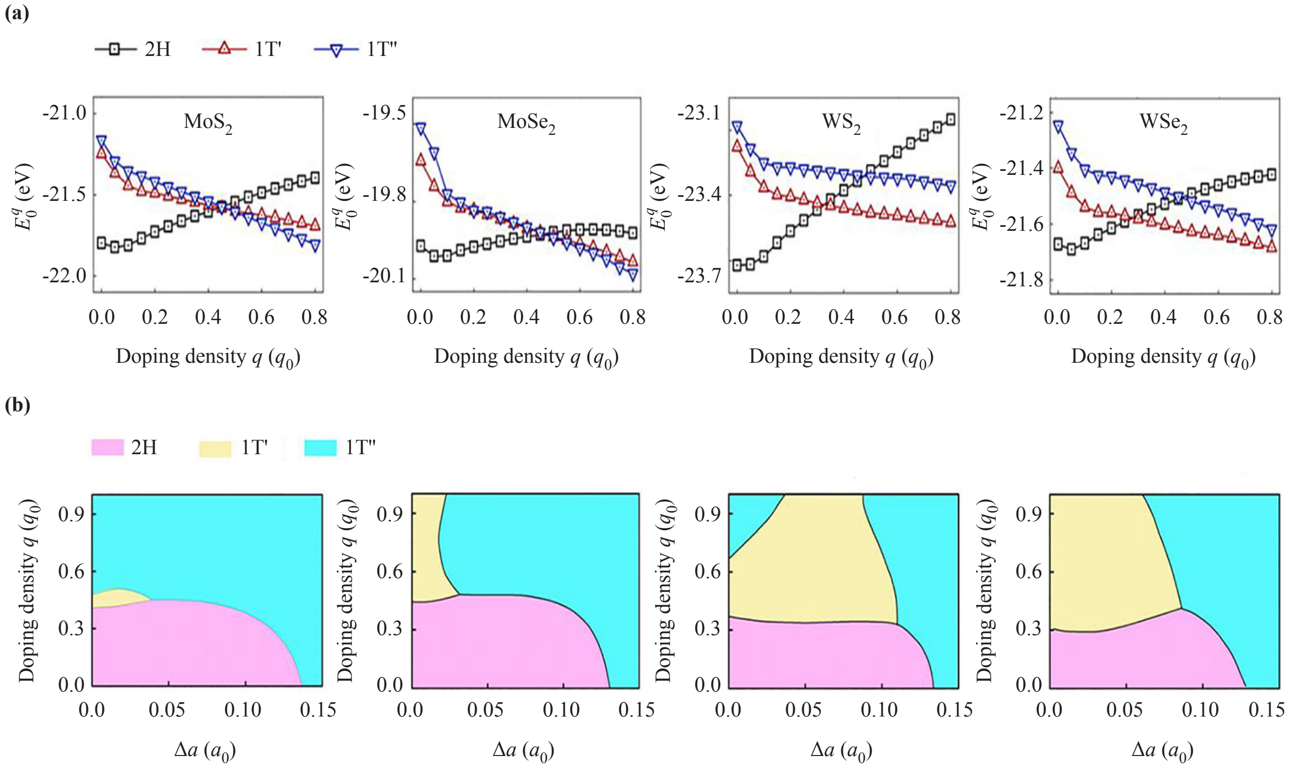

Figure 4. TMD materials' phase stability is dependent on electron doping. (a) The evolution of electron doping density (q) in relation to the total energy per primitive cell (E_0^q). Phase diagram as a function of strain and electron doping (b). The lattice distortion ratio is Δa (a_0) = ($a - a_0$)/a_0, where "a" is the lattice parameter. When the electron doping density (q) and lattice deformation (Δa (a_0)) change, the colored region indicates the energetically favored phase.

The complexity of 2D materials, which include structural, quantum, and electronic/magnetic phases, is reflected in their phase tunability. The physical and chemical properties of 2D materials are significantly influenced by key geometric variables like thickness and lateral dimensions. Because of the atomically thin planar geometry of 2D materials, the quantum confinement effect occurs anisotropically along in-plane and out-of-plane axes in nanometer-scale materials. Furthermore, the dielectric media encircling two-dimensional materials can have a significant effect on their electronic characteristics, leading to modulations in the electronic band structure of different two-dimensional materials based on thickness. A great deal of research has also been done on the function of atomic edges in 2D materials. The lowest energy configurations to explain phase stability have been the subject of numerous investigations. Although a lot of attention has been paid to using first-principles calculations to determine the lowest energy states, it's crucial to remember that these studies have not clearly established intermediate structures during phase transitions. It is difficult to account for these factors in calculations because the addition of heat or kinetic energy to 2D materials through processes such as laser or electron irradiation adds complexity to the system. Surface energy and interlayer interactions interact to further impact a crystal structure's thermodynamic stability. Certain 2D materials can occasionally show critical thicknesses for phase transitions. For example, at a critical thickness of 1.27 monolayers, GaTe experiences a phase transition from monoclinic to hexagonal structures. Similarly, the 2H phase of VSe_2 can be stabilized in thin film geometries, whereas the stable phase of bulk VSe_2 is the 1T phase. It is known that modifications in the lattice constants of 2D materials can generate strain effects, which can be engineered through substrate interactions. Substrates with artificial structures, ferroelectric or piezoelectric properties, and flexible or stretchable characteristics have been employed to induce strain in 2D materials [37]. For example, the use of compressive and tensile strains from a ferroelectric substrate of $Pb(Mg_{1/3}Nb_{2/3})_{0.71}Ti_{0.29}O_3$ (PMN-PT) has led to nonvolatile, strain-induced phase transitions between 2H and 1T' phases in $MoTe_2$ devices at room temperature [38]. Additionally, mechanical methods can apply local strain to 2D materials. For instance, when an atomic force microscope (AFM) tip exerts local pressure on a 2D material, it induces local strain, reduces the activation energy, and lowers the phase transition temperature. This applied force locally modifies the lattice constants of 2D materials, leading to local phase transitions [39]. Furthermore, the application of local strain via AFM indentation has been shown to induce unique ultra-stiff diamine phases characterized by diamond-like sp3 chemical bonds. Researchers have reported phase transitions from hexagonal to monoclinic structures in InSe through AFM tip-driven indentation. These findings highlight the significance of local strain engineering in 2D materials, enabling precise control over their phases. Understanding and harnessing the thermodynamic variables and various phase engineering techniques in 2D materials open up a world of possibilities for tailoring these materials to meet the demands of emerging technologies. From surface charge transfer doping to strain engineering and local phase control, researchers are constantly exploring new avenues to achieve novel phases and transformative material properties in 2D materials. These advancements are central to the development of next-generation electronic and energy devices, as well as the broader goal of overcoming the spatial and technical limitations associated with conventional approaches. As the field of phase engineering in 2D materials continues to evolve, it promises to revolutionize various industries and drive innovative applications.

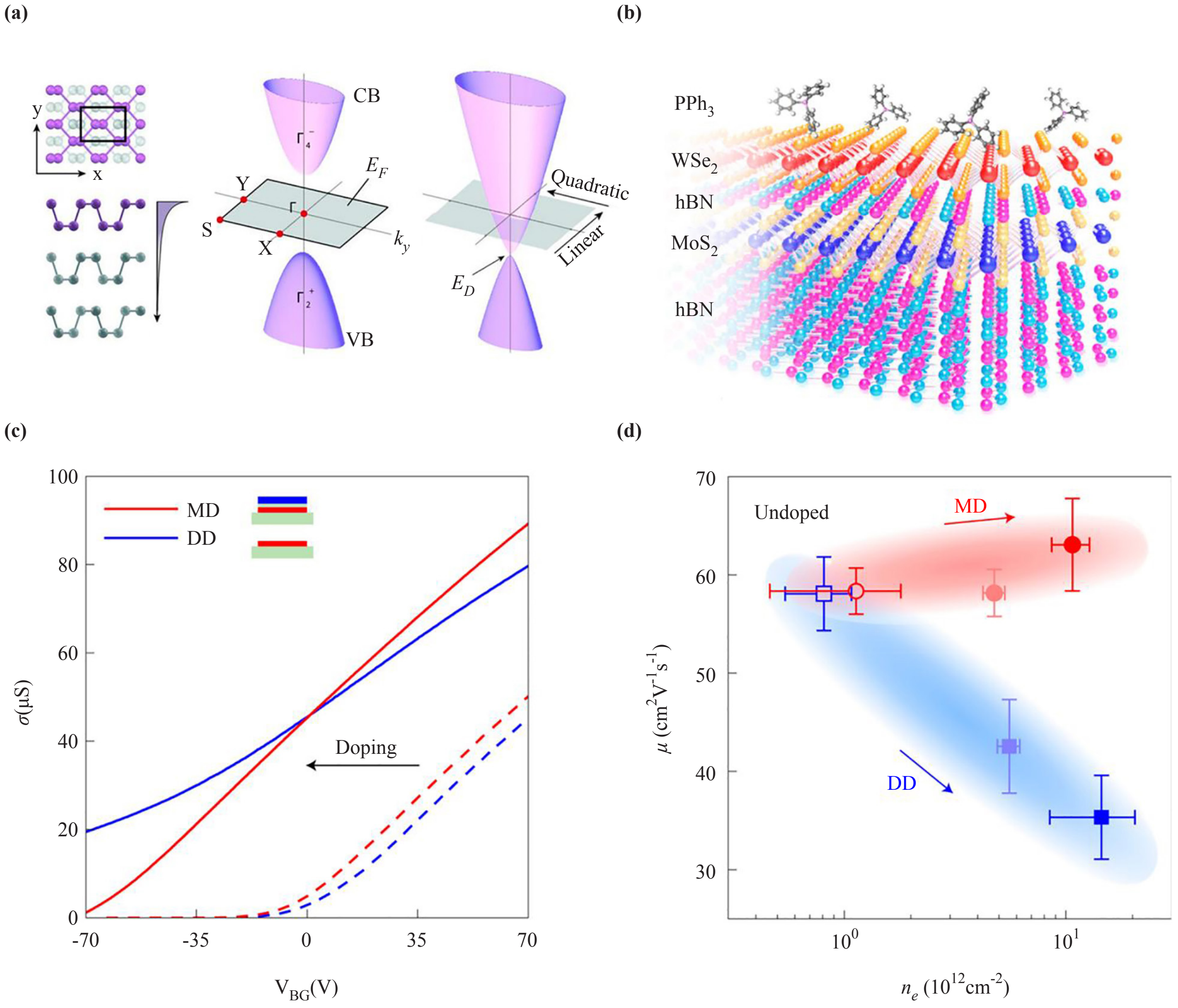

Figure 5. Modifications in electronic properties driven by charge transfer doping are as follows: (a) The atomic structure and charge density profile of BP illustrate a phase transition from a semiconductor to a band-inverted semimetal at the surface of BP. This transition is a result of the high surface charge density. (b) Depicted is a schematic image of the WSe$_2$/h-BN/MoS$_2$ heterostructure designed for remote doping. (c) The electrical sheet conductivity is depicted as a function of the Rewrite VBG as V$_{BG}$ for modulation-doped (MD) and directly doped (DD) MoS$_2$ field-effect transistors (FETs). (d) The field-effect mobility (μ) is plotted as a function of the electron concentration (ne) of the MoS$_2$ FETs both before (open symbols) and after (filled symbols) doping [33].

5. External stimuli for phase tuning

External stimuli for phase tuning play a crucial role in the manipulation of the structural and electronic phases of materials. These stimuli allow researchers to control and optimize the properties of materials for various applications. the key external stimuli used in phase tuning are summarized in Table 1 [40].

Table 1. List of external stimuli, each of these external stimuli plays a specific role in phase engineering, offering a range of options to researchers and engineers when it comes to optimizing materials for specific applications. The choice of stimuli depends on the desired outcome and the material's characteristics

S.No	Type	Description	Applications	ref.
1	Mechanical Strain:	Applying mechanical strain, such as bending or stretching, to a material can alter its atomic structure, leading to changes in its electronic and mechanical properties.	Strain engineering is vital in the development of flexible and stretchable electronics, as well as in the creation of high-performance mechanical and electronic devices.	[41]
2	Temperature	Varying the temperature can induce phase transitions in materials. Different phases may become stable at specific temperature ranges.	Temperature-induced phase transitions have applications in thermoelectric materials, where waste heat is converted into electricity, and in the study of phase change materials for data storage and thermal management.	[42]
3	Chemical Functionalization and Doping:	The introduction of specific atoms or molecules to the material's surface can induce structural changes and modify its properties. This is known as chemical functionalization or doping.	Chemical modification is used to tailor the chemical reactivity and functionalization of materials, leading to enhanced performance in applications like catalysis, sensors, and semiconductor devices.	[43]
4	Light (Optical Stimuli)	Shining light on a material can lead to changes in its electronic properties and induce phase transitions. This is known as photoinduced phase tuning.	Optical stimuli are employed in photodetectors, photovoltaics, and the development of optoelectronic devices.	[44]
5	Electric Fields	Applying an electric field can modify the electronic properties of materials. This is particularly important in the field of ferroelectrics and piezoelectrics	Electric fields are used in devices like field-effect transistors (FETs), piezoelectric sensors, and actuators.	[45]
6	Magnetic Fields	Magnetic fields can induce changes in the magnetic properties of materials and affect their electronic phases	Magnetic field-induced phase transitions are relevant in spintronic devices and magnetic memory storage technologies.	[46]
7	Pressure	The application of pressure, often using atomic force microscopy (AFM) tips or diamond anvils, can induce phase transitions by modifying the material's lattice constants.	Pressure-induced phase transitions have implications for understanding materials' behavior under extreme conditions and developing novel materials	[47]
8	Chemical Reactions	Chemical reactions involving the material's surface can drive phase transitions by changing the material's composition and structure.	Chemical reactions can be utilized in the creation of thin films, surface coatings, and the development of functional materials with tailored properties	[48]

6. Applications

The applications and implications of phase engineering are vast and diverse, especially in the context of two-dimensional (2D) materials. Phase engineering involves controlling and manipulating the structural and electronic phases of materials to achieve specific properties or functionalities.

6.1 *Electronic and optoelectronic devices*

Phase engineering plays a critical role in the development of advanced electronic and optoelectronic devices. By modifying the structural and electronic phases of 2D materials, researchers can tailor their electronic properties to create high-performance components. Applications include Transistors: Phase-engineered 2D materials are used to create high-speed and low-power transistors, essential in modern electronics. Photodetectors: Phase-tuned 2D materials enable the development of sensitive photodetectors for applications in imaging, telecommunications, and remote sensing. Light-

Emitting Diodes (LEDs): The control of electronic phases allows for efficient LEDs, contributing to energy-efficient lighting solutions [49] (Figure 6).

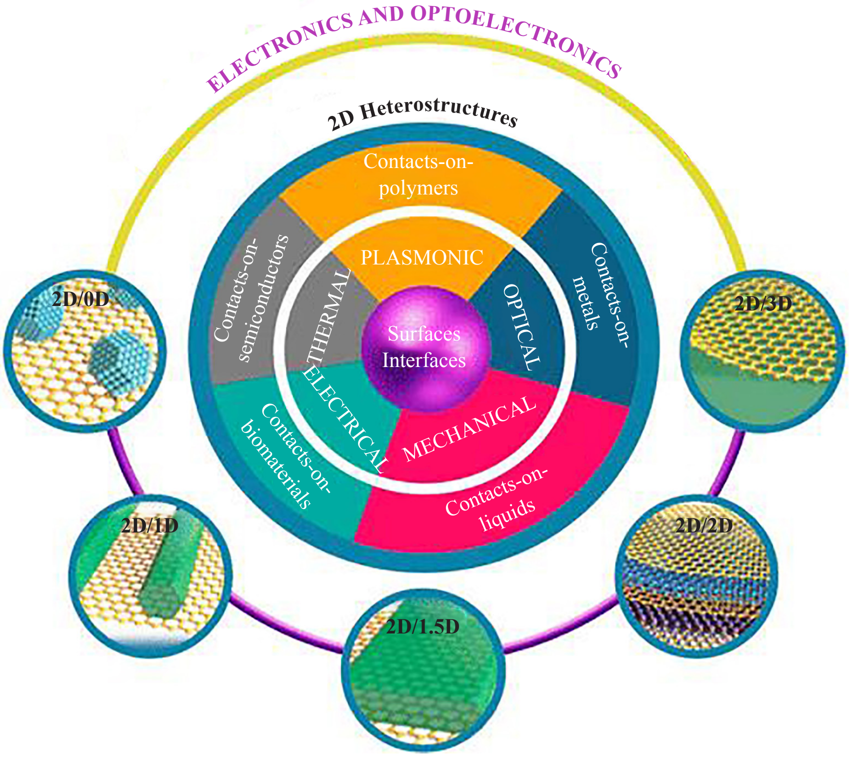

Figure 6. Overview of 2D heterostructures interacting chemically and physically with materials on a variety of surfaces and interfaces in different dimensionalities. For the realization of several electrical, mechanical, thermal, and plasmonic functions necessary for FEO, these 2D heterostructures that create either chemical or physical bonding are important. *Copyright © 2022 The Authors. Published by American Chemical Society* [49]

6.2 *Energy storage and conversion*

Phase engineering has implications for energy storage and conversion technologies, contributing to more efficient and sustainable energy solutions: Batteries and Supercapacitors: Phase-tailored 2D materials are utilized to enhance energy storage capacity and charge/discharge rates in batteries and supercapacitors. Thermoelectric Materials: By controlling the electronic phases, researchers can optimize 2D materials for thermoelectric applications, where waste heat is converted into electricity. Catalysis: Phase-engineered 2D materials have been explored as catalysts for various energy conversion processes, including water splitting and CO_2 reduction [50].

6.3 *Sensing and detection*

Phase engineering enhances the sensitivity and selectivity of sensors and detectors, enabling new possibilities in various industries: Gas Sensors: 2D materials with tunable phases can detect specific gases with high precision, vital in environmental monitoring and safety applications. Biomedical Sensors: Phase-tuned materials are used in biosensors for the detection of biomolecules and pathogens, contributing to medical diagnostics and research. Environmental Monitoring: Phase-engineered materials play a role in creating highly responsive sensors for monitoring pollutants, ensuring clean air and water [51].

6.4 *Flexible and stretchable electronics*

Phase-tailored 2D materials are instrumental in the development of flexible and stretchable electronics: Wearable Devices: Phase engineering enables the creation of wearable electronics that can conform to the body, allowing for comfortable and unobtrusive health monitoring and personal technology. Foldable Electronics: Phase-tuned materials contribute to the development of foldable devices, such as smartphones and tablets [52].

6.5 *Fundamental science and research*

The ability to control and understand phase transitions in 2D materials has broader implications for fundamental scientific research: Quantum Materials: Phase engineering allows for the creation of quantum materials with unique quantum states, leading to advancements in quantum computing and quantum information science. Emergent Phenomena: The study of phase transitions in 2D materials can uncover new emergent phenomena with applications in condensed matter physics and materials science.

6.6 *Novel materials and discovery*

Phase engineering can lead to the discovery of entirely new materials with unexplored properties and applications, expanding the frontiers of materials science. phase engineering of 2D materials is a powerful tool with diverse applications and far-reaching implications. It empowers researchers and engineers to fine-tune material properties to meet the demands of various industries, from electronics and energy to sensing and fundamental research. As the field continues to evolve, we can expect even more innovative applications and transformative discoveries.

6.7 *2D-materials for water desalination and treatment*

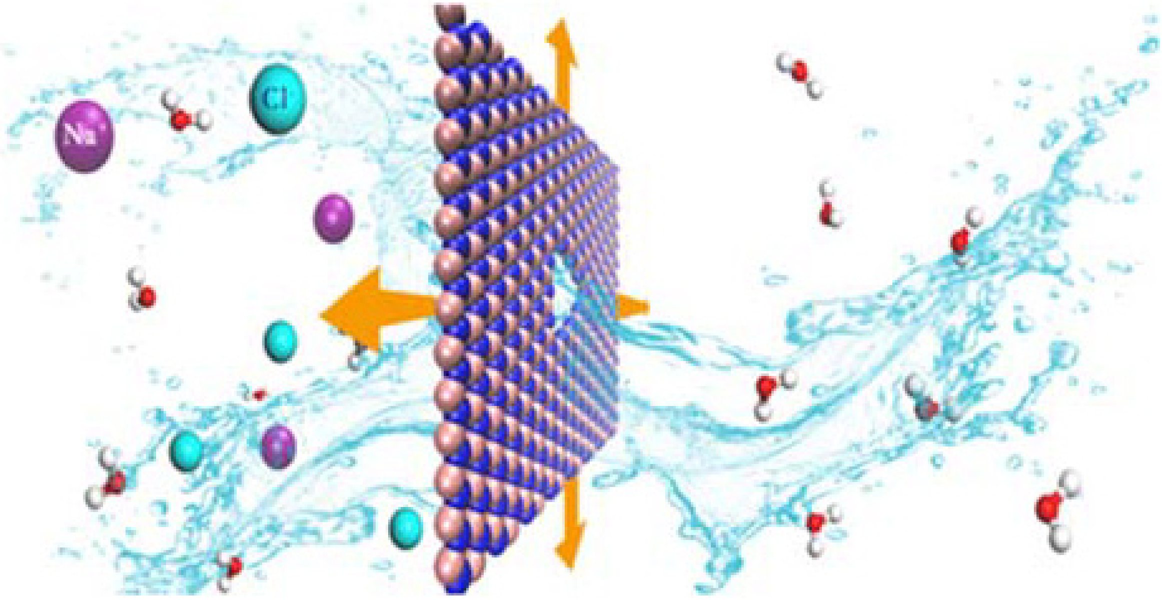

Figure 7. Diagrammatic view of BN nanosheet for water desalination. Copyright 2017. Reproduced with permission from the American Chemical Society [53]

The reproduction approach, which involves a model of a system, is crucial for designing and assessing complex systems. Simulation allows for exploration, analysis, and assessment of circumstances that would otherwise be impossible. Computer simulation methodologies have expanded from macro to nanoscale, with Density Function

Theory (DFT) and Molecular Dynamic Stimulation (MDy) being common tools. MDy simulation has contributed to understanding the connection between microscopic and macroscopic properties of 2-D nanomaterials. MDy simulations are used to examine membrane separation mechanisms, predict the capacity of 2-D nano-porous materials in water desalination, and compute system dynamics like time-dependent fluctuations and transport coefficients. Theoretical simulations of membrane filtration for water treatment have been used to improve the effectiveness of water desalination techniques while reducing costs. Garnier et al. found that BN has a lower surface tension than graphene, resulting in better water wetting. The study also found that nano-porous 2D-BN has greater water permeability than graphene under the same conditions, enhancing water molecules' transit across the nanopore. Advanced research can help develop new separation strategies for water treatment. Gao et al. used MDy stimulation to study water desalination across a BNNS layer. They generated six equilateral three-sided nanopores with two types of pore edges, with external pressure used for water transportation. The study found that pore size, edge chemistry, and applied pressure all impact water flow and salt discharge. The well-planned h-BN film showed excellent porousness, selectivity, and controllability. The water porousness/permeability of the framework with only N iotas at the pore edge was more prominent than the boron-edged framework (Figure 7).

7. Conclusion

Phase engineering of 2D materials presents challenges in comprehending crucial factors and precisely defining phase boundaries across various dimensions. This comprehensive review prioritizes the achievement of atomically well-defined and distinct phase boundaries. To conduct more systematic investigations, techniques like transmission electron microscopy (TEM) and complementary methods such as scanning tunneling microscopy (STM) and tunneling spectroscopy are indispensable. Promisingly, Kelvin probe force microscopy (KPFM) and piezoelectric force microscopy (PFM) show potential for facilitating the study of phase boundaries on a larger scale. The sharpness and structural durability of phase-engineered regions have a direct impact on the overall performance of devices. The strategic implementation of phase patterning and the manipulation of phase interfaces within polymorphic layered materials open up new frontiers in electronic, optoelectronic, spintronic, neuromorphic, and catalytic devices, all of which operate with remarkable energy efficiency. Devices based on phase change materials have ushered in innovative research fields, introducing novel and resilient hysteresis effects in transport and atomic interactions. Phase patterning also serves to eliminate contact resistance in semiconductor-based devices with polymorphic properties, leading to the attainment of exceptional carrier mobility, particularly in field-effect transistor (FET) applications. Furthermore, it has been reported that polymorphic transition metal dichalcogenides (TMDs) exhibit ferroelectric properties through unconventional mechanisms, enabling the development of metallic and superconducting ferroelectric systems. Additionally, the local manipulation of magnetic phases is achievable through the application of optical and electric stimuli. These advancements represent a promising avenue for advancing the control and utilization of magnetic phases in 2D materials.

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Conflict of interest

The author declares no competing financial interest.

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