

THE CHEMISTRY OF 2D MATERIALS FROM GRAPHENE TO BEYOND**Ali Haider**

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Article Info**Abstract**

The advent of two-dimensional (2D) materials has revolutionized materials science, offering a new frontier for research and applications across diverse fields. This review explores the chemistry of 2D materials, beginning with graphene, the pioneering 2D material renowned for its exceptional electrical, mechanical, and thermal properties. The unique atomic-scale thickness of these materials imparts extraordinary characteristics, making them integral to advancements in nanotechnology, energy storage, electronics, and catalysis. Beyond graphene, other 2D materials, including transition metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), and MXenes, have garnered attention due to their tunable band gaps, chemical versatility, and diverse functionalities. The synthesis strategies, such as chemical vapor deposition, exfoliation, and bottom-up approaches, are pivotal in tailoring the properties of these materials for specific applications. Additionally, surface functionalization and chemical modifications are discussed as tools to enhance the reactivity, stability, and compatibility of 2D materials in hybrid systems. The review also highlights the challenges in scalability, reproducibility, and environmental concerns associated with 2D material production. Emerging trends, such as heterostructures and 2D polymers, are presented as promising directions for expanding the application scope. This comprehensive exploration underscores the transformative potential of 2D materials in addressing global challenges, including sustainable energy, environmental remediation, and advanced electronics, while identifying key areas for future research. The ongoing evolution of 2D materials chemistry holds the promise of bridging fundamental science and technological innovation, driving breakthroughs that redefine material capabilities.



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Introduction

Many layered materials have strong in-plane chemical bonds and weak coupling between the layers. These layered structures provide the opportunity to be cleaved into individual freestanding atomic layers. Layers with one dimension strictly restricted to a single layer are called two-dimensional (2D) materials. The density of states for 2D materials exhibits a quasi-continuous step-like increase with increasing excitation energy [1].

Graphene is the latest stable carbon allotrope where the sp^2 carbon atoms are oriented in a two-dimensional honeycomb lattice to form atomically thin layers. The bonding between the adjacent carbons and the delocalization of the bonding electrons throughout the two-dimensional (2-D) lattice contribute to most of the interesting properties of graphene. The term “graphene” originated when studying the intercalation compounds of the parent material graphite, which is the three-dimensional, naturally occurring form of graphene. Graphite, which means “to write” (in Latin) has been known for 500 years and is widely used in pencils (in combination with clays). It is made of graphene layers where the layers are stacked with an interlayer distance of 3.34 \AA . Graphene is considered the ultimate polycyclic aromatic hydrocarbon (including naphthalene, anthracene, pyrene, etc.), and thus, the name “graphene” has been suggested. According to early theoretical calculations, 2-D atomic crystals such as graphene were considered to be thermodynamically unstable [2]. Studies predicted that the 2-D atomic crystals are stable only in a 3-D form as part of a crystal structure, just like they have been seen to be in graphite or thin films grown on solid supports [3]. Calculations showed that the melting point of atomic layers decreases with a decrease in the number of layers, so eventually they segregate into islands of multilayered structures or they decompose at room temperature [4]. This common wisdom was discredited in 2004 by Geim and Novoselov, physicists at the University of Manchester, after their successful isolation of atomically thin, stable free-standing carbon nanosheets from graphite using the “Scotch Tape” method. They were honored with the 2010 Nobel Prize for Physics! This discovery has led to an explosive growth of graphene research ever since. The potential of this technology ensures us to manipulate materials at the nanometer scale, resulting in tools and technologies never visualized earlier, from nanoparticle-based cancer therapy [5] to high-performance composites [6], and thus, nanotechnology opens up new frontiers for innovation in medicine, electronics, materials, etc. In addition to the rise of new technologies, a novel class of low-dimensional systems distinguishes the development of nanoscale sciences. For example, the zero-dimensional (0D) class of quantum dots, a one-dimensional (1D) class of nanoribbons, nanotubes, and nanowires, a two-dimensional (2D) class of single-atom-thick materials, and a three-dimensional (3D) class of nanoballs and nano cones [7]. A main feature that differentiates several categories of nanostructure is their dimensionality. Dimensionality is one of the most fundamental material parameters, which not only defines the atomic structure of the material, but also determines the properties to a significant degree [8]. The same chemical element or compound can exhibit different properties in different dimensions. Carbon nanostructures are a leading material in the nanotechnology field. The discovery and research of carbon materials has considerably contributed to the advancement of modern day science and technology. After the discovery of fullerene and single walled carbon nanotube (CNT), which are zero-dimensional and one-dimensional carbon nanomaterials respectively, the researchers have tried to isolate 2D graphitic material or to make 1D nano-ribbons from 2D crystals. The efforts have started to pay off since 2004 with the first isolation and electrical characterization of graphene transistor reported by Geim and Novoselov [8]. Most of these nanostructures are compiled exclusively of sp^2 hybridized carbon atoms establishing several structures, from the soccer ball like fullerene (C_{60}) to the single atom thick plane of carbon called graphene, to the “rolled up”, tubular sheets of graphene: carbon nanotubes as shown in Figure. 1 [9]. The physicochemical properties of these graphene like structures, even though their being composed of sp^2 carbon, are as different as their atomic structure. From the earliest theoretical investigation into the

electronic properties of graphene and graphite, it has become clearer that graphite has some unusual properties. Later, many more properties of graphite, graphene and CNT have come to light, for example the high charge carrier mobility of graphene and CNT [10]. Physicochemical properties and applications of graphene based materials and reduced graphene oxide had been reported earlier [11]. After the discovery of graphene, many researchers would not realize that more than a dozen 2D materials can be isolated and studied in less than 10 years. Progress in graphene research had a spillover effect by way of leading to an interest in other 2D materials like for example metal nitrides and carbides. 2D nanostructures are one of the greatest widely studied materials because of the unique physical singularities that happen when heat transport and charge is confined to a plane. Due to the unique properties, 2D nanostructures are anticipated to have an important influence on a huge diversity of applications, extending from high performance sensors, electronics to gas separation or storage, catalysis, inert coatings and support membranes, etc. Right now, the 2D materials family includes not just carbon material but also transition metal dichalcogenides (TMDs), and layered metal oxides. One of the most promising applications of 2D materials is in electronic devices [12]. With respect to the electrical properties, one can fabricate a new generation of superconductors, metallic materials, semimetals, semiconductors, insulators from the 2D materials. Even though graphene is the last one to be isolated in the carbon materials family, it serves as the building block for other family members with different dimensionalities. In particular, single layers of TMDs have attracted notable attention because of their diverse properties and natural abundance. Despite the similarity in the chemical formula, MX_2 , where typically M is the transition metal of groups 4–10 (typically Mo, Nb, W, Ni, V, or Re) and X is a chalcogen (typically Se, Te, or S) [13]. While the bonding of the tri-layers are covalent, neighboring sheets are bonded via Van der Waals interactions to grow 3D crystals. There are currently 40 different types of combinations of TMDs with different chalcogen atoms. Based on the coordination and oxidation state of the metal atoms, TMDs ranging from insulators such as HfS_2 , semiconductors such as MoS_2 , semimetal such as $TiSe_2$, to true metals such as $NbSe_2$, which can even exhibit superconductivity at low temperature. Besides, a solid attention in group-IV 2D oxides has been newly developed. These different types of nanosheets whether oxides or TMDs, have been studied experimentally or computationally to understand their electronic structure and compared with graphene [14]. The isolation of monolayer graphene flakes by mechanical exfoliation of bulk graphite opened the field of two-dimensional (2D) materials [15]. Since then, many other 2D materials have been discovered, such as transition metal-dichalcogenides (TMDs, e.g., MoS_2), hexagonal boron-nitride (h-BN), and black phosphorous or phosphorene. The family of 2D materials offers a full spectrum of physical properties, from conducting graphene to semiconducting MoS_2 and insulating h-BN. Moreover, the 2D crystal structures render a unique combination of mechanical properties, with high in-plane stiffness and strength but extremely low flexural rigidity. The 2D materials are promising for various applications [16]. Here we review recent theoretical and experimental studies related to the mechanics and mechanical properties of 2D materials. We emphasize how mechanics is indispensable in studying mechanical properties including interfacial properties and the coupling between the mechanical and other physical properties. Like thin membranes, 2D materials may be deformed by in-plane stretching or by bending out-of-plane. As a result, the elastic properties of 2D materials include both in-plane and bending moduli. With combined stretching and bending, a set of coupling moduli may also be defined theoretically, as noted for graphene being rolled into carbon nanotubes. Large biaxial strain can be applied to 2D materials such as graphene and MoS_2 using a pressurized blister test [17]. By applying a pressure difference across a suspended MoS_2 membrane (diameter $\sim 5\text{--}10\mu\text{m}$) transferred onto etched microcavities in silicon oxide, Lloyd et al. [17] measured the optomechanical coupling directly using a combination of Raman spectroscopy, photoluminescence spectroscopy, and AFM. The pressure difference across the membrane deformed the membrane into a circular blister with a biaxial strain at its center, which resulted in a red-shift in the optical band gap of $-99\text{ meV}/\%$ strain, consistent with theoretical predictions [18]. This technique enables one to apply biaxial strains as large as 5.6% and achieve a band gap shift of $\sim 500\text{ meV}$. Hydrostatic pressure can also enable inter-layer charge transfer in heterostructures, which can further tune

the electronic properties of 2D materials. In a heterostructure composed of monolayer graphene on top of monolayer MoS₂, the graphene was adopted with high carrier concentration ($\sim 2.7 \times 10^{13} \text{ cm}^{-2}$ at a pressure of 30 GPa), an order of magnitude higher than the charge concentration of pristine graphene [19]. This concentration is also comparable to the doping concentration of graphene-MoS₂ heterostructures by gate bias. The objective of this study is to explore the chemistry of two-dimensional (2D) materials, focusing on graphene and extending to other emerging 2D materials, to uncover their potential for advanced applications. While graphene has been extensively studied for its exceptional mechanical, electrical, and thermal properties, the chemical modification and functionalization of 2D materials remain underexplored, particularly for tailoring their properties for specific uses. Furthermore, newer 2D materials, such as transition metal dichalcogenides (TMDs), MXenes, and phosphorene, exhibit unique characteristics but lack comprehensive studies on their chemical reactivity, stability, and integration into practical systems. This research addresses the gap by delving into the chemical interactions, functionalization strategies, and novel synthesis techniques for these materials, aiming to broaden their applicability in fields such as energy storage, catalysis, and electronic devices.

Carbon Allotropes and Related Materials

Carbon was one of the first elements known to humans, and is one of the most remarkable of all chemical elements. The use of carbon materials for a multitude of applications derives from the materials' unique diversity of structures and properties that extend from chemical bonding between carbon atoms to nanostructures, crystallite alignment, and microstructures. Diamond and graphite are both three-dimensional (3D) crystalline forms of the element carbon. Graphite consists purely of sp² hybridized bonds, whereas diamond consists purely of sp³ hybridized bonds. The carbon atoms in diamond are arranged in a lattice, which is a variation of the face-centered cubic (fcc) crystal structure [20]. It has superlative physical qualities, most of which originate from the strong covalent bonding between its atoms (sp³ hybridization). Unlike diamond, graphite in particular is described as consisting of a lamellar (layered, planar) structure [21]. In each layer, the carbon atoms are arranged in a hexagonal lattice with a separation of 0.142 nm (sp² hybridization), and the distance between planes (layers) is 0.335 nm. The two known forms of graphite, α (hexagonal) and β (rhombohedral), have very similar physical properties. The lamellar structures have much stronger forces within the lateral planes than between the planes. Graphitic carbon nanomaterials can be regarded as members of the same group because they consist primarily of sp² carbon atoms arranged in a hexagonal network. This common structure means that they all have some common properties, although they also have significant differences due to their different sizes and shapes. Graphene is the basic structural element of other allotropes, including graphite, fullerene (e.g., C₆₀), carbon nanotube (CNT), graphyne, and other related materials (e.g., carbon fiber (CF), amorphous carbon (AC), charcoal) [22]. (Figure 1). It can also be considered as an indefinitely large aromatic molecule, the limiting case of the family of flat polycyclic aromatic hydrocarbons. Fullerenes (also called buckyballs) are molecules of varying sizes composed entirely of carbon that take on the form of hollow spheres or ellipsoids [23]. Fullerenes were the subject of intense research in the 1990s, both because of their unique chemistry and for their technological applications, especially in materials science, electronics, and nanotechnology.

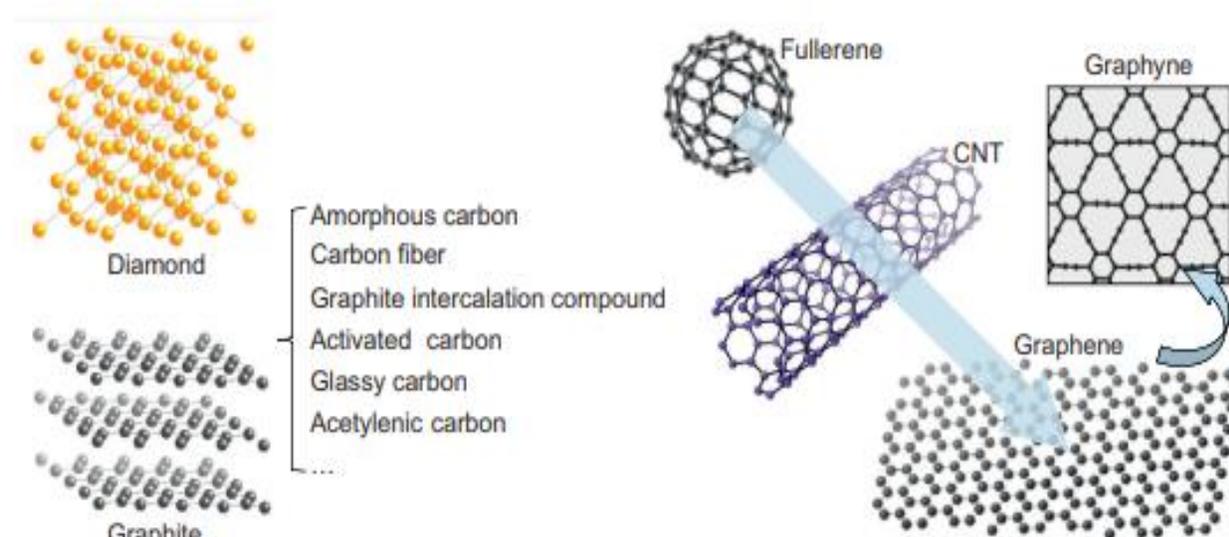


FIGURE 1: Carbon allotropes and related materials. CNT, carbon nanotube

Structure of Graphene:

Graphene, by definition, is an allotrope of carbon in the form of a 2D, atomic-scale, hexagonal lattice in which one atom forms each vertex with sp^2 hybridization. As shown in the length of the carbon-carbon bond is about 0.142 nm. There are three σ bonds in each lattice with strong connections forming a stable hexagonal structure. The electrical conductivity of graphene is mostly attributed to the π bond located vertically to the lattice plane. Graphene's stability is due to its tightly packed carbon atoms and a sp^2 orbital hybridization—a combination of orbitals s , p_x , and p_y that constitute the σ -bond. The final p_z electron makes up the π -bond. The π -bonds hybridize together to form the π -band and π^* -bands. These bands are responsible for most of graphene's notable electronic properties, via the half-filled band that permits free-moving electrons. Graphene can be considered as a unit structure of graphite, CNT, and fullerene, as well as aromatic molecules with infinite size, such as extremely planar polycyclic aromatic hydrocarbons. In other words, graphene is composed of a closely packed single layer of carbon atoms, forming a 2D honeycomb lattice plane. In single-layer graphene, carbon atoms bond with surrounding carbon atoms with sp^2 hybridization forming a benzene ring in which each atom donates an unpaired electron. The thickness of graphene is only 0.35 nm which is 1/200,000th the diameter of a human hair. Nevertheless, the structure of graphene is quite stable. The connection between carbon atoms is tough enough to endure external force by a twisting lattice plane to avoid the reconfiguration of atoms. Graphene, with a limited structure, can exist as a nanoribbon such that an energy barrier occurs near the central point due to a lateral charge movement. Such an energy barrier is increased with a decrease in the width of the nanoribbon [24]. Thus, by manipulating the width of the graphene nanoribbon, the energy barrier can then be precisely controlled, which is a promising characteristic for potential graphene-based electronic devices. In addition to this, similar to a CNT, the edge of graphene can be classified into zigzag and armchair according to different carbon chains as shown in Figure 2. The variety in edges leads to various conducting behaviors. A graphene nanoribbon with a zigzag edge usually behaves like a metal while a nanoribbon with an armchair edge could conduct electricity like either metal or a semiconductor.

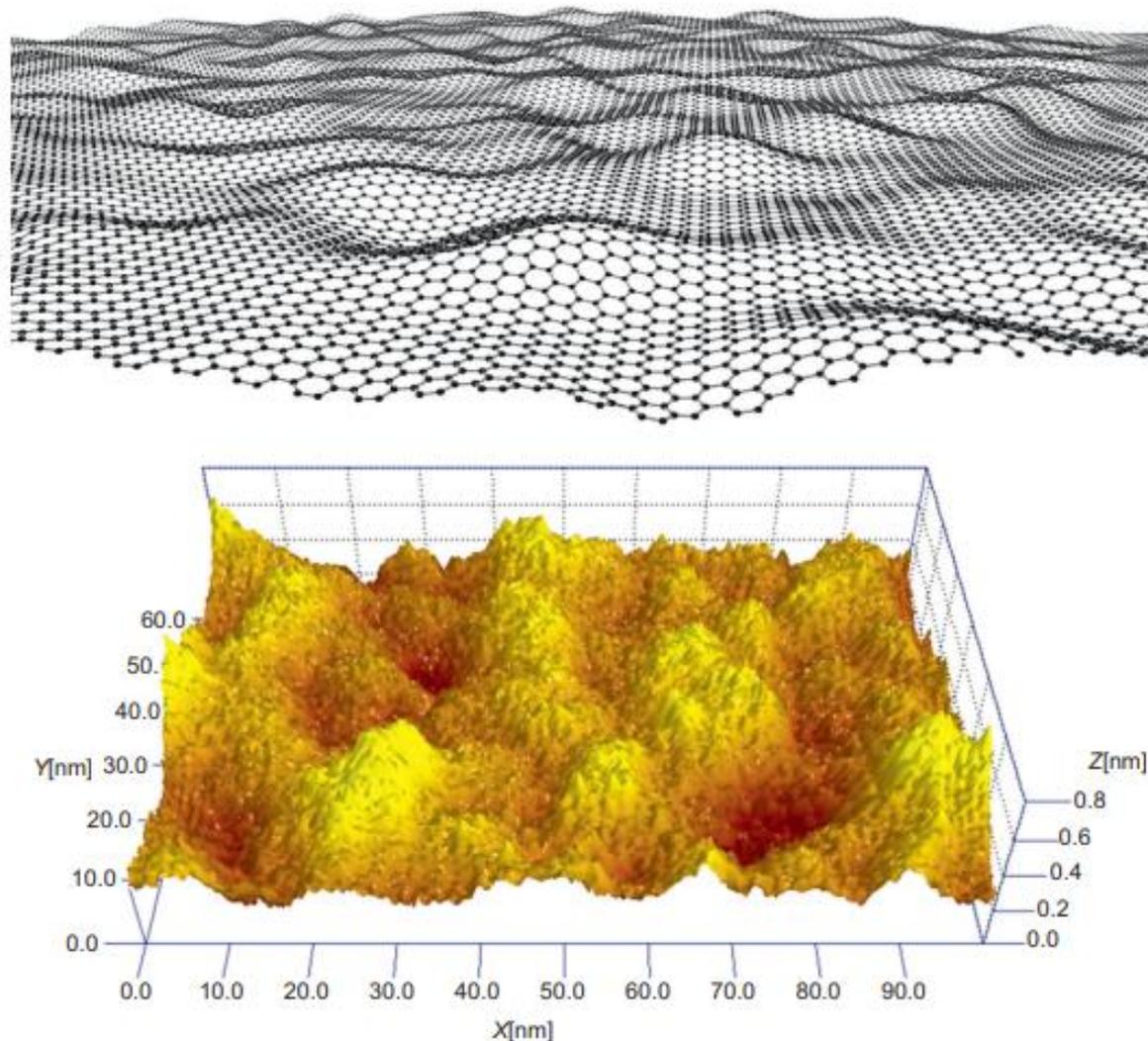


FIGURE 2: Fluctuation of graphene surface [25]

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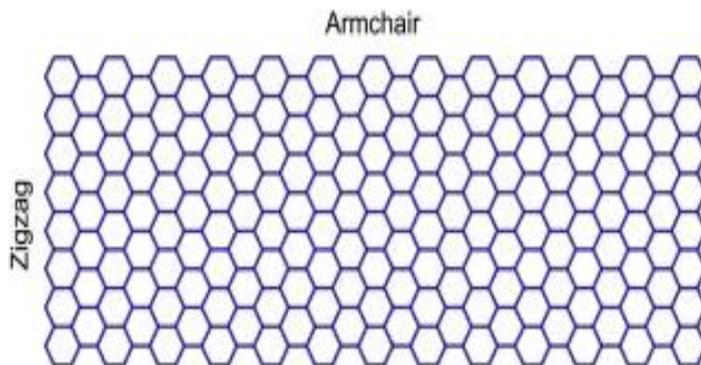


FIGURE 3:Graphene nanoribbon

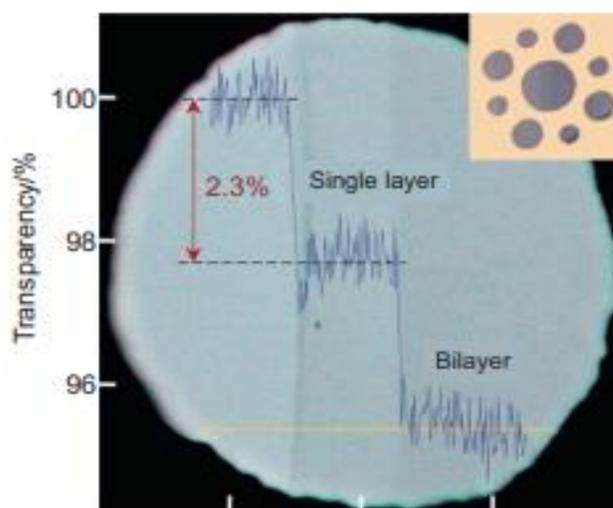


FIGURE 4:Transparency of graphene.

Synthesis methods of Graphene: Chemical vapor deposition

The chemical vapor deposition (CVD) method is an excellent example of convergent evolution in research, where work on two seemingly unrelated problems led to a similar outcome. The first research problem was that of soot formation. Scientists in the 1950s were examining thin sooty films formed on porcelain and graphite when a group led by Walker decided to survey soot formation on many different materials. They discovered that metal surfaces—in particular, nickel surfaces—form carbon films with single crystal sizes much larger than those on ceramics [26]. While this method saw some subsequent development, interest did not increase significantly until the late 1970's, in the course of experiments to determine the mechanism of high-temperature alkylation on catalytic surfaces. When hydrocarbons are exposed to a heated metal surface under vacuum, the metal catalyzes the loss of hydrogen and dissolves the remaining carbon, forming a layer of metal carbide. As the temperature drops, the metal carbide surface layers saturate and graphitic carbon precipitates from the carbide sol [27]. In the 1980s, scientists examined the thin carbon overlayer more rigorously and likely made some of the first observations of graphene's electronic structure and phonon dispersion curves. Researchers in this area were aware that they were making single-layer graphene, a material that they called "monolayer graphite," as is evidenced by the fact that this term appears extensively in the literature of thin graphitic films on metal surfaces during the 1980s and 1990s. After the graphene frenzy began in 2004-2005, many researchers worked to refine the CVD method. A seminal breakthrough came in 2009 when CVD conditions were discovered where graphene growth on copper was self-limited to a single layer, such that very large sheets (side length ≈ 75 cm) of single-layer graphene could be grown (Figure 4) [28]. Single-crystal grain size has increased

steadily; as of January 2014, the largest reported single crystal of graphene is roughly 1 cm in diameter (Figure 5) [29]. Other groups have focused on low-temperature graphene deposition on arbitrary substrates. In this direction, Kwak et al. has deposited single crystals of graphene on the micrometer scale onto arbitrary substrates by allowing carbon to diffuse through a thin overlayer of catalyst metal and graphitize at the metal substrate interface. CVD graphene growth is most commonly performed on copper and nickel surfaces via a thermal method. Plasma-enhanced CVD methods have been reported, but generally produce lower quality films than thermal methods [30]. Thermal growth procedures are quite similar on both metals. Typically, a reannealing run is performed by heating the substrate to around 1000°C under a continuous flow of a hydrogen-argon mixture in a 1:10 volumetric ratio. The growth itself is performed at between 800- 1100°C (nickel growth tends to be somewhat cooler than copper growth), using methane as the carbon source with a small amount of hydrogen to maintain a reducing environment. Argon can be used as a carrier gas to fine-tune the pressure of the growth experiments. One major feature to point out is that the grain boundaries of the graphene do not necessarily coincide with the grain boundaries of the polycrystalline substrate. Grain boundaries in graphene are formed when two separately nucleated. And misaligned single crystals of graphene encounter each other on the surface of the substrate, not by interaction with the substrate itself [28]. That said, it has been found that graphene growth proceeds more rapidly on Cu(111) than on another surface facet. Since the formation of grain boundaries in graphene is inversely dependent on the number of nucleation sites, strategies for CVD growth of single-crystal CVD graphene on copper generally involve suppressing the number of graphene nucleation sites. The most successful method for achieving this so far involves the introduction of oxygen impurities on the copper substrate before growth. These impurities dramatically reduce the nucleation density of graphene, which in turn allows single-crystal domains to grow much larger than if the nucleation density were high [31]. Other methods of suppressing nucleation, including electrochemical polishing of the copper surface and using copper enclosures to limit the partial pressure of the carbon seed gas at the growth site, are also effective at promoting large single crystal growth. Very recently, another avenue toward single crystal growth has been presented by Lee et al. [32]. This group used hydrogen-terminated germanium(110) as a growth substrate. Since the surface of this material has an anisotropic symmetry axis, a large number of nucleated graphene crystals all grow with the same orientation, and individual grains are therefore much more readily stitched together than CVD material grown on copper or nickel, whereas the orientation of the graphene crystals is random, leading to grain boundaries as the crystals grow into one another.

Chemical exfoliation

The chemical method is one of the most appropriate methods for synthesis of graphene. In chemical method colloidal suspension modifies graphene from graphite and graphite intercalation compound. Different types of paper like material polymer composites [33], energy storage materials and transparent conductive electrodes have already used chemical methods for the production of graphene. In 1860 graphene oxide was first manufactured Brodie [34], Hummers and Staudenmaier [35] methods. Chemical exfoliation is a two-step process. At first reduces the interlayer van der Waals forces to increase the interlayer spacing. Thus it forms graphene intercalated compounds (GICs) [36]. Then it exfoliates graphene with single to few layers by rapid heating or sonication. For single-layer graphene oxide (SGO) uses ultrasonication and various layer thicknesses using Density Gradient Ultracentrifugation. Graphene oxide (GO) is readily prepared by the Hummers method involving the oxidation of graphite with strong oxidizing agents such as KMnO_4 and NaNO_3 in $\text{H}_2\text{SO}_4/\text{H}_3\text{PO}_4$ [37]. Ultrasonication in a DMF/water (9:1) (dimethyl formamide) mixture was used and produced single-layer graphene. For this reason, interlayer spacing increases from 3.7 to 9.5 Å. For oxidization high density of functional groups, and reduction needs to be carried out to obtain graphene-like properties. Single-layer graphene sheets are dispersed by chemical reduction with hydrazine monohydrate [38]. Polycyclic aromatic hydrocarbons (PAHs), has used for synthesis of graphene. Using a dendritic precursor transformed by cyclodehydrogenation and planarization. produce small domains of graphene. Poly-dispersed hyper

branched polyphenylene, precursor give larger flakes [39]. The first were synthesized through oxidative cyclodehydrogenation with FeCl_3 . Variety of solvents are used to disperse graphene in perfluorinated aromatic solvents, orthodichloro benzene [98], and even in low-boiling solvents such as chloroform and isopropanol. The electrostatic force of attraction between HOPG and the Si substrate use in graphene on SiO_2/Si substrates. Laser exfoliation of HOPG has also been used to prepare FG, using a pulsed neodymium-doped yttrium aluminum garnet (Nd:YAG) laser [40]. Thermal exfoliation and reduction of graphite oxide also produce good-quality graphene, generally referred to as reduced graphene oxide (RGO)

Mechanical exfoliation

Mechanical exfoliation can be categorized based on directional routes such as normal force and shear force vectors (Figure 5). One of the recent studies on the normal force synthesis route is the peeling of graphite using advanced machinery of ultra-sharp single crystal diamond wedge [41]. This method eliminates the need for manual operation, and saves time and labor cost. Another method uses a three-roll mill machine, an established technique in rubber industry, to produce graphene of 1.13–1.41 nm. The major drawback of this method is the cost of adhesives such as polyvinyl chloride (PVC) and the purification of graphene from the adhesive. The removal of PVC was achieved by heating in a muffle furnace at 500 °C for 3 h. Thus, residue PVC elimination could lead to high energy consumption and hence high production cost. The two approaches, however, still lack in-depth synthesis and parametric studies. The shear force-based methods such as ball milling and fluid dynamic methods have been gaining much attention recently. Ball milling which is commonly used in grinding minerals, ceramic, cement and fertilizer, utilizes grinding media in the form of balls to generate mechanical force via impact and attrition, exfoliating graphite to form graphene flakes. This technique facilitates exfoliation and fragmentation of graphite to graphene of nano-size thickness, mixing between graphene and composite materials and even functionalization of graphene. The quality of graphene produced by ball milling synthesis is controlled by process parameters such as grinding media type, time, matrix, speed and precursor initial size. Exfoliation of graphene using ball milling is a time consuming process. The reaction time for the process could vary from 24 to 48 h which is undesirable for largescale production. Notwithstanding the suitability of ball milling for batch and continuous processes, this undesirable factor needs to be resolved to ensure scalability[42].

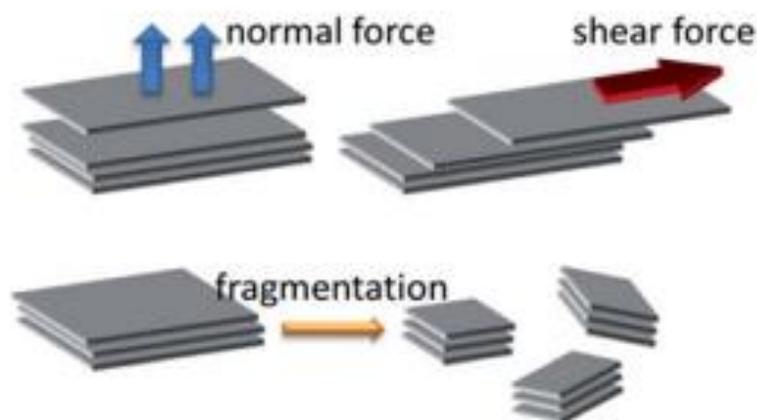


Figure 5: Mechanical exfoliation of graphene based on different mechanical routes [42].

BEYOND GRAPHENE

After the discovery of graphene in 2004, a distinct branch of research in 2-D materials rapidly evolved. Atomically thin layers of several such materials, with high surface area and specific chemical compositions, showed superior properties when compared to the corresponding bulk materials. These 2-D materials are being extensively tested for applications in electronics, catalysis, and biomedicine.41 Detailed descriptions of these materials and their applications will be given in Chapter 4, Inorganic analogs

of graphene: synthesis, characterization and applications, and Chapter 5, Graphene composites with inorganic 2-D materials, but a short introduction is given here. The “hunt” for other, stable, thin atomic layers, other than graphene has begun with h-BN nanolayers (discussed below) [43].

TRANSITION METAL DICHALCOGENIDES

As the name indicates, TMDs are formed from a transition metal and group 16 elements (oxygen group: chalcogens). These compounds with the general formula MX_2 (M, metal; X, halogen) have zig-zag bonding pattern with XM_2 bonds, where the chalcogen has out-of-plane orientation concerning the metal plane (Figure 6). Oxides, sulfides, selenides, and tellurides of transition metals such as molybdenum (Mo) and tungsten (W) form layered structures similar to graphite.⁴⁸ A wide variety of TMDs are known to exist in monolayer form and the most widely studied member is molybdenum sulfide (MoS_2) because of its availability in bulk form and a band gap that is comparable to many semiconductors (band gap of 1.21.9 eV), depending on the number of layers. CVD, exfoliation from bulk and molecular beam epitaxy techniques, can synthesize ⁴⁹ TMD monolayers. Apart from the chalcogens, nitrides, carbides, or carbonitrides of transition.

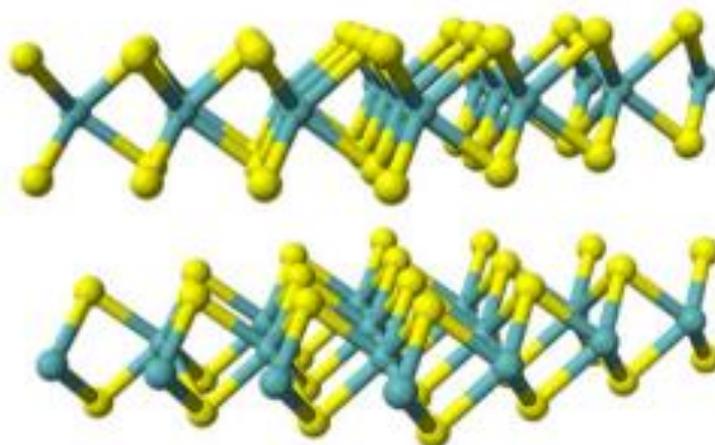


FIGURE 6: MoS₂ monolayer structure

MXENES

MXenes are 2-D layers derived from MAX phases, where M is a transition metal (Ti, V, Cr, etc.), A is a group A element (e.g., Si, Al, etc., Groups 1, 2, 12, 13, 14, 15, 16, 17 in current IUPAC naming) and X represents carbon and/or nitrogen.⁵¹ They have the general formula M_nAX_n , where $n = 1, 2, \text{ or } 3$, for example, Ti_3AlC_2 . Nanolayers of MAX phases are achieved by acid etching (usually hydrofluoric acid) of the bulk material to yield composition of M_nAX_n (Fig. 1.9), named as a graphene family member, MXenes (e.g., Ti_3C_2).⁵⁰ MXenes find versatile applications in supercapacitors, electromagnetic interference shielding, batteries, and many more [44].

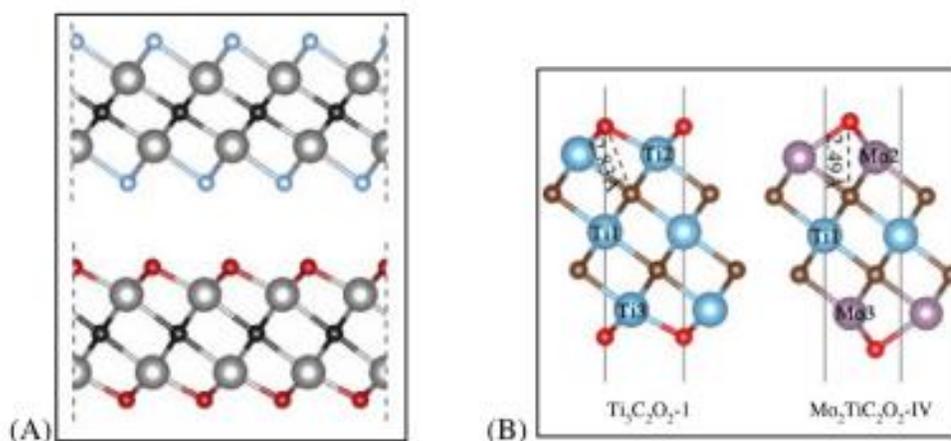


Figure 7: Bonding in Ti_2CF_2 (top) and Ti_2CO_2 . Most energetically favorable structures of $Ti_3C_2O_2$ (A) and $Mo_2TiC_2O_2$ (B).

PHOSPHORENE

A single-atom-layer allotrope of phosphorous, analogous to graphene was also realized in 2014, by micromechanical exfoliation of black phosphorous. Unlike graphene, phosphorene has a band gap of B2.0 eV, perfect for semiconducting applications when compared to that of silicon (B3 eV).⁵³ Liquid-phase exfoliation methods are also established for phosphorene, which promises its large-scale applications. Since phosphorene is highly reactive to oxygen, deoxygenation of solvents and stabilizing agents or suitable solvent is needed. Phosphorene is stable in water in the absence of oxygen. Regardless of its sensitivity to air, phosphorene was demonstrated to be useful in transistors, sensors, and catalysis. Phosphorene, like single-atom layers of boron (borophene), antimony (antimonene), and so on, are known to exist, but stability and scalable production are still to be realized for practical applications [44].

Graphene's success has stimulated the rise of a group of new materials: two-dimensional (2D) materials.^{1,2} These include, but are not limited to, graphene, silicene, germanene, borophene, phosphorene, hexagonal boron nitride (h-BN), transition metal dichalcogenides (TMDCs), MXenes, and layered oxides.^{3–8} Some of them are present in the form of 2D atomic crystals such as graphite, h-BN, TMDCs, and micas, while others e.g. silicene and borophene are purely synthetic and need to be supported on substrates [45]. The 2D materials present strong in-plane bonding but weak van der Waals-like interaction between neighboring layers. More excitingly, single layers with one-atom or few-atom thickness can be stable in their freestanding state. In the 2D materials the charge and phonon transport are strongly confined within each layer, and it is expected that the 2D materials present unusual physical properties which are different from their 3D bulk counterparts. Taking graphene as an example, the interaction between electrons and the honeycomb carbon lattice causes the electrons to behave as massless fermions, which give rise to novel physical phenomena such as anomalous room temperature quantum hall effect and extraordinarily high carrier mobility [46]. Similar to graphene, a 2D honeycomb arrangement of Si atoms has an electronic dispersion resembling that of the relativistic Dirac fermions. The rich new physics exhibited by the 2D materials has stimulated extensive research efforts in both fundamental physics and technological applications in the past decade. The chemistry of 2D materials is less explored. Nevertheless, many important advances have been made in recent years.^{16–25} The 2D materials have open double-sided surfaces and in principle, all atoms are subject to surface reactions. By reacting with other atoms or molecules, each single layer can be chemically functionalized which creates a new family of 2D materials. For example, graphene reacts with atomic hydrogen and transforms into graphane or graphene [47]. Hydrogenation of a silicene phase on Ag(111) forms half-silicane.²⁸ Oxidation of graphene produces graphene oxides (GOs), which contain reactive oxygen-containing functional groups and show many interesting chemical properties. Besides the surface functionalization,

small parts of atoms in the 2D materials can be substituted by heteroatoms. The dopants acting as donors or acceptors change the electronic states of the neighboring atoms in the 2D matrix and produce new active sites. N-doped graphene is the most widely investigated heteroatom-doped 2D material, which finds many applications in electrocatalysis. Finally, one kind of 2D material can be combined with another one to form heterostructures or supported on other solids. The chemical properties of the top 2D layer can be strongly modulated by the underlying substrates [45].

Most studies in the chemistry of 2D materials have made use of the open surfaces of the 2D layered structures. Chemical processes such as surface functionalization, chemical modification, surface synthetic chemistry, and surface catalytic reactions almost exclusively occur on the surfaces of the 2D layers [48]. As discussed above, the 2D materials are characterized by their weak interaction between layers such that atoms and molecules may be trapped under the 2D layers and furthermore reactions occur underneath. Accordingly, we suggest that new chemistry can be done under the surfaces of the 2D materials (Figure 8). Intercalation of 2D atomic crystals such as graphite, h-BN, and TMDCs is an old topic. For example, intercalation and de-intercalation of graphite-based materials form the basis of lithium ion batteries. Recently, intercalation reactions are often employed to exfoliate the 2D atomic crystals, producing individual atomic and molecular layers. The endothermic opening of layers in the 2D atomic crystals is well compensated by the interaction energy among intercalants and the 2D sheets. Similarly, intercalation of 2D material overlayers supported on solid surfaces is also energetically favored since the energy cost to decouple van der Waals interaction between 2D material overlayers and substrate surfaces can be offset by the energy gain from interaction of the intercalants with the substrates. Considering the feasible intercalation into the 2D atomic crystals and the interfaces between 2D materials and solid surfaces, we suggest that there should be plenty of room for new chemistry in the space confined under the 2D covers, which has been extensively explored in the past few years [48].

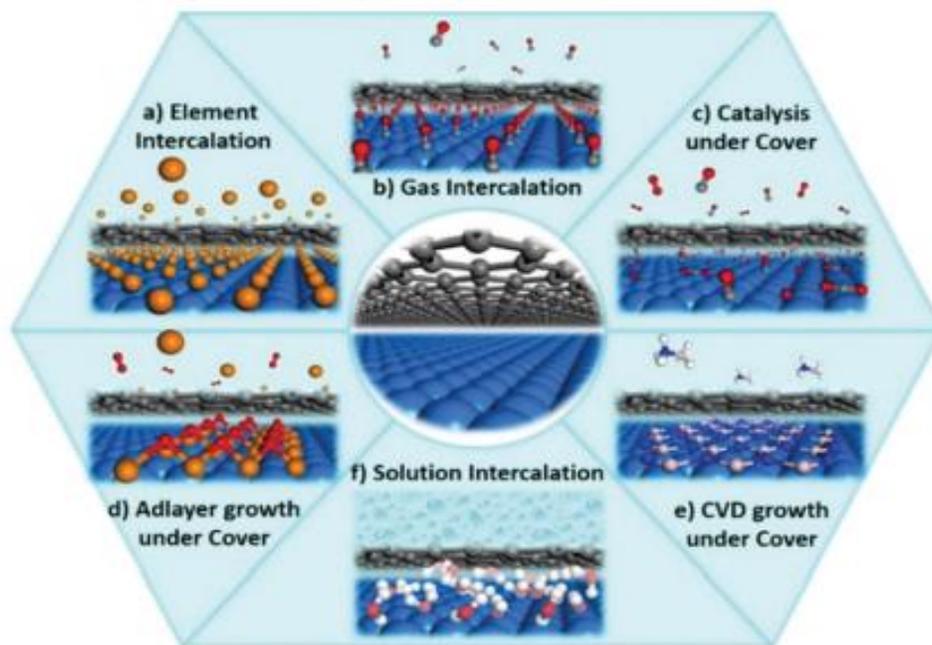


Figure 8: Chemistry under the 2D materials. Various chemical processes under the 2D materials were illustrated. Here, graphene was used as an example. (a) Atom intercalation; (b) molecule intercalation; (c) catalysis under cover; (d) surface adlayer growth under cover; (e) CVD process under cover; and (f) solution intercalation [49].

Application of 2D materials:

2D Materials Transistor and Device Technology A field-effect transistor (FET) is a three-terminal device with a semiconducting channel material forming the conducting path between the source and the drain, which can be modulated by the gate electrode. FETs are the primary elements in modern integrated circuits

(ICs). Figure 9 depicts the basic structure of a top-gate transistor with 2D materials as the channel materials in the classical metal-oxide-semiconductor field-effect transistor (MOSFET) structure. R_S and R_D are the source and drain access resistance. R_i is the intrinsic resistance. $g_{m,i}$ is the intrinsic transconductance. g_0 is the output transconductance. C_{ds} is the source-drain capacitance. C_{gs} and C_{gd} are the gate-source and gate-drain capacitances. R_G is the resistance in the gate electrode. Currently, the existing channel materials of commercial FETs are dominated by bulk semiconductors including silicon, GaAs, SiC, GaN, and so on. FETs based on these bulk semiconductors have been successfully scaled down to the micro and nanometer scale in the 50 years of Moore's law. To keep sustaining Moore's law and meet the technological demand for next-generation semiconductor devices, new materials, and device geometries will be needed to address the challenges in transistor technology. In the following, we introduce the operation and characteristics of 2D materials-based FETs to understand the advantage of using 2D materials as the channel materials in FETs. Then, several considerations for FET performance optimization are discussed. Finally, important figures of merit (FOM) are defined and introduced to evaluate their performance and compare them against channel materials of other types [50].

Sensing functions

2D semiconductors have a surface-to-volume ratio unmatched by other structural materials and have a natural advantage in responding to surrounding physical or chemical signals. Light, atmosphere, temperature, and humidity are prone to cause rapid changes in electron transport at 2D surfaces. And these changes are fast response, high sensitivity, easy to achieve sensor miniaturization, which can play a significant role in improving sensor sensitivity and reducing sample usage, especially for in vivo, in situ and real-time detection in biological science[51]. Its suitable bandgap provides better biocompatibility and lower detection limits for biological targets, which is advantageous in the detection of complex biological samples at low concentrations. The MoS_2 nano-biosensor has already achieved the detection of various biomolecules such as DNA, RNA, and proteins. Compared to resistive or capacitive sensors, biosensors based on field-effect transistor structures are typically used as 2D semiconductor channels for transduction, where the detection mechanism lies in the electrical signal in the biomolecule altering the carrier distribution in the channel. So, high mobilities are important for detection [52]. To improve the detection sensitivity of the target, different structures or surface modification functionalization's of the channel have been used [124,125]. The principle is similar to detecting some molecules or ions as chemical sensors. One of the problems of detection in solution is that long-time immersion can easily damage the channel material or structure of the transistor, thus the controllability of the device is poor and non-reusable. 2D semiconductors can also provide sensitive detection of pressure, yet pressure puts high demands on the stability of the device as well. For use on electronic chips, gas and light detection is non-invasive for 2D semiconductors and is generally more widely used. The sensing of gases by 2D semiconductors generally stems from the electron transfer mechanism between the gas molecules and the channel. A suitable bandgap allows for the transfer properties to enhance the sensing capability [53]. Different gases touching or disassociating from the channel will cause the channel resistance to change accordingly. The direction and magnitude of the variation in channel resistance are used to analyze the composition and concentration of the gas to be measured. It is valuable for the detection of flammable and toxic gases [54].

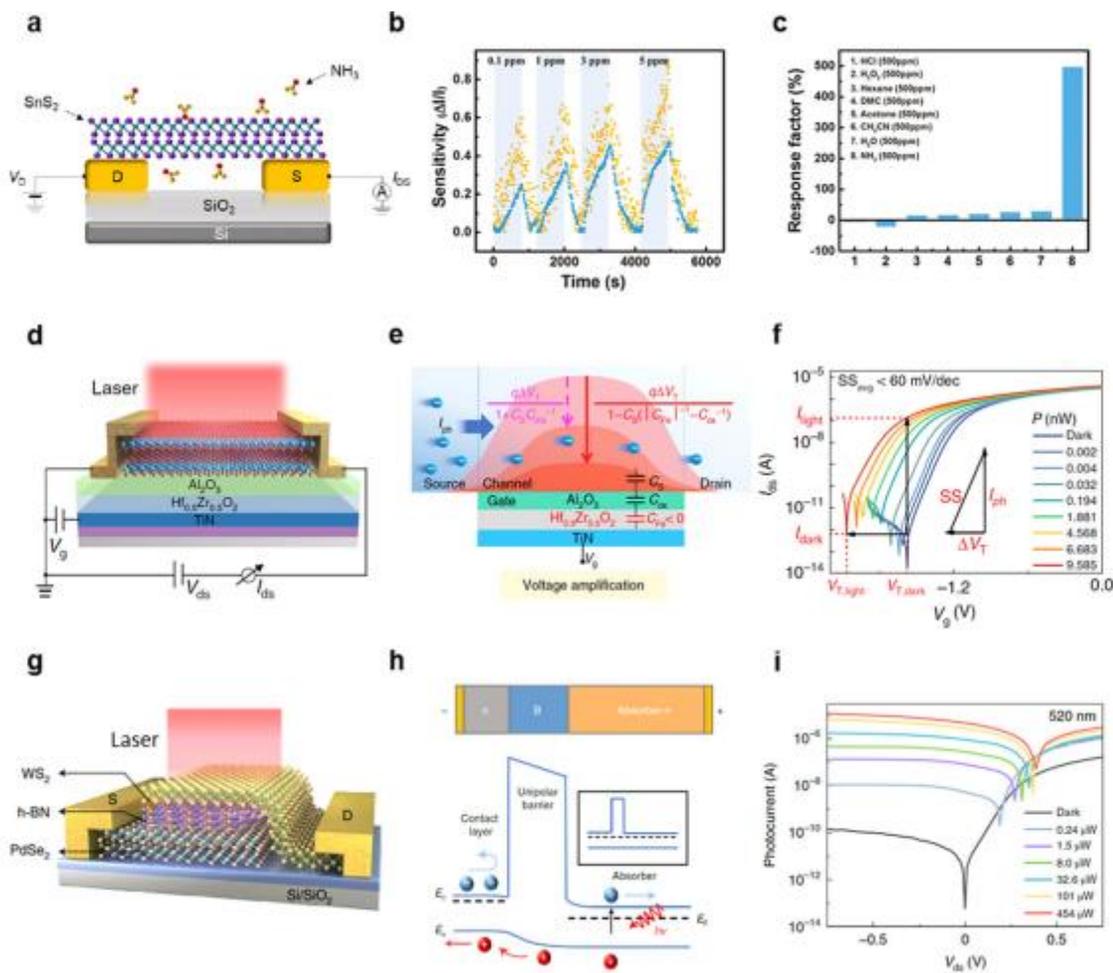


Figure 9: 2D semiconductors for sense.

A schematic of a suspended SnS2-based gas sensor. b Responses of the suspended SnS2-based sensor under different vapor conditions. c The selectivity of the suspended SnS2-based sensor in different gases and solvent vapors. a–c is reproduced from ref. [55]. d Schematic of a MoS2-based photoconductive mode detector with the ferroelectric HZO thin film in the gate dielectric stack. e Mechanism of ultrasensitive optical detection in the negative-capacitance MoS2 phototransistor. f Transfer curves of the NC MoS2 phototransistor under different light. d–f is reproduced from ref. [56]. g Schematic of vdW unipolar barrier phototransistors. h Band alignment of the vdW unipolar barrier phototransistors. i Output curves of the vdW unipolar barrier phototransistors under different light. g–i are reproduced from ref. [57].

Application of 2D materials to Optoelectronics

Graphene has received much interest because of its exceptional optical and electrical characteristics. Due to the unique electronic band structure of graphene, it can absorb 2.3% of incident light [58]. and generate a photocurrent through photo thermoelectric effects (the temperature difference by light illumination is converted to an electric voltage). In addition, the huge carrier mobility (about 200000 cm² V⁻¹ s⁻¹) of graphene can be exploited in ultra-fast 2D-material-based optoelectronic applications. A monolayer of MoS2 was used in optoelectronic devices by Mak et al. [59] as a new 2D semiconductor material with a wide direct bandgap (Eg = 1.88 eV). This allowed high light absorption over a wide spectral range (visible to near-infrared). Other TMDs (e.g., MoSe2, WS2, and WSe2) have also been reported to have a direct

bandgap in the monolayer structure. This discovery of graphene and TMD could open the door for next-generation 2D-material-based optoelectronic applications. In this section, we review the development of 2D-material-based optoelectronic devices: i) photodetectors, ii) photovoltaic devices, and iii) LEDs [60]. The ever-increasing demands of electrical vehicles and power station utilization promote the development of rechargeable batteries with superior electrochemical performances. To further enhance the energy and power densities, the design of new electrode materials with higher specific capacities, especially beyond their theoretical capacities, is desirable. Such a task is of high priority. Two-dimensional (2D) nanostructures represent a material family with various layered ensembles. These include graphene, transition metal dichalcogenides (TMDCs), phosphorene, $g\text{-C}_3\text{N}_4$, MXenes, [61]. h-BN, [30,31] and layered double hydroxides, among others. Most of these 2D materials, and their derivatives, have been adopted as electrodes in energy-storage devices, especially for rechargeable batteries. They indeed exhibit a superior Li/Na storage performance. Interestingly, one of the most important features of 2D materials is their self-assembly and richness of micro-/nanostructures, which provide many more newly generated geometric sites for storage of the guest ions. This is a newly emerging discipline in regard of the required mathematical concept, materials design, and fabrication, as well as electrochemistry, which in short can be termed “geometry-driven” energy storage. These approaches have greatly promoted the investigation and application of 2D-based materials as electrodes in secondary batteries. The topic of “geometric sites” energy storage has witnessed a rapid development in recent years. Thus, a comprehensive review summarizing the present progress is indeed timely and warranted for a fundamental understanding and further optimization of electrode performance. Geometric sites (beyond the normal guest-ion storage sites that include inner/inter spaces of 2D layered materials). The progress in mechanism studies, especially based on in situ transmission electron microscopy (TEM) techniques, is also discussed with respect to geometric-site evolution and kinetic features during insertion/desertion of guest ions. This review is organized based on the following issues. (1) Most of the rechargeable batteries (lithium-ion battery [LIB] is representative) based on the intercalation/deintercalation of guest ions (Li^+ , Na^+ , K^+ , Mg^{2+} , Al^{3+} , etc.) into/from host electrode materials, have been named “rocking chair” batteries. [39] Their capacities are dependent on the theoretical sites for accommodation of guest ions. Materials with a 2D layered morphology show great promise for energy storage, as displayed in Figure 11. Importantly, new 2D electrode materials, with a capacity far beyond their theoretical values, have indeed been reported and have drawn increasing attention. [8,9] Some of “extra capacity” has been derived from newly generated geometric sites within 2D layered materials [62]. To shed new light onto the materials design, the formation and functions of such geometric sites will be sorted and discussed concerning point-like, line-like, and hierarchical geometry structures. The electronic structure, which has profound effects on energy storage performance, will also be elucidated. The self-assemblies or template-directed assemblies of 3D hierarchical structures, constructed from 2D layered materials, may also create new energy-storage sites.

Application of 2d in biomedical:

In recent years, increasing interests have been attracted towards 2-D Ms. Investigating this type of Ms is one of the most attractive research areas in physics that may be due to their unique electrical, mechanical, magnetic, and optical characteristics. The main techniques for preparation of 2-D Ms include the chemical vapor deposition, hydrothermal, and epitaxial growths. Each technique is associated with advantages or disadvantages [63]. 2-D Ms have shown different properties as compared to the bulk materials. Enhanced surface areas of these ultra-thin structures remarkably elevate their chemical and physical reactivity and affect 2-D wave functions via the quantum restraint effects. 2-D Ms could be applied in a variety of fields including the photonics, optoelectronics, and biomedicine. They are suitable templates for fabricating the robot and soft actuators backbones. Interestingly, 2-D Ms are capable of mimicking the human skin functionalities because of their fascinating physiochemical characteristics including high chemical and thermal stabilities [64]. This might inhibit small molecule penetration or reduce harmful substance spread.

2-D Ms in association with ML approaches enable accelerated analysis of the biomedical data. These Ms may also be applied for constructing highly efficient photo-catalytic conversion systems. Using 2-D Ms and photo-electric controlled hetero-structures for designing the neuronal elements as well as 2-D vW synapses enables achieving various bio plasticity with efficient photo-electric versatility and dual modulation. 2-D hetero-junction synapses have shown superior biological characteristics and plasticity that provide novel paradigms for imitating the synapses in combination with 2-D inorganic or organic Ms. 2-D WSe₂/h-BN vW hetero-structures with synaptic performance and optical sensing capabilities have been shown promising for colored pattern recognizing. Photonic memory platforms have also attracted interest by which data could be read, written, and erased optically. This type of devices have been investigated for the chip-scale, all-photonic processing of information. For instance, integration of the phase change Ms onto the photonics-based chip has enabled optical signal multiplication [65]. Based on the controlling synaptic behavior mechanism, 2-D Ms-based synaptic electronics and ANNs could be divided into the conductive bridge/electro-chemical, metallization electron ion/electrostatic, thermochemical, or phase change synapses. Ultra-thin 2-D Ms have shown superior electrical, magnetic, and optical characteristics that might be due to 2-D electron confinement. Atomic thickness of these Ms provide a highly-specific surface area, rapid production rate of photo-carriers, and short distance of migration for the photocarriers. The properties of 2-D Ms are satisfying for the photocatalysis (via altering the absorption of light) and separation and transportation of carriers. 2-D Ms could be the key parts of the next generation transistors, capacitors, photodiodes, and memory elements [66]. This might facilitate construction and transferring of the nanoelectronics circuits. Devices composed of 2-D Ms are capable of bypassing the problems associated with traditional electronics that might be due to their advantages such as low-energy implementations, high turn on currents, high limits of strain, and suitable gate control. Besides overcoming the scaling-related limitations of transistors, providing highly-efficient integrations including those associated with wafer-based technologies, it would be possible to improve the performance of various devices including the magnetic ones or in-memory techniques of computing that eliminate energy intensive and time-consuming interactions of data leading to the significantly improved efficiency of computations. The units of computational memory usually have various in memory cores which are connected via the on-chip networks and may have digital units of processing, buffers, and registers [67].

2-D Ms for drug delivery

Nanoplatforms for bio-inspired computing have been shown promising in various fields including the delivery of theranostics. They could be programmed for performing multi-step and sophisticated computations leading to the accelerated detection of Ms or development of the advanced devices for targeted delivery of therapeutic agents with improved outcomes [68]. Besides automatic collection of data and creation of more reliable records by eliminating inaccurate information, the miniaturized electronics-incorporated drug delivery systems could protect against the overdose of drugs or increase patients' compliance via providing controlled and targeted drug delivery in a more precise fashion leading to the reduced dose and dosage frequency and improved treatment outcome at low energy consumption and costs. In recent years, the capabilities of 2-D Ms for conjugating with a variety of molecules (via non-covalent or covalent binding) or bio-imaging have attracted considerable interests. GO with broad surface area, suitable biocompatibility, solubility, and stability as well as the capability of loading drugs by chemical conjugation or physisorption appears as a promising carrier for delivery of drugs. In the pharmaceutical industry, designing the controlled release oral products has usually been a challenging issue. Application of the electronics-based technologies for controlling and integrating the multiple source-based data appears quite helpful for more reliable and precise control of drug delivery within the gastrointestinal (GI) tract [69]. For development of the programmable electronic systems for oral delivery, the elements such as drug reservoir, fluid pump, microprocessor, temperature and pH sensors, and

receiver/transmitter (transceiver) for wireless communications are incorporated into the systems leading to the accelerated in vivo assessment of drugs which are delivered at exact rates and targets. It would also be possible to continuously measure and record the pH, temperature, or drug residence time in the specific parts of the GI tract. Electronic transdermal delivery of specific drugs (e.g., wireless patches for transdermal applications) could make a key contribution to the clinical practice that might be due to the improvement of drug delivery efficiency as compared to the traditional routes. Because of the remarkably broad surface area, 2-D nanomaterials are promising carriers for delivery of therapeutics including the anticancer ones. Another MXene family member, 2-D niobium carbide, can be applied as biodegradable 2-D photo-therapeutic vehicle for PT eradication of tumor. Surface modification with polyvinyl pyrrolidone improves the biocompatibility and stability of the nanosheets [70].

Theranostics potentials of 2-D Ms against the COVID-19

COVID-19 pandemic has induced negative impacts on the healthcare systems or other global infrastructures. Special characteristics of the pathogen necessitates developing more suitable theranostics. Nanotechnology-based advancements enable providing advanced platforms and techniques for acquiring a better knowledge of disease pathophysiology and more efficient treatment outcomes. Because of the suitable physicochemical characteristics which facilitate cell membrane penetration, targeted delivery of theranostics, improved drug bioavailability, and reduced drug adverse effects or resistance, nanomaterials particularly the multivalent and immune-targeted ones could be applied against the coronavirus-induced infections [71]. Application of the scalable nanomaterials with capabilities of penetration into the tissues, accelerated detection or killing the virus, genome editing, or smart therapeutic delivery might be of remarkable importance against the treatment or management of disease. Gp as one of the most investigated 2-D Ms with superior electronic characteristics and high surface-to-mass ratio, has been suggested as a promising candidate for detecting or fighting against the bacterial infections which have shown resistance towards various drugs. Its capability of light absorption is of great significance for sterilization of Ms or heat generation. Furthermore, the presence of oxygen on Gp surface provides appropriate sites for functionalization with nucleic acids, proteins, or enzymes [72].

2D materials for disinfection

Pathogens like bacteria and viruses as well as organic and inorganic wastes are considerable environmental pollutants causing health problems. For example, illnesses caused by *Escherichia coli* (*E. coli*) and transmission *via* contaminated water brings about many childhood deaths worldwide. Conventional bacterial and viral disinfection approaches such as ultraviolet (UV) light, chlorination, and ozonation reagents can usually be ineffective due to environmental pollution, toxic byproduct generation, high energy consumption, and related cost. Besides, it is not practical to directly use natural enzymes like peroxidase as antimicrobials because of poor stability, high production cost and complicated purification [73]. Thus, 2D materials such as GO, MoS₂, and MXenes with much more favorable intrinsic material properties were explored by researchers, and their innate antimicrobial behaviors have been investigated over the last decade. They exhibit large specific surface area, remarkable stability, good catalytic activity, minimal cytotoxicity, and unique energy-conversion ability. Several groups have suggested that 2D materials possess photo-induced antimicrobial activity by inducing oxidative stress on pathogens *via* the generation of reactive oxygen species (ROS) and photothermal effect *via* the activation by near-infrared light (NIR) [74].

2D materials as nanotherapeutics against pathogens

The design of new drug delivery systems for antimicrobial therapy focuses on being affordable and lowering the adverse side effects of antimicrobial drugs when patients take high drug doses. In order to achieve such a goal, nanotechnology-based drug delivery systems represent an essential option to achieve because 2D materials may offer unique physicochemical properties such as high surface area,

ease of chemical functionalization and photoactivity. Thanks to these properties, 2D materials show antimicrobial activity through different mechanisms

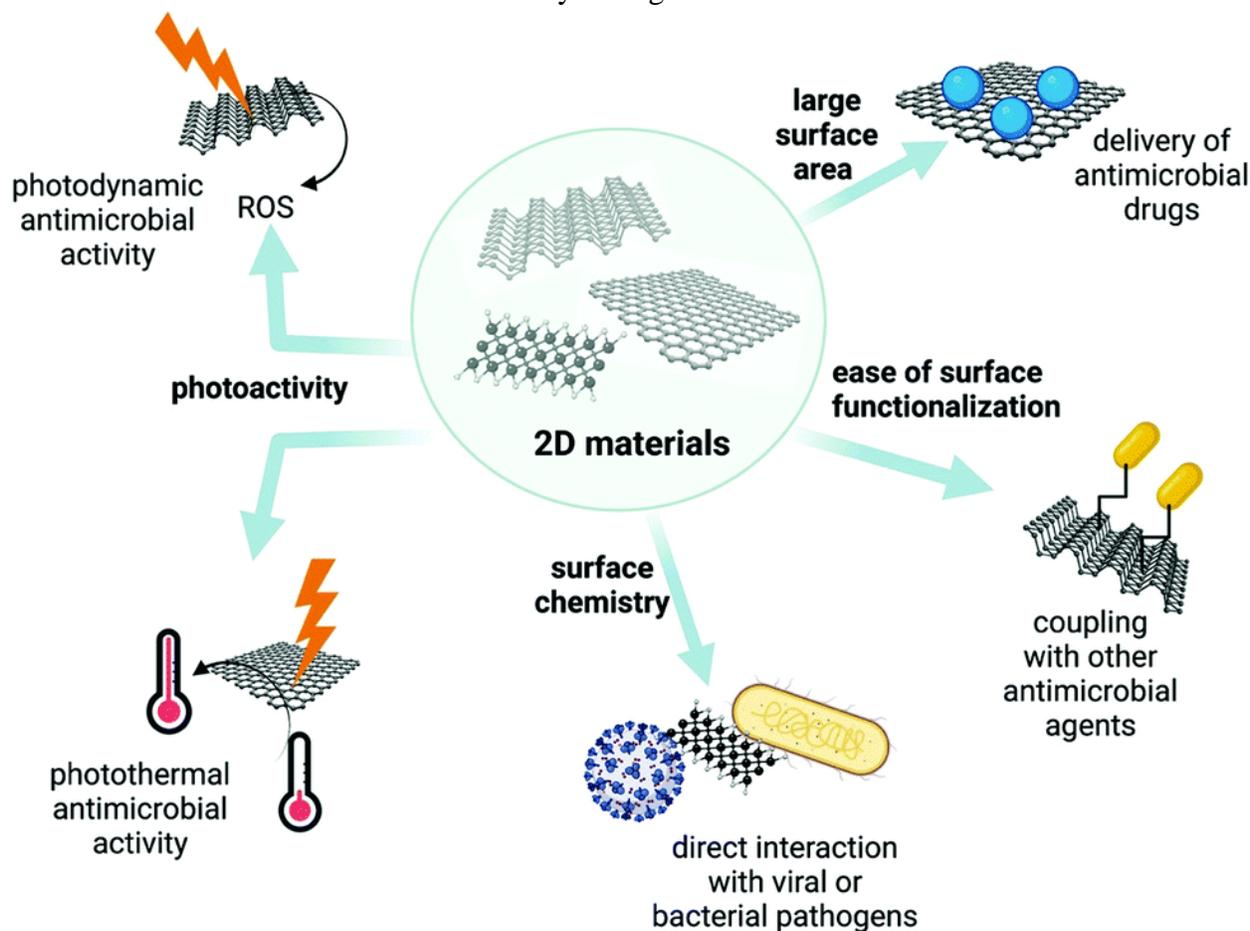


Figure 10: Intrinsic properties of 2D materials allow their use in antimicrobial applications.

2D materials have unique optical, electrical, and mechanical properties enabling their use in antimicrobial applications. The large surface area allows efficient delivery of antimicrobial drugs. The ease of surface functionalization enables the coupling with other antimicrobial agents. Due to their surface chemistry, 2D materials show direct interactions with pathogens. Finally, their photoactive properties allow their use in photothermal or photodynamic antimicrobial applications [75].

Application of 2D in environment

Two Dimensional (2D) materials have appeared as a novel material platform due to their unique properties such as high surface area, large reactive sites, flexibility, tunable configuration to change the band gap, thickness at the atomic level, high conductivity, magnetic and fluorescence. These unique characteristics of the 2D materials make them an exceptional candidate for various end applications mainly environmental remediation, energy, and biomedical application. Since the discovery of single-layer graphene using mechanical exfoliation method by Andre Geim and Kostya Novoselov [76], a new era of 2D materials has led that aided advantages in developing a next-generation innovative device with miniaturization and flexibility by assembling a single nanosheet. Moreover, high surface area with enormous active sites to move electrons, and mechanical stability are incorporated advantages of 2D materials. Numerous 2D materials such as Transition Metal Chalcogenides (TMDs), MXene, WS₂, silicene, germanene, and phosphorene are another class of 2D materials having a surge of scientific and engineering interest as

these materials are fulfilling the demand of advanced materials for energy, environmental, and biomedical application. Additionally, their cutting edge properties such as reduction/oxidation ability in-plane electric conductivity, high reactivity, and high biocompatibility significantly aided advantages for energy and biomedical applications. In this concern, electronic structure modulation with changes in the design and synthesis process of 2D materials to create featurerich functional micro-architectures for sustainable energy, clean technologies, and biomedical applications remain a challenge. In this context, researchers continue to develop newer strategies to synthesize 2D materials that efficiently improve applicability in end applications [77].

Various synthesis methods such as mechanical/ liquid exfoliation, microwave synthesis, Chemical Vapor Deposition (CVD), hydrothermal, and self-assembly etc., have been used for the development of 2D materials. CVD is the most widely used method to synthesize the high-quality 2D material without defects or vacancy in the electronic structure. Moreover, the self-assembly method has attracted other methods for the synthesis of 2D materials because 2D-nano-architecture lacks intermolecular interaction such as hydrogen bonding or hydrophobic interaction during layer assembly that reduces agglomeration and restacking, thereby well-defined nano-architecture. The process of self-assembling is different in the case of 2D material as this material exhibits wide distributed in-plane shape, and size. However, the other process is limited by their severe restacking and irreversible aggregation. In this regard, tailoring the geometry of nano-architecture with exploiting the material properties is one of the significant tasks to design several nano-composite materials for next-generation materials for energy, environment, and biomedical application [78].

2D materials for environmental remediation

2D materials offer a new avenue to explore high-performance filtration materials with high permeability and selectivity compared to other nanomaterials. Controlled pore size distribution, functional sites, and creation of heterojunction to lower the band gap can be utilized in separation process using 2D materials. Numerous studies focused on synthesizing several 2D materials for environmental remediation application; for example, Ikram, et al. [79] synthesized MoS₂ nano petals for dye degradation. Iqbal, et al. [80] synthesized La and Mn-co-doped Bismuth Ferrite/Ti₃C₂ based composites for photodegradation of Congo red dye. Another study by Zhu, et al. [81] synthesized MOF on BiOBr based 2D-nanosheet to degrade rhodamine, methylene blue, and methyl orange dye. These studies are based on 2D-nanosheet, and their composite for efficient degradation of various organic contaminants attributed active sites of the 2D materials binds with analyte and also create heterojunction. The heterojunction reduces the band gap position of CB and VB that improve photoelectron adsorption in visible range and degrade organic contaminants by taking part in redox reactions, subsequently support in the removal of contaminants from water

2D materials for energy applications

2D materials possess several unique properties such as mechanical robustness, high surface area, functional sites, and mass transport in advanced electronic devices. The working mechanism behind the success of 2D material in energy storage is based on their ability to capture charge and effectively transport or store it inside the structure or migrate through the ions on the surface. Researchers found several ways, such as doping, intercalation, altering the chemical composition, etc., to enhance the spacing of the layers of 2D materials to store or transport charge to control charge effectively. To synthesize a promising electrode material, foreign ions can be intercalated between the layers of 2D materials as the layers are stacked together through weak interactions, which allow ions or molecules to pass through them or store inside them to form active sites [82]. The particle size and morphology are also significant to enhance charge storage performance. For example, Feng et al. synthesize MoS₂ nanoflake having curves

to form nanotube-like morphology. This morphology allows Li^+ to intercalate easily and increase the battery performance compared to MoS_2 nanosheets. Another study by Teng, et al.[83] synthesized MoS_2 nanosheet grown over graphene. The MoS_2 is grown vertically over graphene using the hydrothermal method. This creates an enormous oxygen functional group on the surface result in enhance charge transport, subsequent high-rate performance, and cycling stability as lithium-ion battery electrodes. Liu synthesized V₂C MXene by self-discharge method for hybrid batteries that allows Li ions to pass through the interlayer space and increase the spacing between the layers, which provides ample space for ion diffusion. These studies suggest that the intercalation of foreign ions enhances battery performance by increasing the gap between layers to facilitate ions' transport in advance battery performance [84].

Future perspective:

The future of "The Chemistry of 2D Materials from Graphene to Beyond" holds immense potential for advancing science and technology. Researchers are expanding the library of 2D materials beyond graphene, focusing on transition metal dichalcogenides, boron nitride, phosphorene, and MXenes. These materials offer diverse properties that can be tailored through functionalization, doping, and defect engineering. The integration of 2D materials into next-generation electronics and optoelectronics promises breakthroughs in flexible devices, ultra-fast transistors, and quantum computing components. Additionally, their applications in energy storage and conversion, such as high-capacity batteries, supercapacitors, and photocatalysts for hydrogen production, are revolutionary. In environmental science, 2D materials are being explored for water purification, pollutant sensing, and bioremediation. Their biocompatibility also opens doors in biomedicine for drug delivery, diagnostics, and tissue engineering. Industrially, they enhance the strength, flexibility, and functionality of nanocomposites, coatings, and 3D-printed structures. Advances in computational modelling and AI are accelerating the discovery and optimization of 2D materials, while challenges like scalability, stability, and sustainability are being addressed through innovative green chemistry approaches. The multidisciplinary integration of 2D materials, from It to aerospace, marks a transformative era in material science, with applications that promise to redefine technology and sustainability.

Conclusion:

In conclusion, the chemistry of 2D materials, from graphene to beyond, represents a transformative frontier in material science with vast implications for technology, energy, health, and the environment. These materials, with their extraordinary mechanical, electronic, and chemical properties, have demonstrated the potential to revolutionize numerous fields. By expanding the scope of 2D materials to include transition metal dichalcogenides, boron nitride, MXenes, and other emerging compounds, researchers are unlocking unprecedented opportunities for innovation across multiple disciplines. Functionalization, doping, and defect engineering continue to enhance their tunability, making them adaptable for highly specific applications. From next-generation electronics and sustainable energy solutions to advanced biomedical applications and environmental remediation, 2D materials are paving the way for a smarter, more efficient, and sustainable future. Their integration into flexible devices, ultra-fast transistors, quantum computing components, and renewable energy systems highlights their role in addressing global technological and environmental challenges. Furthermore, their potential in water purification, pollutant detection, and biocompatible medical applications demonstrates their versatility and value in improving human health and environmental sustainability. Addressing critical challenges, such as scalability, stability under ambient conditions, and the environmental impact of their synthesis, remains vital for the widespread adoption of these materials. Advances in green chemistry, machine learning, and computational modelling are expected to accelerate the discovery of novel 2D materials and their optimization for industrial-scale applications. The multidisciplinary integration of these materials into

fields like aerospace, artificial intelligence, and the Internet of Things (IoT) underscores their potential to redefine the boundaries of modern technology. As research continues to bridge the gap between laboratory studies and real-world implementation, the future of 2D materials is poised to bring about groundbreaking advancements that can reshape industries, drive sustainable innovation, and address pressing global challenges. This transformative journey from graphene to beyond promises to establish 2D materials as a cornerstone of 21st-century science and technology.

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