

ROADMAP

The 2D materials roadmap

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Abstract

Over the past two decades, two-dimensional (2D) materials have rapidly evolved into a diverse and expanding family of material platforms. Many members of this materials class have demonstrated their potential to deliver transformative impact on fundamental research and technological applications across different fields. In this roadmap, we provide an overview of the key aspects of 2D material research and development, spanning synthesis, properties and commercial applications. We specifically present roadmaps for high impact 2D materials, including graphene and its derivatives, transition metal dichalcogenides, MXenes as well as their heterostructures and moiré systems. The discussions are organized into thematic sections covering emerging research areas (e.g. twisted electronics, moiré nano-optoelectronics, polaritronics, quantum photonics, and neuromorphic computing), breakthrough applications in key technologies (e.g. 2D transistors, energy storage, electrocatalysis, filtration and separation, thermal management, flexible electronics, sensing, electromagnetic interference shielding, and composites) and other important topics (computational discovery of novel materials, commercialization and standardization). This roadmap focuses on the current research landscape, future challenges and scientific and technological advances required to address, with the intent to provide useful references for promoting the development of 2D materials.

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1. Introduction

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The advent of two-dimensional (2D) materials has revolutionized condensed matter physics and materials science, offering unprecedented opportunities to explore exotic physical phenomena, engineer novel functionalities, and address critical technological challenges across diverse fields. Over the past two decades, the exploration of 2D materials has expanded beyond graphene, encompassing a vast library of atomically thin crystals and their heterostructures. These materials exhibit extraordinary electronic, optical, thermal, mechanical, and chemical properties, and hold promise for breakthroughs in electronics, optoelectronics, quantum technologies, energy storage, catalysis, thermal management, filtration and separation, and beyond. Many exciting new physics and phenomena continue to emerge, while select 2D materials, such as graphene, h-BN, and the semiconducting transition metal dichalcogenides (TMDCs), are transitioning from laboratory-scale demonstrations to industrial applications. In this context, a holistic understanding of synthesis, structure-property relationships, integration, and performance optimization is essential. This roadmap reviews the multifaceted challenges and opportunities in 2D materials research, focusing on the synthesis, properties and applications of representative systems including graphene and its derivatives, TMDCs, MXenes as well as their heterostructures and moiré systems.

Scalable and reliable synthesis

As research on many 2D materials progress beyond the 'laboratory demonstration' phase, the consistent and scalable production of high-quality materials has become a critical bottleneck. This challenge is equally relevant to fundamental research, where precise control over structure, doping, strain, and contamination is required, and commercial applications, which demand large-scale production while maintaining material integrity. To address this challenge, we see two pathways. The first is the robotic automation of mechanical exfoliation and stacking to reproducibly produce microscopic single-crystal (SC) flakes. This versatile approach offers an unprecedented ability to rationally design and fabricate 2D

material assemblies with customized configurations. Provided that transfer-induced inhomogeneities can be minimized, this approach would provide sufficient throughput for fundamental research and some customized high-end devices.

The second approach is wafer-scale synthesis of 2D SC films (e.g. graphene, TMDCs and Moiré materials) or large-scale cost-effective production of bulk micro-flakes (e.g. graphene oxides (GO) and MXenes), representing a mainstream solution to the industrial production of materials that inherit the superlative properties demonstrated with microscale flakes. Technological progress requires not only the precise growth and transfer of large-area high-quality crystals, but also the development of complete pathways to heterogeneous integration, quality control and cost reduction at every process stage. Another perspective is to combine the two approaches towards automated wafer- or even roll-to-roll (R2R) based lamination systems, creating large-scale heterostructures on demand. In addition, the issues such as limited controllability, environmental pollution, and high cost in the mass production of micro-flakes necessitate the urgent development of novel, more eco-friendly synthesis techniques.

New directions in synthesis research are emerging to refine synthesis control and deepen our scientific understanding. Site selective synthesis of microscale 2D crystals via direct growth on patterned substrates is a growing topic of interest as a pathway to avoid complications of layer transfer. Electrochemical exfoliation has shown a great potential for the sustainable, low cost, and controlled large-scale synthesis of micro-flakes. To transition from empirical, trial-and-error methods to scalable and application-specific synthesis, a shift toward data driven strategies is underway. Artificial intelligence (AI)-assisted simulations of growth dynamics in combination with operando characterizations and real-time process control will substantially improve the yield, consistency and repeatability.

Discovery of novel 2D materials

In addition to the controllable synthesis of established materials, the discovery of novel 2D materials is an exciting frontier. Density functional theory (DFT) and first-principles calculations have become powerful tools for predicting the stability, properties, and potential applications of hypothetical 2D materials—especially those without bulk counterparts. AI-driven approaches will undoubtedly play a crucial role in this field by integrating machine learning (ML) algorithms with high throughput computational screening. However significant challenges persist. Realistic assessment of synthesizability and stability, accurate modelling of moiré materials and reliable predictions of electronic/magnetic properties

remain open questions. This necessitates further and close collaboration between computational and experimental scientists.

Van der Waals (vdW) and three-dimensional (3D) assemblies

Moiré materials are at the forefront of research in strongly correlated electron systems, including unconventional superconductivity and topological phases, offering immense potential for applications in quantum electronics, photonics, and polaritonics. However, many challenges persist in understanding and manipulating these exotic quantum states, including establishing direct correlation between the atomic-scale properties and emergent mesoscopic phenomena, developing robust sources and detectors for non-classical states of light, new theoretical frameworks for modelling strongly correlated and topological states, and advancing computational methods for predicting multi-electron interactions.

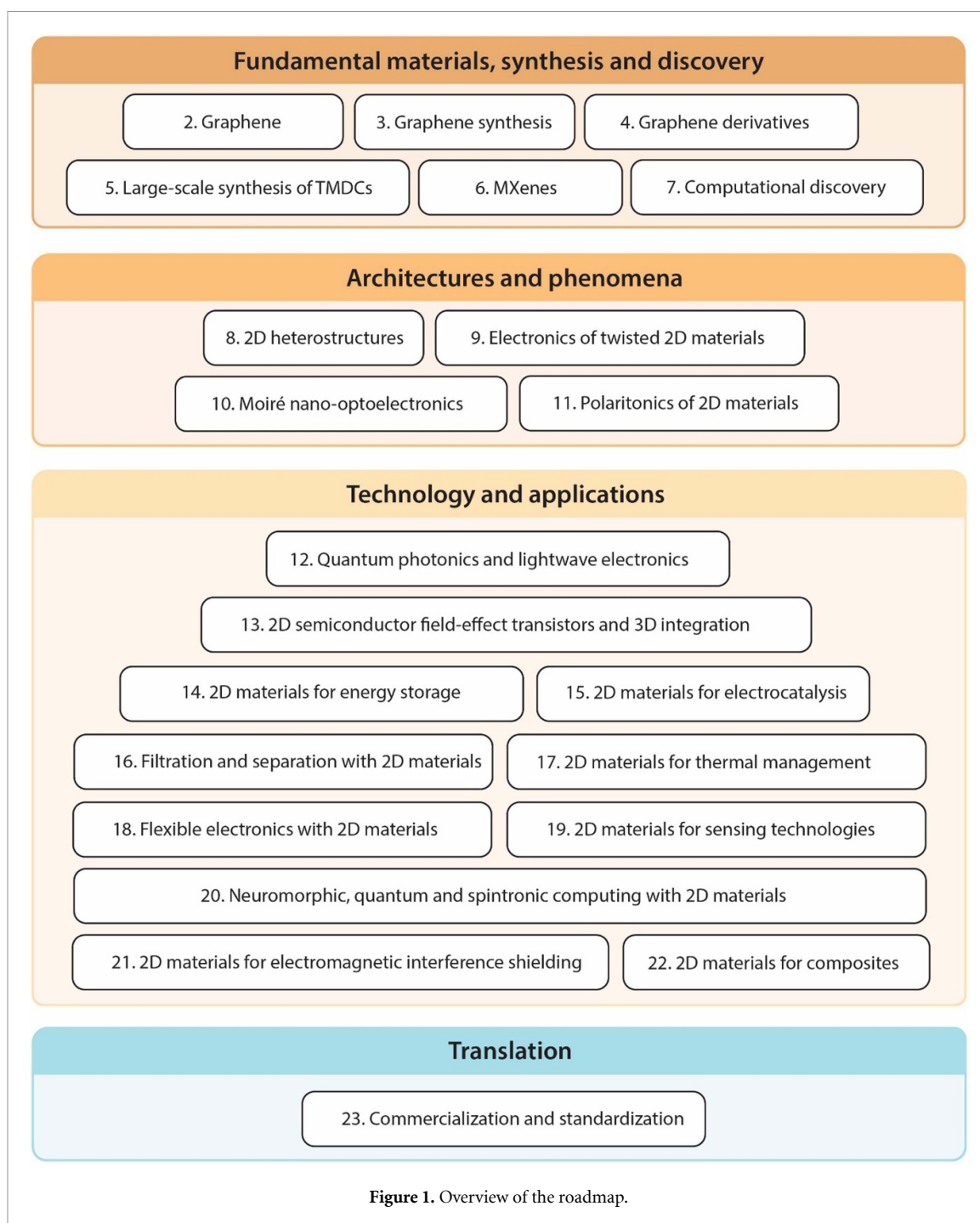
Similarly, the fabrication of 3D assemblies significantly expands the application of 2D materials in areas such as energy storage and thermal management by enhancing their functionality and compatibility. However, a lack of comprehensive structure-property mappings hampers precise engineering for tailored properties and the realization of new functionalities. The complex hierarchical structures and dynamic operational behaviours of 3D assemblies necessitate multimodal characterization techniques to decode their intricate architecture and correlate them with macroscopic properties. To advance this field towards consistent and scalable production of high-quality materials, it is necessary to develop new techniques for controlling their properties as well as advancing theoretical modelling capabilities for understanding and predicting new properties in emerging materials and systems. The integration of AI with advanced characterization and modelling tools will be pivotal for addressing challenges in microstructural recognition and property prediction.

Real-world applications

2D materials have demonstrated their potential to deliver transformative impact on diverse applications including, but not limited to, electronics, optoelectronics, energy storage, catalysis, filtration and separation, thermal management, flexible electronics, sensing, electromagnetic interference (EMI) shielding, and composites. To date, several applications such as thermally conductive films, functional coatings, and conductive additives for lithium-ion batteries have been commercialized. A key consensus within the 2D materials community is that scalable production of 2D materials with consistent properties is essential for realizing real-world applications. Furthermore, field-specific challenges must be addressed to bridge the gap between laboratory-scale

demonstrations and industrial implementation. In electronics, the integration of 2D materials into 3D device architectures has emerged as a groundbreaking approach to overcome the limitations of traditional silicon-based technologies. This enables the development of task-specific, energy-efficient, and versatile electronic systems, making it a promising candidate for next generation device components for storage and computation. To realize the vision of industrial-scale adoption, research and development efforts must prioritize scalable and reliable fabrication processes, which require holistic solutions across material, process, and architecture dimensions. For interdisciplinary fields such as flexible electronics, neuromorphic computing, quantum technologies, spintronics, and sensing, advancing material property engineering, improving mechanistic understanding, scaling up high-performance device fabrication, and integrating with mainstream architectures are essential for commercialization. For energy storage, electrocatalysis, filtration and separation, thermal management, EMI shielding, and composites, future efforts should be devoted to improving performances at relatively low cost to compete with existing technological solutions. Application-driven design and long-term stability should be prioritized in optimization efforts, which require precise structural control of both the materials and their assemblies. This structural and process optimization should be based on in-depth mechanistic insights, which will benefit from the combination of atomic-scale characterizations, real-time simulations and progress in theory and modelling. The development of hybrid systems and novel 2D materials may offer pathways to resolving fundamental trade-offs in performance, scalability and selectivity while operating under realistic conditions. In this process, identifying critical and irreplaceable applications for 2D materials remains a high-priority task for researchers in academia and industry alike. In addition to addressing the above technical challenges with an increased focus on reproducibility and consistency, establishing accurate international standards is crucial for efficient communication across the commercialization chain. While terminology and measurement standards are under development or have been published, a coherent, hierarchical structure of international standards is needed to finally achieve commercialization of 2D materials.

The 2D Materials roadmap marks a decisive transition in the field of 2D materials research from isolated studies of individual materials, phenomena, and processes toward comprehensive, application-oriented development strategies. Building on recent advances in synthesis, computational methods, and system-level integration, the research community is now in a position to realize the full potential of 2D materials. This can and should



enable a new generation of advanced and sustainable technologies, but will require sustained interdisciplinary collaboration and a concerted effort to translate into tangible societal and industrial impact.

In this roadmap, research leaders assess the current status of the field as well as future challenges, goals and directions, condensed into 22 chapters as overviewed in figure 1.

2. Graphene

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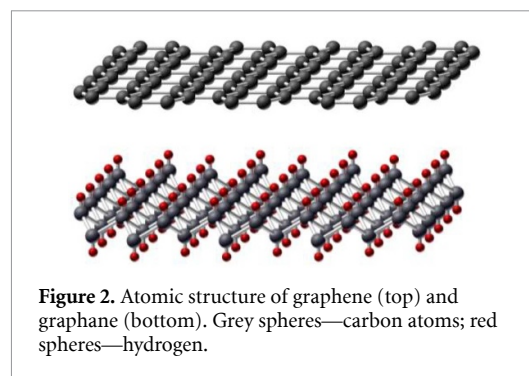
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Graphene [1] is probably one of the simplest possible materials—monolayer of carbon atoms (and carbon is one of the lightest atoms) arranged in a honeycomb lattice, figure 2. And yet, despite its simplicity, it is one of the most popular materials to study. One reason is the very high quality of the crystals widely available—carbon-carbon bonds are very strong, so it is relatively easy to obtain samples without any defects. Electron mobility in modern graphene devices can be as high as tens of millions $\text{cm}^2\text{V}\cdot\text{s}^{-1}$ with the mean free path of a few tens of microns at low temperatures. Another—is the linear electronic spectrum. Apart of the zero bandgap, which ensures possible applications in low-energy photonics (THz and far infrared), such linear dispersion relation provides chiral properties to the quasiparticles.

The basics

The linear dispersion relation is not unique to graphene, but graphene is the first material where the linear dispersion was demonstrated to determine the majority of the electronic and optical properties. Thus, for the large part of the spectrum (ranging from THz, practically to ultra-violet, where the deviation from the linear dispersion is not too large), the optical adsorption (and the optical conductivity) is given simply by the combination of the fundamental constants: $\pi\alpha = 2.3\%$ (here $\alpha = e^2/4\pi\epsilon_0\hbar c$ is the fine structure constant) [2]. More importantly, the linear dispersion relation implies the chiral properties of electrons in graphene—the specific relation between the electron's momentum and its pseudospin (the phase between the components of the electron wavefunction which reside at different sublattices). For electrons in graphene their pseudospin is always either collinear or anti-collinear with the momentum (depending on the valley), and it has more complex relations for bilayer graphene. This has an immediate effect on the scattering properties of electrons in graphene, as any changes of the electrons momentum would imply a change in the electrons pseudospin (sublattice composition), which would require very special symmetry of the scattering potential. This partly explains the Klein paradox (electron penetration through any rectangular barrier is always 100%) and, as a consequence, the high mobility of the charge carriers. Other consequences of the linear dispersion relation are the half-integer quantum Hall effect in graphene



[3, 4] and the chiral quantum Hall effect in bilayer graphene.

The chemistry

Honeycomb lattice of graphene implies that each of the carbon atoms has three neighbours. Thus, out of its four valence electrons, three are involved in forming the σ -bonds, leaving one electron in the delocalized π -states, which determines the electronic and optical properties of this material. However, the same electron can be utilized for the formation of yet another chemical link, thus creating new chemical compounds. Historically, the first chemical derivative of graphene was graphane [5], when one hydrogen atom is attached to each of the carbon atom (the most stable configuration being when the two sublattices of graphene are hydrogenated from two different sides), figure 2. Unlike graphene—graphane is an insulator with a few eV bandgap. Interestingly, the process is completely reversible—hydrogen can be removed (for instance, by annealing), bringing the material back to the pristine, zero-bandgap state of graphene. Later, other chemical derivatives have been demonstrated, including fluorographene (the 2D analogue of Teflon, where one fluorine atom is attached to each carbon).

One of the popular derivatives, which also offers a viable production route for graphene, is GO. Obtained via exfoliation of oxidized graphite, this material is hydrophilic (unlike graphene, which is hydrophobic, but lipophilic) and thus can form suspensions in water, which significantly simplifies its processing. GO is a rather disordered material, with a variety of hydroxyl, epoxy and carboxyl groups. The typical carbon-to-oxygen ratio is around 1.5–2.5, and can be varied to balance the conductivity and the hydrophilicity. The hydrogen bonds allow the formation of stable laminated multilayer structures, known as GO paper [6] (or graphene paper, if a succeeding reduction has been used). Such structures are very efficient for a variety of water and ion filtration applications.

The possibility of functionalisation of graphene offers multiple opportunities for the use of this 2D crystal for a variety of sensing applications. Graphene can be functionalized with various receptors, which can selectively bind certain chemicals. The process

of binding is usually accompanied with the changes in the electrical environment, which influences the electronic transport in graphene (effectively the layer of molecules on the surface act as a floating gate on the graphene channel). Since the distance between graphene and the absorbed molecules is very small, the sensitivity achieved can be significantly higher than that for similar structures based on silicon.

The use

Clearly, graphene applications are not limited only to the chemical sensors. One niche, though very important, application is the use of graphene for quantum metrology as a resistance standard. For years, III–V GaAs/AlGaAs heterostructures have been used for the measurements of the von Klitzing constant in the quantum Hall regime. Such structures, however, require complex MBE growth facilities, milliKelvin temperatures and significant magnetic fields. Graphene, grown on silicon carbide (SiC), on the other hand, demonstrates pinning of the zero Landau level, due to charge exchange with the substrate, which, in conjunction with very large cyclotron gap for massless quasiparticles, allows observation of a very high-quality quantized resistance plateau at helium temperatures and at very modest magnetic fields.

Apart from this, graphene has been following the very usual pathway of any new material in terms of applications. Applications in composites to improve strength and toughness and reduce weight become very popular. Interestingly, graphene does the same to concrete: the addition of a fraction of a percent of graphene to concrete improves its strength by up to 100% (the numbers in the literature vary from 20% to 100%). This result is extremely important for our sustainability goals, as concrete industry is one of the largest CO₂ emitters. Functional composites are being utilized as well, where graphene improves their conductivity or fire retardancy. Large amounts of graphene is now used for batteries applications as a conductive material for electrodes as well as a host for nanosilicon particles.

Graphene ink is used for printable electronics. Graphene's high thermal conductivity is now utilized for thermal management in electronic devices (in this case reduce GO paper is usually used). A number of optoelectronic applications are in the developing stage, where graphene is being adopted as an optical modulator in silicon photonic circuits. In terms of electronic applications, graphene is being tried for a variety of roles as well, from the active channel to interconnects. The recent progress in chemical vapour deposition (CVD) of graphene [7, 8] makes such applications more and more realistic.

The stack

The isolation of graphene confirmed the very possibility of the existence of single atom thin 2D

materials. This gave rise to many other 2D crystals to be isolated and studied [9]. Today we are talking about several hundred of those investigated experimentally and many more being predicted theoretically. Having access to such 2D crystals means that one can stack them into heterostructures, by placing one crystal on top of another. Interestingly, very high-quality interfaces, practically free of contaminants, could be achieved this way, so the crystals then occur in the very close proximity to each other and mainly interact via vdW forces. Sandwiching graphene with crystals that contain heavy atoms (for instance tungsten, as in WS₂) has been demonstrated to promote spin-orbit interaction in graphene. High-quality hexagonal boron nitride (hBN) is being used as a protective layer to screen graphene from the environment, as well as a very thin, high-quality dielectric for applying the gate. As the lattice constants of graphene and hBN are very close to each other (2.460 Å for graphene and 2.504 Å for hBN), if aligned, these crystals form a moiré structure (corresponding to the periodic variations of the atomic stacking between the two crystals) with a period of up to 14 nm (and even larger if hBN is allowed to be compressed, as, for instance, happens in the case of monolayer hBN). The moiré structure acts as an additional scattering potential for electrons, which results in strong spectrum reconstruction at the corresponding wavevectors. In fact, the reconstruction results in the formation of the replicas of the linear Dirac spectrum with locally linear dispersion relations as well. Furthermore, as the period of the moiré is large enough so that one can fit a flux quantum in experimentally achievable magnetic fields—it opened up the possibility of studying the Hofstadter physics in such devices [10–12].

The twist

A very special type of heterostructures with peculiar and highly unusual properties has been obtained by simply stacking two graphene layers under a small angle. The interplay between the Bragg scattering in the moiré potential and the vdW interaction between the layers leads to the formation of the flat electronic bands [13] (the specific angle at which it happens has been dubbed the magic angle and is about 1.1°). These flat bands trigger a number of electron-electron correlation effects, including superconductivity, the Mott insulator and orbital ferromagnetism.

The future

It is amazing that even after twenty years of intensive research, graphene still brings us surprises. At the same time, it is already becoming one of the platform materials, similar to silicon, being used in many areas of scientific research due to its unique properties: as a transparent electrode; as a substrate in transmission electron microscopy; as nanoreactor, etc. It is

impossible to forecast where the next breakthrough in graphene research will happen—in the study of its electronic, chemical, or mechanical properties—but one thing it is possible to predict with high accuracy: it *will* happen. A similar situation exists for the applications of this material. It looks like we have lived the full cycle: from the denial (graphene is too difficult to produce, so it is unlikely that it will be used in applications)—to euphoria (in the future everything will be made from graphene)—to disappointment (why we do not see graphene everywhere). In fact, the penetration of graphene into our life is gradual but steady, and we expect it to con-

tinue at the ever-increasing pace for the years to come.

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3. Graphene synthesis

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Introduction

Graphene has spearheaded research into 2D materials, accelerating the development of various material systems in its wake. The term 'graphene and related materials' has since evolved into a broad label that encompasses a wide range of materials. However, grouping these distinct materials together can obscure important factors. Even the simple concept of the 'cost of graphene' is often expressed in USD per ton to match bulk applications like inks and composites. This can overshadow the unique challenges and opportunities specific to high-quality graphene films (GFs) and wafers. Starting from a brief review of the progress on the synthesis of continuous films, this section discusses the challenges ahead for continuous graphene to fulfil its potential as a core material in future technology.

In 2007, small, exfoliated graphene domains ($\sim 1000 \mu\text{m}^2$) had become commercially available. The development of CVD graphene and SiC growth methods soon enabled larger films (see figure 3), with today's global providers offering large-area CVD GFs at costs $< 1 \text{ EUR cm}^{-2}$, a factor of 10^8 lower than the exfoliated, microscopic flakes initially traded on a one-by-one basis. The production of GFs has advanced to the foundry pilot line stage [14], with industrially compatible infrastructure for manufacturing of basic opto-electronic device architectures at technology readiness level approaching 8. Technological progress thereby requires not only the capability to grow large, high-quality crystals but development of complete pathways to heterogeneous integration, and adequate characterisation and quality control at every process stage.

We here review the progress in the view of holistic graphene integration pathways beyond individual process steps, as integration represents an Achilles heel of all current 2D material-based roadmaps and translation of their widely hailed unique properties to scalable technology. We structure our reflections accordingly, starting from the currently dominant 'general purpose' approach of CVD growth on Cu support and subsequent graphene transfer, to highlight a range of developments and discoveries that can serve the needs of future application-specific integration. Addressing yield and reproducibility

thereby arguably requires a deeper scientific understanding and overcoming the 'black-box' that such processing often presents by new characterisation approaches.

Current and future challenges

General-purpose GFs. The strong in-plane bonding that gives graphene its excellent mechanical properties and chemical stability comes at the cost of requiring high energy input during synthesis to achieve high crystallinity. This motivates the use of transition metal growth substrates, i.e. a catalytic CVD approach [15]. Cu was found to not only present a broad process window for monolayer film CVD [7], but subsequently also enable effective graphene release, helped by interfacial decoupling or its dissolution in etching solution. Subsequent graphene transfer allows general-purpose utilization compatible with a wide range of substrates, from silicon to plastics. Cu-based CVD has become the most widespread approach, driving a large fraction of the current graphene commercialisation, be it batch-to-batch (B2B) or R2R manufacturing processes. While much of the early work utilized polycrystalline Cu foils, substrate design has progressed to epitaxial metallisation and surface alloying, such as SC Cu(111) and CuNi(111) on sapphire wafers, in order to promote planarity and lateral graphene domain orientation control for their effective merging to a SC film.

Compared with the growth step itself, the subsequent transfer and handling of large, continuous atomically thin films remains a critical bottleneck. While progress has been made in polymer handling layers [16, 17], it still faces challenges of cracking and wrinkling and strain, especially when scaling up. The polymer and liquid solvents inevitably lead to contamination effects, compromising e.g. achievable graphene channel mobilities, and complicating further processing and functionalisation. The decoupling relies on diffusion of oxygen or water species at the interface between the graphene and the growth substrate, which significantly slows down the transfer process for high-quality, defect-free graphene. This makes dry transfer of industrially relevant graphene particularly challenging. This epitomizes the need for combined process optimisation [18], which comes with a vast parameter space, where many important parameters remain hidden. Despite progress towards streamlining and processes and robotic automation, successful transfer generally depends on skilled individuals. The economics and sustainability of transfer-based routes is also influenced by the reusability or recovery of the growth substrate and the transfer handle.

Application specific routes. While general-purpose metal-catalysed CVD and wet transfer techniques have introduced GFs to commercial markets, numerous integration challenges remain unresolved. This

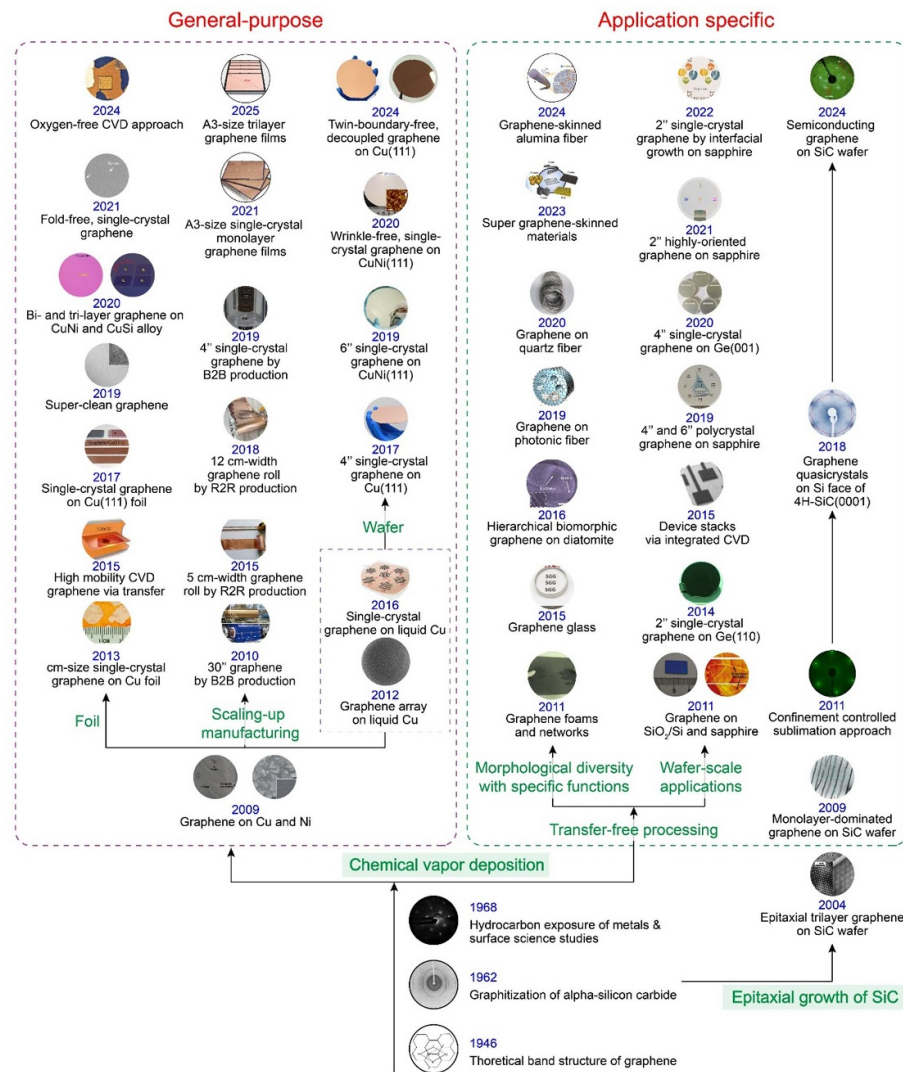


Figure 3. Development of graphene CVD processes & technology. 1946, theoretical band structure of graphene [20]; 1962, graphitization of alpha-silicon carbide [21]; 1968, hydrocarbon exposure of metals & surface science studies [22]; 2004, epitaxial tri-layer graphene on SiC wafer [23]; 2009, graphene on Cu and Ni [7, 24]; 2009, monolayer-dominated graphene on SiC wafer [25]; 2010, 30'' graphene by B2B production [26]; 2011, graphene foams and networks [27]; 2011, graphene on SiO₂/Si and sapphire [28, 29]; 2011, confinement controlled sublimation of silicon carbide approach [30]; 2012, graphene array on liquid Cu [31]; 2013, cm-size single-crystal graphene on Cu foil [32]; 2014, 2'' single-crystal graphene on Ge(110) [33]; 2015, high mobility CVD graphene via transfer [34]; 2015, 5 cm-width graphene roll by R2R production [35]; 2015, graphene glass [36]; 2015, device stacks via integrated CVD [37]; 2016, single-crystal graphene on liquid Cu [38]; 2016, hierarchical biomorphic graphene on diatomite [39]; 2017, single-crystal graphene on Cu(111) foil [40]; 2017, 4'' single-crystal graphene on Cu(111) [41]; 2018, 12 cm-width graphene roll by R2R production [42]; 2018, graphene quasicrystals on Si face of 4 H-SiC(0001) [43]; 2019, super-clean graphene [44]; 2019, 4'' single-crystal graphene by B2B production [45]; 2019, 6'' single-crystal graphene on CuNi(111) [46]; 2019, graphene on photonic fibre [47]; 2019, 4'' and 6'' polycrystal graphene on sapphire [48]; 2020, Bi- and tri-layer graphene on CuNi and CuSi alloy [49, 50]; 2020, wrinkle-free, single-crystal graphene on CuNi(111) [51]; 2020, graphene on quartz fibre [52]; 2020, 4'' single-crystal graphene on Ge(001) [53]; 2021, fold-free, single-crystal graphene [54]; 2021, A3-size single-crystal monolayer graphene films [55]; 2021, 2'' highly-orientated graphene on sapphire [56]; 2022, 2'' single-crystal graphene by interfacial growth on sapphire [57]; 2023, super graphene-skinned materials [58]; 2024, oxygen-free CVD approach [8]; 2024, twin-boundary-free, decoupled graphene on Cu(111) [59, 60]; 2024, graphene-skinned alumina fibre [61]; 2024, semiconducting graphene on SiC wafer [19]; 2025, A3-size tri-layer graphene films [62]. Figure is adapted from References [7, 19, 20], and [8, 21–62]. Reprinted figure with permission from [20], Copyright (1947) by the American Physical Society. Reproduced from [21], with permission from Springer Nature. Reprinted from [22], Copyright (1968), with permission from Elsevier. Reprinted with permission from [23]. Copyright (2004) American Chemical Society. From [7]. Reprinted with permission from AAAS. Reproduced from [25], with permission from Springer Nature. Reproduced from [26], with permission from Springer Nature. Reproduced from [27], with permission from Springer Nature. Reprinted with permission from [29]. Copyright (2011) American Chemical Society. Reproduced with permission from [30]. [insert copyright line, if specified]. Reproduced with permission from [31]. [insert copyright line, if specified]. From [32]. Reprinted with permission from AAAS. From [33]. Reprinted with permission from AAAS. From [34]. Reprinted with permission from AAAS. Reprinted with permission from [35]. Copyright (2015) American Chemical Society. Reprinted with permission from [36]. Copyright (2015) American Chemical Society. Reprinted with permission from [37]. Copyright (2015) American Chemical Society. Reprinted with permission from [38]. Copyright (2016) American Chemical Society. Reproduced from [39], with permission from Springer Nature. Reprinted from [40], Copyright (2017), with permission from Elsevier. Reprinted with permission from [41]. Copyright (2017) American Chemical Society.

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situation has driven alternative approaches. CVD on Ge, sapphire, SiC or SiO₂ substrates offers metal-free processing. However, such approaches require higher temperatures and/or result in poorer crystallinity of the graphene due to the reduced catalytic activity of the substrate. To meet these challenges, numerous efforts have been made such as confined space CVD and co-catalysis CVD. For semiconductor/dielectric substrates the complexity and importance of surface preparation typically increases, as studies on sapphire surface orientation/termination and miscuts have shown. On select stepped sapphire or e.g. Ge(110) surfaces graphene domains have been shown to align in select orientation, i.e. highly crystalline graphene can be achieved by merging of such domains.

Processing without transfer necessitates incorporation of the substrate into the device design and demands precise interfacial control, due to the high sensitivity of the exposed single-layer films to numerous external influences and imperfections. The many discoveries that contributed to the successful development of graphene growth directly on SiC via surface thermal decomposition over the last decades highlight the importance of such interface control and engineering [19]. Motivated by CMOS back-end integration, low temperature processing enabled by e.g. plasma or hot filament enhanced CVD or ALD type processes has been explored. This may lead to a significant reduction of graphene crystallinity and layer control. Localized heating is another strategy for specific applications, such as sensor platforms.

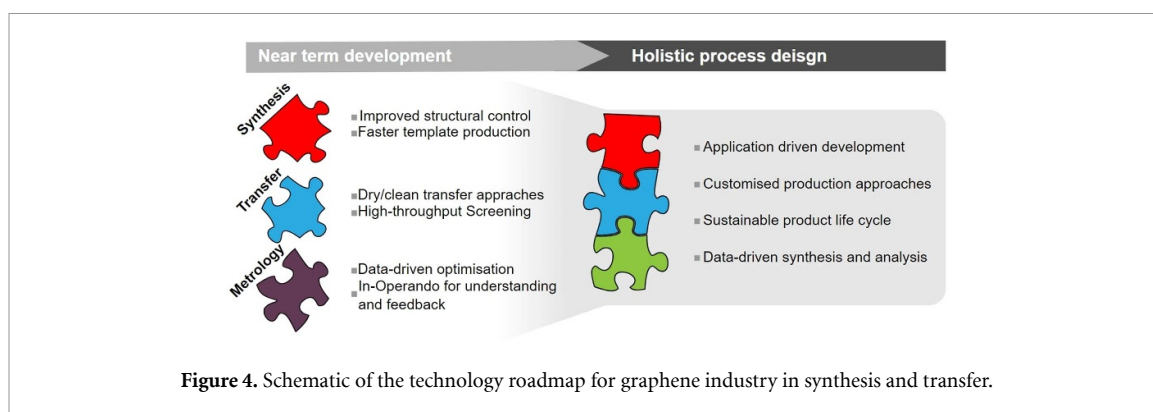
Graphene CVD synthesis generally affects the substrate and its surface, i.e. process steps should not be thought as being just additive. Rather, system design is required, and holistic approaches need to be tailored and matched to application specific requirements. The ‘Catch 22’ is that more specific development tends to spring from more specific application pull. While for general purpose growth the graphene quality is typically seen in ‘absolute’ terms, e.g. single crystallinity/defect density, for application specific growth it is the functionality, robustness and consistency achieved with graphene in the concrete application scenario that should be taken as a measure.

Transfer-free integration with direct graphene CVD on metals that form part of the device structure, such as on ferromagnets for spintronics, ferroelectrics in memristors or as diffusion barrier on contacts, but also graphene-skinned materials that cultivating on engineering materials with various morphologies, such as glass fibres, powders, 3D metal foams, and zeolites [58], present diverse examples where CVD process integration pathways have started to be explored.

Advances in science and technology to meet challenges

Industrial production of graphene materials is the prerequisite for the commercialization of graphene products and motivated scientific research in this field (see figure 4). Improving quality control and reducing production costs are long-term critical concerns in the materials industry. Currently, the expense associated with producing continuous GFs and wafers exceeds market demand, limiting their industrial applications. The field is still far from being able to scale-up all the superlative properties demonstrated at small flake level for individual ‘hero’ devices, using complex, often manual assembly strategies. Increasing automation of R2R or B2B will be crucial for production with high reproducibility [63]. Technological maturing requires standardisation that also feeds into health and safety protocols. This reflects a need for scalable screening methods not only for the general-purpose route but supporting each tailored process development step.

Arguably, graphene is the major model system for process development at atomically thin level. The vast parameter space, intrinsic and extrinsic disorder and distinct reaction kinetics need more scientific underpinning. The story of synthetic graphene clearly highlights that the empirical, trial-and-error development is inadequate in terms of reaching stable, cost-effective application scenarios. Today, growth control is mainly limited to monolayers. Achieving bilayer and few-layer (3–10 layers) graphene with high uniformity and controlled stacking order remains fundamentally challenging, primarily due to



uncontrolled adlayer nucleation and complex growth kinetics between the basal plane, edges and defects of pre-existing layers. This underscores the need for **novel theoretical frameworks** to capture the extreme reaction anisotropies of 2D materials and to serve as basis for **novel reaction design** to effectively exploit rather than combat such strong anisotropy for controlled atomic scale processing.

Different applications also require varying graphene properties. To proceed towards commercially viable graphene applications, synthesis needs to be seen in a holistic perspective as part of an increasing portfolio of process capabilities at monolayer level, including film handling and transfer, which need to tie in with diverse existing manufacturing pathways across targeted application areas. While, for instance, large-area, transparent conductive films may not demand SC graphene, they still require high-quality, homogenous films; electronic applications require significantly more uniform and clean graphene, as even minor inconsistencies can lead to issues with performance and variability. Modelling of yield, **driven by end-application performance**, will guide the optimization of graphene production processes, ensuring the highest possible device yields within specific performance thresholds. This approach will allow graphene manufacturers to **customize production** for different industries, enhancing both yield and performance across diverse applications. We also anticipate that graphene will more frequently serve as a key supporting component in an evolving portfolio of materials and applications, rather than being the primary focus or centrepiece material.

Many graphene growth processes are optimized and communicated without much concern regarding subsequent integration and performances, which limits the ability to optimize yield and reproducibility of end devices at an industrial scale. To address this, the field is shifting towards **data-driven synthesis and assessment**, where automation and improved process control will make a substantial improvement in repeatability and application specific process understanding. Incorporating real-time, *in operando* methods [64], and AI will allow for continuous feedback, analysis, and adjustment, enabling increasingly automated optimisation through statistical methodologies already prevalent in mainstream manufacturing. Such a transition is crucial for aligning the quality of graphene with the performance demands of a wide range of industries, moving from trial-and-error methods to a more systematic, scientific approach.

Improving the environmental footprint often remains an after-thought after a material/application reached mass market. **Sustainable product life cycle design** has driven the exploration of carbon source alternatives to highly purified gases, from waste gases to organic waste. There are many carbon waste streams and graphene growth can offer new routes to up-cycling. Therefore, eco-friendly process is another aspect that should be judged by much more holistic metrics.

Concluding remarks

At this 20 year anniversary, the celebrations often focus on the fundamental science discoveries in properties and functionalities. If the 2D material

research and innovation communities are serious about impactful commercialization, much more appreciation and attention should be given to the science of crystal growth and scale-up, keeping integration and the needs of the end-application in mind. Automation, high-throughput and *operando* characterization approaches now allow us to go beyond ‘black-box’ reactor and process calibrations, allowing us to make a large leap from ‘black magic’ to systematic, data-driven science.

Acknowledgments

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4. Graphene derivatives

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Status

Graphene derivatives, chemically modified or structurally altered forms of graphenes, are designed to enhance or diversify the already remarkable properties of graphenes for various applications. Their exploration dates back to 1859, with the discovery of graphite oxide, long before pristine graphene was isolated in 2004 by Andre Geim and Konstantin Novoselov. These derivatives are especially valuable due to their chemical versatility and ease of production. For instance, GO is notable for its dispersibility in water and potential for chemical modifications, making it ideal for use in energy storage, flexible electronics, and biomedical applications. Reduced graphene oxide (rGO), which is produced by deoxygenation of GO, restores part of the sp^2 carbon network, providing a balance between conductivity and functionality for electronic devices and sensors.

As graphene derivatives continue to evolve, researchers are exploring new structural forms that enhance their functionality and open new application areas. One important advancement in this field is the development of 3D graphene derivatives, in which graphene nanosheets—typically GO or rGO—are assembled into 3D structures, such as fibres, membranes and aerogels. The added structural variety introduces valuable features. For example, the nanoporous network, particularly the nanochannels formed between two adjacent layers, creates a transport pathway for ions and molecules, thus enabling the applications such as ion/molecules sieving and separation [65]. Their flexible carbon skeleton also supports rapid electron transfer and electromechanical responses, making them highly beneficial for the development of wearable electronics, where flexibility, lightweight, and quick response times are crucial [66]. Additionally, these structures enhance composite materials by improving interlaminar strength,

adhesion, and toughness in polymers, and aiding stress relief and phase control in metal matrix and ceramic composite.

The ease of processing and diversity in properties make graphene derivatives integral to many large-scale commercialized products, including composites, anticorrosion coatings, separation processes, and energy storage. Over the next decade, various commercial graphene products are expected to emerge, underscoring the critical importance of ongoing research in graphene derivatives.

Current and future challenges

Over the past years, a range of graphene derivatives have been developed, each presenting unique challenges. Here, we specifically focus on the challenges associated with graphene derivatives used in large quantities for practical applications, particularly GO, rGO, and their assemblies. While our review centres on these specific materials, the insights and challenges discussed may also be relevant to other graphene derivatives.

Large-scale, cost-effective production with controlled and consistent quality. The variability in production quality arises from the complexities in controlling the synthesis and functionalization processes of graphene materials. For instance, the nonstoichiometric nature of GO and rGO results in varying ratios of carbon, hydrogen, and oxygen. These variations pose fundamental issues in determining the reproducibility of rGO by just comparing the atomic ratios of each sample, making it difficult to evaluate the consistency of product quality of graphene derivatives. Additionally, diverse synthesis methodologies for rGO and its precursors lead to significant variations in their defects, clustering of functional groups, sheet size and overall composition. These variations complicate efforts to achieve good uniformity in one batch and reproducibility across different batches.

Structural characterization and control at multiple length scales. The challenges of structural characterization and control ranges from atomic structure of building blocks to the assembled stacking structure. In specific, GO, as the commonly used building blocks of graphene assembly, has a broadly understood elemental composition; however, the precise distribution and arrangement of its functional groups at the local and long-range scale remain unclear. The surface chemistry and interfacial effects of functional groups on GO—particularly their interaction with solvents—require further research to fully understand their role in regulating their assembly process. Moreover, defects, in-plane pores and corrugations of nanosheets complicate the interactions between the building blocks and the resultant stacking patterns. Consequently, structure irregularities and disorder occur at different length scales, including the

variation in the interlayer features, formation of intermediate structure unites, and the existence of large voids [67]. The difficulty to accurately characterize and describing those structural irregularities complicates efforts to precisely engineer the hierarchical structure of those assemblies to achieve optimized performances for given applications.

Establishing proper structural-property relationship. Even though advanced characterization techniques can provide insights into the local atomic structure and hierarchical organization, understanding how these structures influence macroscopic properties across multiple scales remains incomplete. For example, studies report two diverse trends of sheet size effects on the mechanical properties of graphene membranes [68]. These seemingly controversial discoveries indicate how this lack of comprehensive structure-property mapping hampers the precise engineering of graphene derivatives for targeted applications.

Exploring new properties and translating it into real-world applications. Studies have shown that graphene derivatives hold great promises in many advanced applications including flexible electronics, energy storage, and ion separation. However, in most studies, only principal concepts have been demonstrated. Gap exists in the practical applicability of these materials in real-world applications. For example, graphene assemblies with controlled nanochannels have been theoretically predicted and experimentally demonstrated to exhibit ultra-fast ion transport, remarkable ion selectivity and storage properties [65]. Although these properties are promising in catalysis, energy storage and filtration field, their integration into commercially viable products remains limited.

Advances in science and technology to meet challenges

Graphene derivatives are now being produced at industrial scales, marking a pivotal era for designing graphene-based materials with broader commercial applications in the coming years. While many technical advancements and applications are discussed elsewhere in this roadmap, three often-overlooked aspects are critical for advancing graphene derivative research (figure 5)

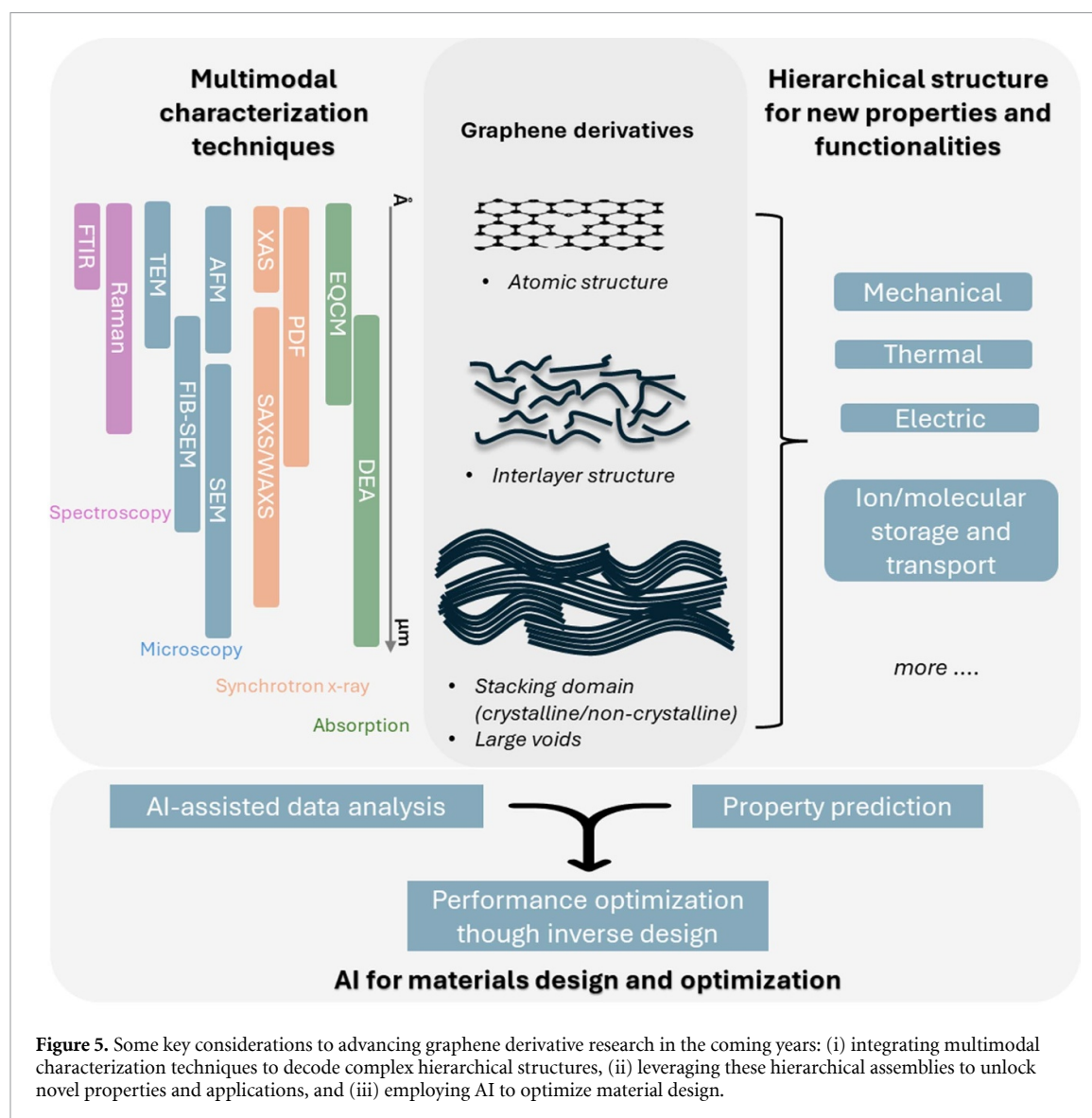
Integrating multimodal characterization techniques. Recent advancements in characterization techniques have significantly enhanced our understanding of graphene assemblies. Spectroscopic tools such as Raman and FTIR spectroscopy remain fundamental for identifying defects, sp^2/sp^3 domains, and oxygen-containing functional groups in graphene nanosheets. Microscopic tools such as SEM, AFM,

and focused ion beam SEM (FIB-SEM) provide nanoscale insights into atomic and nanoscale structure of graphene derivatives. For example, FIB-SEM nanotomography has recently been employed to reveal intricate morphological details in printed graphene networks, including porosity, tortuosity, surface area and sheet orientation [69]. Synchrotron-based methods, including XAS, pair distribution function analysis, and small-angle/wide-angle x-ray scattering, address intrinsic structural complexities of graphene assemblies by offering exceptional spatial and spectral resolution for multiscale characterizations from sub-nm to μm and enabling *in situ* and operando observations [67].

Despite these advances, the complex hierarchical structures and dynamic operational behaviours of graphene assemblies demand more integrated approaches. Fully understanding these assemblies also requires complementary methods, such as dynamic electroadsorption analysis and electrochemical quartz crystal microbalance (EQCM), which use small ions and molecules as probes to obtain pore surface area, surface chemistry and active sites [70]. Together, these techniques provide structural information at different dimensions to systematically decode the intricate architectures and correlate it with collective properties of graphene derivatives.

Harnessing hierarchical structures of graphene assemblies. Research on graphene-based bulk materials has traditionally focused on utilizing the intrinsic properties of individual graphene sheets, such as mechanical strength and thermal or electrical conductivity. However, increasing research has found that the performance of graphene assemblies is influenced more by the hierarchical organization than by the properties of individual sheets. For example, Mechanical properties and thermal conductivity of assemblies depends heavily on the inter-sheet bonding and connectivity [66]. Moreover, controlled stacking of graphene sheets creates nanochannels structures showing unique ion transport behaviours, critical for energy storage and filtration applications [71]. Particularly, the hierarchical porous structures are shown to remarkably enhance molecules/ion transport efficiency, demonstrating the importance of architectural design [72].

Structural features within assemblies can sometimes conflict, necessitating trade-offs and precise multiscale characterization and structural control. For instance, while maximizing surface area and porosity benefits ion transport efficiency, it can also reduce volumetric energy density in energy storage electrodes and ion selectivity in separation applications [73]. Advances in understanding interfacial interactions during GO assembly have enabled tailored internal microstructures, balancing surface



area and packing density. Approaches such as solvent-controlled removal and capillary compression have produced rGO hydrogels with superior volumetric performance while maintaining high gravimetric capacitance [73]. These developments highlight the need for deeper exploration of hierarchical assembly processes to unlock new applications.

Implementing AI for graphene derivative research. The structural complexity and diverse property requirements of graphene derivatives present significant challenges for material design and optimization. AI offers transformative potential in this domain through microstructural recognition, property prediction and performance optimization [74]. As the field evolves, combining AI with advanced characterization and modelling tools will be important in addressing the multifaceted challenges of graphene research. Specifically, by integrating AI with advanced

characterization techniques and computational models, researchers can correlate hierarchical structures—such as nanochannels and defect distributions—with macroscopic properties like conductivity and ion transport behaviour. This approach uncovers intricate structure-property relationships and guide the optimization of graphene assemblies, from sub-nanometre channels for high-efficiency filtration to dense nanosheet packing for next-generation batteries.

Concluding remarks

The discovery of graphene has revolutionized materials science, while its derivatives continue to expand the field's horizons with their ease of production and diverse properties. From GO's dispersibility to the newly introduced functionalities of graphene assemblies, these materials have reshaped the landscape of technological applications of graphene. However,

challenges remain in ensuring consistent production quality, precise structural characterization, hierarchical stacking controlling and real-world applications integration. Addressing these with advanced characterization, new structural control strategies, and AI-driven design will be key. As graphene derivatives and their applications transition from conceptual innovations to practical solutions, they hold the promise of revolutionizing industries and driv-

ing transformative progress in addressing global challenges.

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5. Large-scale synthesis of TMDCs

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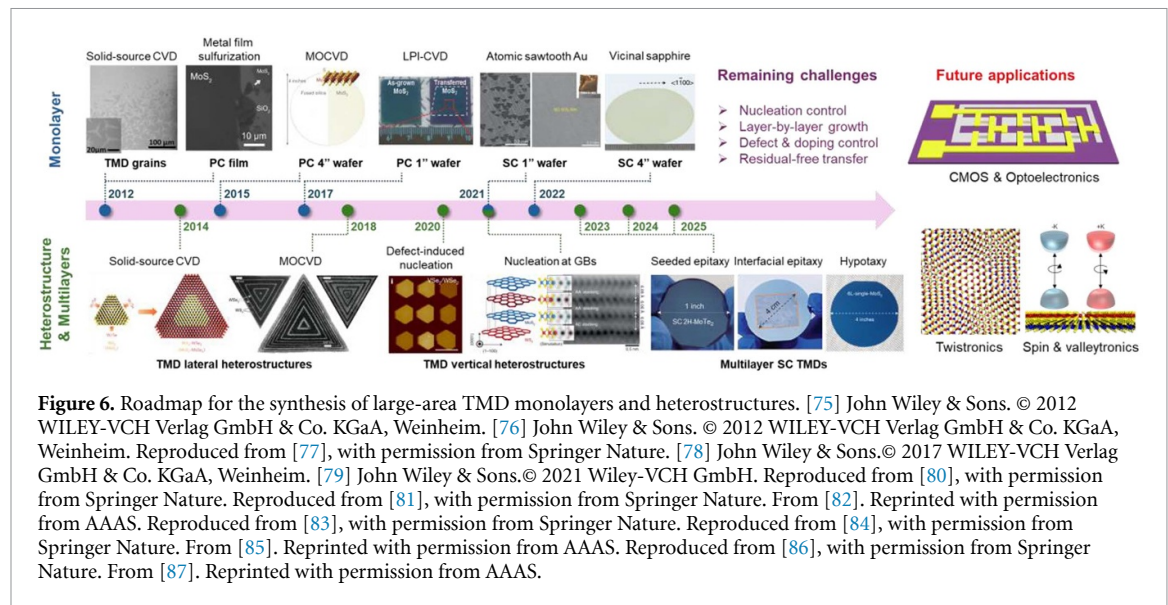
Status

Despite extensive research on the remarkable physical and chemical properties of TMDs, there are still significant challenges in large-area synthesis techniques toward practical applications. In this section, we will provide an overview of the historical development of large-area synthesis techniques for TMD materials (see figure 6).

To achieve large-area TMD films, various techniques have been applied, including pulsed laser deposition, molecular beam epitaxy, atomic layer deposition (ALD), and CVD. Among them, CVD is the most extensively studied technique for economically viable large-area TMD film synthesis. In 2012, solid-source CVD method was developed to synthesize TMD grains of a few tens micrometres in size by vaporizing or supplying transition metal oxide powder and chalcogen powder precursors [75]. At the same time, the different approach was proposed to synthesize large-area poly-crystal (PC) TMD films with uniform thickness [76]. This approach involves the deposition of transition metal films onto substrates, followed by subsequent heat treatment in a sulphur or selenium atmosphere. However, this method often produces TMD films with poor crystallinity due to uncontrolled reactions with chalcogens, leading to a substantial reduction in charge carrier mobility in the field effect transistor (FET). In 2015, monolayer PC TMD films were successfully synthesized on 4-inch wafers using metal-organic CVD (MOCVD) [77]. This approach enables precise control over the supply of volatile solid or liquid precursors, facilitating the successful synthesis of high-quality TMD films at a large scale. Furthermore, liquid-precursor-intermediated (LPI) CVD method was developed to synthesize the large-area polycrystalline TMD films by spin-coating the liquid transition metal precursor onto the substrate,

followed by controlled thermal annealing in chalcogen atmosphere [78]. This method offers precise control of the film coverage by adjusting the precursor concentration and spin coating speed, ensuring reproducibility and versatility in the growth. Moreover, different transition metal precursors are incorporated to result in the doping in TMD materials. This significantly broadens the range of potential applications. Meanwhile, recent research has progressed on the synthesis of SC TMD films to address the degradation of their intrinsic properties such as mechanical strength, chemical stability, and carrier mobility, caused by grain boundaries (GBs) in PC TMD film. As a result, single crystalline monolayer TMD films have been successfully synthesized with sizes of up to 2 inches using substrates including atomic sawtooth Au and miscut sapphire substrate [79, 80].

Lateral and vertical TMD heterostructures offer unique physical phenomena for electronic and optoelectronic devices including Coulomb drag, Bose-Einstein condensation, band renormalization, inter-layer excitons, etc. Initially, diverse physical phenomena and applications from TMD heterostructures have been investigated through the transfer of each TMD layers. The presence of residuals at the heterostructure interface during the transfer process often obscures intrinsic interface physics. Therefore, developing direct synthesis techniques of heterostructures has been highly desired to achieve clean interfaces. In 2014, TMD lateral heterostructure grains were synthesized by sequentially supplying powder precursors in a two-step process [81]. Furthermore, by utilizing the MOCVD technique, the width of the heterostructure can be precisely controlled up to a few tens nanometres [82]. On the other hand, several problems still remain in the synthesis of vertical heterostructure. Among various challenges, most important issue is the nucleation on dangling bond-free surface. To address this, artificial defects were introduced on TMD surface to enable controlled nucleation for the patterned synthesis of vertical heterostructures [83]. However, the utilization of micrometre-scale defects concerns regarding potential degradation in the intrinsic properties of TMD layers. In 2021, large-scale vertical TMD superlattice has been successfully synthesized through the nucleation at GBs within polycrystalline TMD films [84]. More recently, several strategies have been proposed to realize wafer-scale, SC multilayer TMD films. Using a 2H-MoTe₂ seed crystal, the growth of SC multilayer 2H-MoTe₂ has been demonstrated [85]. By creating opening in the seed crystal, the flux of the Te precursor was constrained to pass solely through them. Building on this concept, a hypotaxy method—replacing the seed crystal with SC monolayer graphene as the seed layer—has been established, enabling multilayer SC growth beyond 2H-MoTe₂ to additional



TMD systems [86]. It has also been reported that SC rhombohedral (3R) TMD films can be grown via precursor diffusion-precipitation, referred to as ‘interfacial epitaxy’ [87].

To date, the synthesis techniques for achieving large-area SC TMD films from monolayer to multilayer have been successfully developed. However, while multilayer SC TMD films have been successfully grown by novel approaches, the techniques for synthesizing TMD heterostructures are predominantly limited to grain growth methods and PC films. With further advancement of CVD techniques, the performance of current electronic and optoelectronic devices will be significantly improved, and the scaling issues faced by silicon-based devices could be addressed.

Current and future challenges

Progresses of TMD materials synthesis have been remarkable in the past decade for large-area TMD films. These advances are anticipated to support both 2D-material counterparts of existing applications (CMOS, optoelectronics, etc.) and entirely new paradigms exploiting phenomena that arise in twisted 2D structures and vdW heterostructures. However, despite these notable achievements, several critical challenges persist for the commercialization of large-area TMD film. In this section, we will discuss the key issues.

(i) Nucleation on dangling-bond-free surface for TMD heterostructures

To date, the synthesis techniques for TMD heterostructures have been primarily focused on the limited number of materials, and the synthesis of large-area heterostructure films has been predominantly achieved in the polycrystalline materials. Heterostructures with single crystallinity and well-defined stacking order

and orientation are deemed necessary. One important key for TMD heterostructure is the nucleation on the dangling-bond-free surface of TMD materials. While defect-induced nucleation has been developed, the recovery of film damage resulting from defect formation still remains to be solved.

(ii) Defect control in TMD materials

Despite intensive efforts to eliminate GBs in large-area TMD films, defects such as vacancies, antisites, and interstitials within grains remain abundant and insufficiently addressed. Recent advances, including two-step flux and chalcogen-monomer supply methods [88], have yielded highly crystalline TMD crystals with substantially fewer intragrain defects; however, progress via CVD remains modest in minimizing them. To address these limitations, future research should focus on achieving deterministic defect control and, where possible, defect elimination. Equally important is advancing the understanding of structure–property–performance correlations and developing high-throughput, wafer-scale defect characterization techniques.

(iii) Other issues

Various dopants could be doped in TMD materials using LPI-CVD and MOCVD techniques. Yet, the dopant uniformity is of primary concern. In addition, the current synthesis techniques require a transfer process of large-area TMD films onto another substrate prior to the fabrication of devices. In this transfer process, wrinkles and tearing on TMD films and contaminations caused by the chemical residues inevitably arise. Thus, the development of residual-free transfer techniques is highly desired.

Advances in science and technology to meet challenges

Although recent novel approaches have enabled the growth of SC multilayer TMD films, additional strategies based on alternative growth routes are still needed due to their complexity and restricted substrate comparability: (1) thickness-controlled synthesis of few-layer TMD islands followed by their coalescence, or (2) layer-by-layer epitaxy. Bi-layer SC MoS₂ film has been successfully synthesized via thickness-controlled nucleation on miscut sapphire substrates [89]. Due to the higher thickness of step edges on the sapphire substrate, coherently aligned bi-layer MoS₂ islands predominantly synthesized, resulting in the formation of bi-layer SC MoS₂ film. Furthermore, 3–5 layer SC hBN and SC rhombohedral BN films have also been synthesized on Ni (111) and vicinal Ni (100) substrates, respectively, via the coalescence of thickness-controlled BN islands [90, 91]. Thus, similar approaches could enable the synthesis of few-layer SC TMD films. The layer-by-layer homo- and heteroepitaxy is an ideal approach to synthesize few-layer SC TMD films as well as SC TMD heterostructures. Therefore, the development of techniques to precisely control the surface energy of TMD materials is highly desired, while maintaining a defect-free surface. This could offer the synthesis of various TMD materials with a precisely con-

trolled thickness. In addition, from the perspective of modulating the electronic structure of TMD materials, the development of novel doping techniques or post-processing strategies for dopant redistribution could lead to the uniform distribution of dopant elements within the film.

Concluding remarks

For the practical application of TMDs in various fields, significant advancements have been made in the development of CVD techniques for the synthesis of large-area TMD films. Nevertheless, further progress is still required for layer-by-layer epitaxy or transfer techniques that enable precise control of TMD film thickness and stacking orders for next-generation electronic/optoelectronic devices.

Acknowledgments

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6. MXenes

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Status

Since the first report on unconventional physical properties in graphene, materials with 2D morphology and one or a few atoms in thickness have been attracting increasing interest. This led to the discovery of many new 2D materials, including a family of 2D transition metal carbides/nitrides (MXenes), which continue growing and show remarkable potential in many applications. MXenes have a general formula of $M_{n+1}X_nT_x$, where M is an early transition metal, X is carbon or nitrogen, T_x is the surface terminations that bonded to the outer M layers, $n + 1$ and n is the respective numbers of layers of M and X atoms. The diverse compositions and versatile structures endow MXenes with tunable physical and chemical properties, which are useful in various applications. This article provides a brief perspective on the latest advances in synthetic methods, surface chemistry, and applications of MXenes. We further give an insight into the future opportunities for the MXenes materials.

Synthesis methods & surface chemistry

Since the first discovered MXene $Ti_3C_2T_x$ was obtained using HF to etch the Ti_3AlC_2 MAX phase in 2011, selective etching of the A-site element of MAX phases in fluorine-containing aqueous solutions has become the most widely used method to prepare MXenes [92]. Besides HF, fluorine-containing etchants such as $LiF + HCl$, bifluoride salts (e.g. NH_4HF_2), and fluorine-containing molten salts are used for the synthesis of MXenes [93]. Besides, fluorine-free etching methods such as electrochemical etching, alkaline hydrothermal etching, HCl-hydrothermal etching, halogen etching, and Lewis acidic molten salts have been developed [94]. In contrast to the above 'top-down' synthetic approaches, a direct synthetic route through the reactions of metals and metal halides with graphite, methane, or nitrogen was proposed in 2023 [95]. It enables CVD growth of MXene carpets and spherulite-like morphologies. It is important to mention that the fluidized bed CVD synthesis of Ti_2CCl_2 MXene from titanium chloride (an intermediate product of TiO_2 synthesis) and methane (natural gas) can provide large amounts of chlorine-terminated MXenes at the price level

between titania and multiwall carbon nanotubes [96], which are produced using similar processes.

The synthetic route determines the surface terminations of MXenes, enabling property tuning and broadening their application scope. Fluorine-containing aqueous etching methods inevitably result mixed $-O$, $-OH$, and $-F$ terminations. Fluorine-free etching methods enable a wide range of surface terminations. For instance, gaseous halogen etching produces halogen-terminated MXenes with uniform surface terminations [97]. The Lewis acidic molten salt etching methods can form MXenes with pure terminations of $-Cl$, $-Br$, $-I$ and their combinations [98]. Substitution and assembly of the MXene terminations in molten salts can further transform MXenes with terminations such as $-NH_2$, $-S$, $-Se$, and bare MXenes (no surface termination) [99]. Furthermore, chemical scissors-mediated structural editing, based on the molten salt chemistry, can form MXene with $-P$ and $-Sb$ terminations [100]. The rich surface chemistry of MXenes facilitates their functionalization for various applications.

Properties & applications

The 2D structure and diverse elemental constituents endow MXenes with a unique combination of properties, including a large exposed surface area, high electronic and ionic conductivity, outstanding mechanical properties inherited from bulk carbides and nitrides, and a hydrophilic nature, particularly when terminated with oxygen or hydroxyl groups. These characteristics are vital for a multitude of applications, such as electrochemical energy storage, sensing, microwave absorption, EMI shielding, catalysis, and more.

In the field of energy storage, MXenes are widely used as an electrode material for lithium/sodium/potassium-ion batteries, supercapacitors, and metal-air batteries due to its high specific capacity and rapid ion diffusion capability. For instance, $Ti_3C_2T_x$ MXene can achieve a volumetric capacitance of $>1000 \text{ F cm}^{-3}$ in supercapacitors [101], while its open interlayer channels facilitate efficient electrolyte ion transport.

In the sensing field, MXenes exhibit high sensitivity to minor strains, gas molecules, and biomarkers, making it suitable for flexible strain sensors (e.g. monitoring human motion), gas sensors (e.g. NH_3 , NO_2 detection), and biosensors (e.g. glucose, DNA detection) [102]. The abundant surface functional groups of MXene can be further modified to enhance selectivity and stability.

In the microwave absorption/EMI shielding field, MXenes effectively attenuate electromagnetic waves owing to its high dielectric loss and conductive network. Its lightweight nature surpasses traditional metal shielding materials—for example, $Ti_3C_2T_x$ can achieve an electromagnetic shielding effectiveness (SE) of $>60 \text{ dB}$ in the X-band

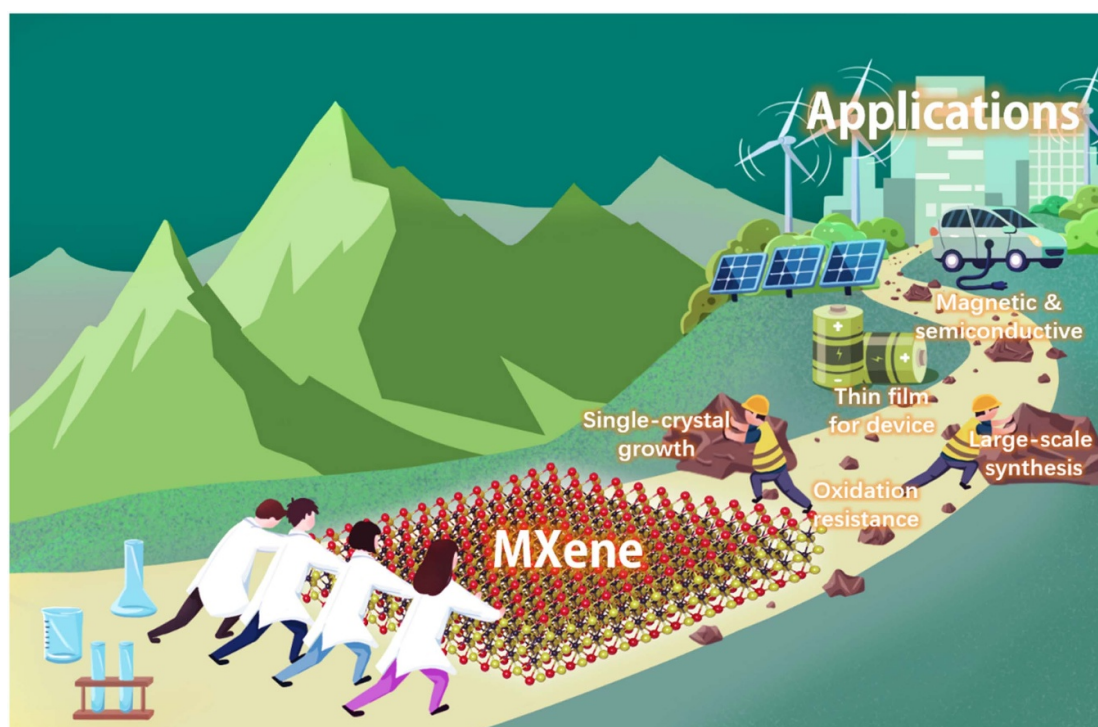


Figure 7. The challenges and opportunities for the MXenes.

(8–12 GHz), highlighting the advantage of fabricating micrometre-thin, free-standing films [103].

In the catalytic field, MXenes serve as supports or active components, demonstrating excellent catalytic activity and stability in reactions such as the hydrogen evolution reaction (HER), oxygen reduction reaction, and CO₂ reduction. For instance, Mo₂CT_x MXene acts as an efficient HER catalyst due to its low overpotential and high conductivity [104].

Although MXenes exhibit outstanding performance in various applications, the edge defects and vacancies in MXene sheets make them susceptible to oxidation. The oxidation of MXenes is usually accompanied by a decrease in electrical conductivity and mechanical properties, which further degrades their performance in applications. Therefore, researchers have dedicated considerable efforts in recent years to solving the oxidation problems. Strategies such as defect passivation, surface modification, and antioxidant solvent dispersion have been proposed to prevent MXenes oxidation [105]. These efforts are expected to advance future MXenes applications.

Outlook

The research on MXene materials is rapidly evolving, with significant advancements made in recent years. The development of new synthetic routes has greatly expanded the elemental composition of MXenes, endowing them with novel properties and enhancing their applicability (see figure 7). These advancements

also allow for better control over surface chemistry and have the potential to substantially reduce production costs. We anticipate further expansion in MXene research in the near future, with the following key issues warranting attention:

- (1) Expansion of elemental composition: the incorporation of lanthanide and actinide elements at the M-site, and non-metallic elements such as oxygen, boron, nitrogen, and phosphorus at the X-site, with multi-element terminations as T_x groups.
- (2) Structural stability in varied environments and working conditions: strategies to resist oxidation and performance degradation must be implemented.
- (3) Synthesis of large-sized SC MXene nanosheets: techniques to derive large-size SC MXene nanosheets directly from MAX phase single crystals or via bottom-up methods (such as CVD) are crucial for studying their fundamental physical properties.
- (4) Heteroepitaxial CVD growth techniques: the development of heteroepitaxial CVD growth methods will provide a new route for producing high-quality MXenes or complex layered nano-architectures with tailored properties.
- (5) Exploration of intrinsic physical properties of MXenes: it is crucial to investigate the physical properties of MXenes, focusing on

- semiconductive and magnetic behaviours that have never been reported.
- (6) Large-scale production: scaling up the synthesis of MXenes through etching approaches or CVD techniques will be essential for industrial applications.
 - (7) Emergence of MXene-analogous layered materials (LMs): the layered transition metal carbodichalcogenides, such as $\text{Nb}_2\text{S}_2\text{C}$, which can be considered analogous to Nb_2CS_x MXene but with doubled sulphur terminations, are promising to combine the merits of both TMDCs and MXenes.
 - (8) Applications of MXenes: given their unique properties, MXenes promise breakthroughs in various fields. Potential applications include conductive transparent, flexible, and wearable electronic and optoelectronic devices, energy harvesting and storage, electromagnetic shielding, epidermal and implantable electrodes, tissue engineering, soft robotics, thermal insulation, and beyond. The ongoing and future research efforts will undoubtedly unlock new potentials for MXenes, making them pivotal in addressing technological challenges across multiple domains.

7. Computational discovery of novel 2D materials

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Status

First-principles calculations based on DFT are increasingly used to guide and accelerate the search for new materials. In the field of 2D materials, a number of computational databases have been created to support this development and to provide an overview of known as well as hypothetical (potentially synthesizable) 2D monolayers. For example, the Computational 2D Materials Database (C2DB) [106] contains about 16k monolayers with a large variety of calculated properties (mechanical, electronic, magnetic, topological, linear- and nonlinear optical) while the 2D Materials Cloud [107] and the 2D Materials Encyclopedia [108] contain respectively 3k and 6k monolayers and their electronic band structures.

The strategies used to generate new 2D materials can be categorized as ‘top-down’ or ‘bottom-up’ approaches. In the top-down approach one starts with a 3D bulk crystal and calculates whether single layers can be exfoliated from it either mechanically [107, 109] (relevant for weakly vdW bonded layers) or chemically [110] (relevant when specific elements binding the layers together can be selectively etched away). The mechanical exfoliation approach facilitates predictions based on a straightforward calculation of the interlayer binding energy using a vdW compliant exchange-correlation functional. The chemical exfoliation approach is more involved as it is necessary to have a representation of the chemical processes involved, including how to passivate the obtained surfaces by, e.g. O, F, or OH terminations. Large-scale computational studies of chemical exfoliation, such as MAX to MXene conversion, have identified stable 3D precursors [111] by evaluating exfoliability based on Pourbaix diagrams (for electrochemical etching) and assessment of the exfoliation free energy (for conventional etching with imposed electroneutrality) [112].

Several different ‘bottom-up’ approaches have also been employed. The simplest uses a known 2D monolayer as scaffold structure and generates new ones by substituting the atoms by chemically similar ones [106]. The crystal symmetry approach starts from an abstract space group (or more precisely layer group) and systematically decorates the Wyckoff

sites by different elements [113]. In the intercalation approach one starts with a known homobilayer and inserts atoms into the vdW gap to produce new covalently bonded 2D crystals [114]. Fusion of entire monolayer structures with similar in-plane lattice constants, has also been used as strategy to generate new classes of 2D materials [115]. Finally, AI-based generative models trained on existing 2D materials databases have been successfully used to produce new stable monolayers with a high degree of chemical and structural diversity [116]. A key question concerns the stability of the resulting structures. Here an important indicator is the *energy above the convex hull*, which is defined as the energy of the given structure relative to all other competing phases (including mixed phases) of the same chemical elements and stoichiometry. A hull energy close to zero indicates thermodynamic stability at low temperature and in the absence of any other chemical species. A systematic analysis of experimentally realized 2D materials suggest that free-standing monolayers are unlikely to exist if their calculated convex hull energies exceed 0.2 eV [106]. Considering that freestanding layers of 2D materials are typically not thermodynamically stable with respect to their 3D counterpart, the important convex hull indicator can be complemented by evaluation of properties or processes leading from 3D to 2D, e.g. exfoliation energies or forces, in combination with assessment of the dynamical stability of the 2D derivatives. Experimentally, bottom-up synthesis is typically based on specific substrates and a clever choice of substrate may even facilitate growth of metastable compounds—as in the case of silicene. Such effects are highly challenging to include in computational approaches although preliminary steps have been taken to identify ideal substrates [117].

First-principles calculations have been pivotal for the development of several classes of 2D materials that have recently emerged or attracted renewed interest. These include high-entropy alloys (HEAs) of TMDs [118] and MXene [119] containing four or more metal elements with low mixing energy. The HEAs exhibit enhanced stability at elevated temperatures and show promise as e.g. (electro)catalysts. Natural vdW bilayers, i.e. homobilayers in naturally occurring stacking configurations, are attractive due to their good stability and easy production (compared to twisted bilayers) as well as their highly tunable and switchable properties arising from the stacking/sliding degrees of freedom. A systematic computational exploration of all natural bilayers resulting from stacking of 1k different monolayers was recently reported [120]. Inspired by the synthesis of MoSi₂N₄ [121], computational fusion of MZ₂ layers (e.g. MoS₂) with A₂Z₂ layers (e.g. In₂S₂) was used to predict a new class of MA₂Z₄ structures

exhibiting a wide range of electronic and magnetic properties [115, 122]. TMD homobilayers with native metal atoms filling a periodic pattern of sites in the vdW gap comprise a class of ultrathin, covalently bonded 2D crystals with stoichiometry dependent properties [123]. Computations show that self-intercalation generally promotes magnetism, metallicity, and basal plane reactivity [114]. On a more conceptual level, but supported by material-specific calculations, the general class of Moiré structures, in particular heterostructures and twisted homobilayers, have been proposed as a robust and easily accessible quantum simulation platform enabling the study of strongly correlated physics and topology [124]. For classes of 2D materials made from non-vdW structures, theoretical predictions have facilitated development of 2D materials from selective etching, beyond MXenes. Through identified reduced interlayer interaction via alloying, and screening procedures targeting optimal compositions for chemical exfoliation, both a 2D metal boride, *boridene* [125], and 2D sheets based on primarily Ru and O have been realized [110]. Both materials show promise as catalysts.

The discovery of new 2D materials with optimal properties for specific applications has largely been driven by high throughput computational screening studies. Such approaches usually take existing databases as a starting point [106–108] and apply workflows to compute properties systematically for thousands of materials [126–128]. Magnetic order in 2D materials is arguably one of the most interesting properties with rather direct prospects of applications for 2D spintronics [129]. In this regard the most pertinent challenge is to find a compound that remains magnetic at room temperature [130] and high throughput computations have been applied to compile lists of promising 2D magnets [131, 132] for room-temperature applications. Such studies comprise important seeds for further analysis of physical properties—for example multiferroic order [133] or altermagnetic band splitting [134]. Other classes of 2D materials that have been characterized systematically by first principles calculations include topological insulators [135–137], ferroelectrics [138, 139], superconductors [140], thermoelectrics [141], high mobility semiconductors [142], catalysis [143] and non-linear optical properties [144, 145].

Current and future challenges

It is evident that first-principles electronic structure codes in combination with big data analytics and AI models comprise a powerful tool for accelerated digital discovery of novel materials. Yet, a number of outstanding challenges must be overcome before its full potential can be leveraged and fully benefit

the field of 2D materials. One is related to the development of deep generative models to autonomously create materials with prescribed properties. While methods like crystal diffusion, with proper training data, can generate stable and chemically meaningful structures [116], the problem of property conditional structure generation is still in its infancy. As computer power continues to increase and automated workflow management software and generative AI tools become more available, the computational throughput will grow tremendously. This situation entails a risk of the field being flooded by potentially interesting hypothetical materials. To mitigate this risk, it is crucial that computational discovery studies invoke more careful assessment of candidate materials. This includes a more serious evaluation of the synthesizability of proposed structures and their stability under realistic conditions, i.e. beyond the ‘low formation energy’ paradigm, as well as a characterization of the materials most basic properties. Another long-standing challenge in the field concerns the accurate modelling of twisted 2D materials and general vdW heterostructures because large number of atoms per unit cell of such structures (many thousands) simply precludes conventional first principles descriptions. Such calculations have been performed in specific cases, but are currently limited to carbon-based systems, where the simulations are feasible with a minimal basis set [146].

Advances in science and technology to meet challenges

The upcoming exascale supercomputers provide an opportunity for expanding computational studies to larger structures and more complex processes. However, as these supercomputers are GPU-based, the current simulation codes must be ported, which is a rather demanding endeavour. Emerging ML interatomic potentials will enable more realistic simulations of 2D materials including dynamics and growth processes. They may also permit determination of the detailed atomic structure of materials with thousands of atoms per unit cell, e.g. twisted Moiré structures. However, the potentials are currently limited to the prediction of total energies and forces and cannot provide electronic or magnetic properties, which are essential for many envisioned applications of these materials.

Concluding remarks

The computational development of novel 2D materials is an exciting frontier in materials science, driven by advancements in computational techniques and high-throughput screening methods. By employing DFT and ML algorithms, one may predict the stability, properties, and

potential applications of hypothetical 2D materials before experimental synthesis. However, challenges remain in accurately modelling the synthesizability, necessitating further collaboration between computational and experimental scientists.

ML will undoubtedly play a crucial role for future materials discoveries, leveraging the vast amounts

of computed data available in publications and databases.

Acknowledgments

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8. 2D heterostructures

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Status

Stacking individual 2D crystals into heterostructures offers the unprecedented ability to rationally design functional materials at the atomic level with nearly limitless configurations. The large library of 2D materials (2DM) with diverse electronic properties can be used to assemble complex devices layer-by-atomic-layer, allowing for novel material combinations and interfaces that cannot be realized through direct growth methods. Over the past decade, numerous proof-of-principle devices have been demonstrated, however for many the prospect for commercialisation is currently remote. Transfer-induced inhomogeneity and interfacial contamination drastically limit the clean area of heterostructures as the number of layers and interfaces increase, impeding the development of high end-applications.

This problem is especially acute for applications where high electronic quality and large-scale uniformity is essential, such as in optoelectronics, quantum technologies and aerospace. While 2DM can substantially impact these fields, the transition from micrometre-scale prototypes to large-scale manufacturing has become a critical bottleneck. Despite this, advances in 2D material growth and transfer techniques are starting to yield viable commercial products, albeit those with less stringent requirements for electronic grade material quality. This discussion outlines the state of the field and the developments necessary to enable the commercial applications where tailored vdW heterostructures can really shine.

Current and future challenges

The major challenge, for both academic investigation into vdW heterostructures and their industrial utilisation, is repeatable fabrication of homogenous 2D crystal stacks. While layer-by-layer growth techniques show promise [147, 148], they are limited to specific systems with compatible chemistry, demonstrated over small areas, and incapable of generalizing to more complex arrangements, such as controllable crystalline misalignment. This makes transfer of individually grown 2D materials an attractive option, although it presents its own set of problems and integration challenges.

Considerable progress has been made in thin film growth of 2D materials in the last 5 years, despite its thermodynamic disadvantage compared to bulk crystal formation. However, challenges remain. For instance, few-layer grown hBN, the key dielectric crystal employed in the majority of vdW

heterostructure devices, exhibits limited uniformity and poor crystalline quality compared to exfoliated crystals. The rapid development in this field instils optimism that the quality of few-layer grown hBN will match that of exfoliated crystals within a few years [149], although it currently falls short of the necessary standards.

The primary issue for 2DM devices occurs as individual crystals are stacked to form a heterostructure. Currently, this process is performed in air or inert gases, resulting in the adsorption of a wide range of volatile atmospheric species on the crystal surfaces. These contaminants subsequently become trapped at the interfaces within the heterostructure (figure 8). This contamination remains mobile, and can diffuse to form isolated pockets (also called ‘bubbles’ or ‘blisters’) leaving micrometre-scale regions of atomically clean interface behind. This phenomenon, typically referred to as ‘segregation’, has been both a blessing and a curse for the field. Whilst it provides small clean areas perfect for device prototyping, it prevents scale-up via dense patterning, and large area devices. Segregation occurs regardless of whether the 2DM is exfoliated or grown, however it does not occur if one of the surfaces is not atomically flat or has high defect density. In such cases the contamination is pinned, forming a continuous film at the interface. While certain techniques can remove most of the trapped contamination after transfer [150], these are time consuming, limited to small areas, and do not necessarily restore the interface to a pristine state. An additional problem stems from the use of polymeric transfer methods. Polymer carrier films are widely used to delaminate and support fragile atomically thin crystals. These soft layers have drastically different thermal expansion coefficients compared to those of 2DM. In combination with the difference in topography between the growth and target wafer, this leads to formation of wrinkles and cracks in transferred 2D materials.

Due to these issues, despite 12 years of intensive development, all currently demonstrated assembly techniques suffer from large scale interfacial inhomogeneities. Atomically clean areas are limited to tens of microns at most, even in the simplest 3-layer heterostructures. Homogeneous areas decrease with each additional layer in the stack, compounding the issue in more complex devices such as LEDs, where the optically active area is typically limited to a few micrometres due to contaminants at the numerous interfaces. Another issue relates to studies of the rotational misalignment, or ‘twist’, between each crystal. Controllable misalignment enables the formation of novel optoelectronic states and fine tuning of material properties. Such structures are extremely sensitive to small local strain variations, resulting in a complex and unpredictable moiré superlattice. Even using state of the art transfer processes, significant twist angle disorder, typically $\sim 0.1^\circ$, is observed over

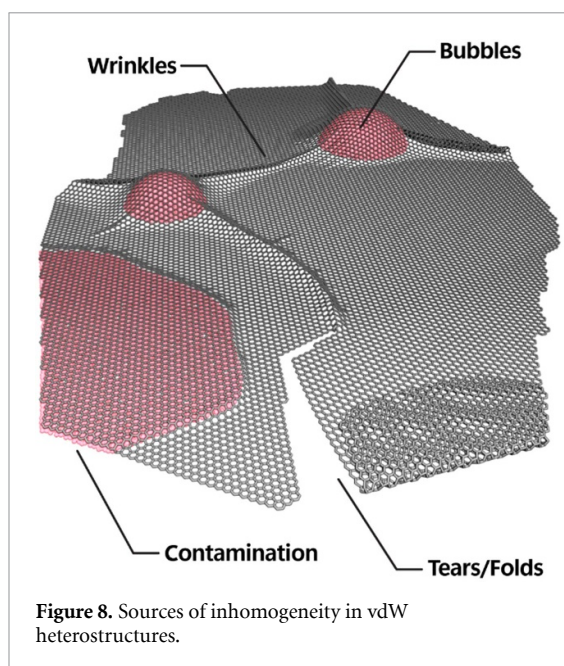


Figure 8. Sources of inhomogeneity in vdW heterostructures.

~100 nm length scales [151]. This, together with the sensitive dependence on twist angle of the electronic behaviour, means that measurements on nominally identical stacks display considerable variation. This variation prevents repeatability, external verification of results, and targeted testing of hypotheses, let alone the development of applications.

Advances in science and technology to meet challenges

An obvious solution to address these challenges is to modify the operational conditions during layer assembly. Alternatives include high or ultra-high vacuum (preceded by surface conditioning, e.g. annealing) or performing assembly with interfaces submerged in solvents capable of stripping away surface contamination. However, such alternative environments remain unattainable due to the use of polymeric carriers in all 2DM transfers. These polymers exhibit low glass transition temperatures (100 °C–200 °C), a loose molecular matrix which is prone to outgas in vacuum, and poor chemical resistance against solvents capable of removing hydrocarbon surface contamination. In initial experiments contamination persists even in high vacuum environment due to use of these polymeric carrier layers. Turning away from polymers in favour of inorganic materials to transfer 2DM (e.g. metal foils, nitride or oxide films) should significantly improve the situation, allowing for higher processing temperatures, and providing more closely matched thermal expansion rates, low outgassing in vacuum, and the ability to employ more aggressive chemical treatments.

Regarding compatible scale-up methods, we foresee two major pathways (illustrated in figure 9). One obvious and widely explored route of development is to apply the current research best-practice techniques

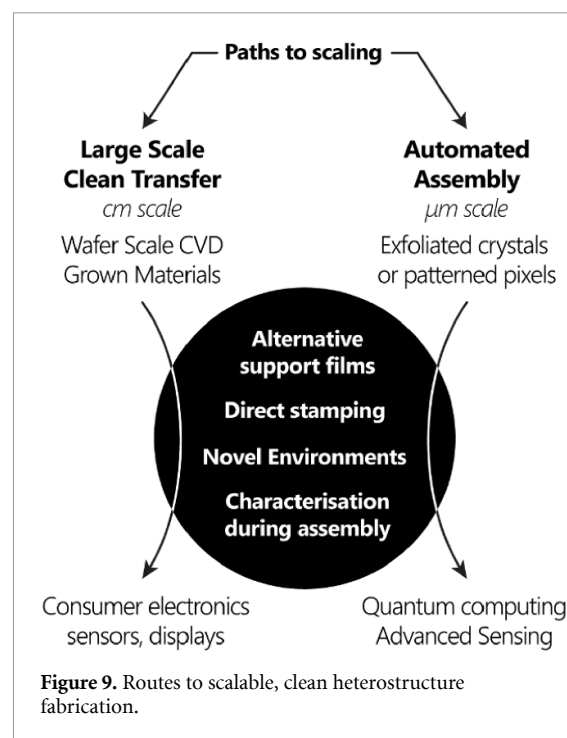


Figure 9. Routes to scalable, clean heterostructure fabrication.

at a large scale to CVD-grown materials. These are polymer based ‘dry’ delamination techniques, where 2D materials are transferred from low adhesion growth substrates to higher adhesion atomically flat 2DM. These avoid any contact with polymers or liquids on the vdW heterostructure interfaces, confining most contamination to an outer encapsulation layer. As almost any potential inorganic replacements for the carrier would be less pliable than polymers, techniques will also require extremely low roughness of the 2D materials (and thus growth substrates) at the large scale to ensure conformal contact with the pickup layer, as well as relatively weak bonding to the growth substrate. Various pathways to achieve this at scale have recently been demonstrated for multiple materials, for example growth of CVD graphene on ultra-flat Cu and subsequent oxidation to enable stamp transfer [152], or direct growth of weakly bonded graphene on polished SiO₂ [153]. Such processes will need to be optimized and applied to a larger section of the 2DM library for commercial applications.

An alternative approach for both research and commercialisation is the automation of the manual stacking of small-area crystals. VdW heterostructures with unprecedented numbers of layers have already been fabricated by automated transfer systems using both automatically identified mechanically exfoliated crystals [154], and lithographically defined sections of grown materials [155]. Although interlayer contamination remains an issue, if the aforementioned transfer problems are reduced, automated stacking may provide sufficient throughput for specialized segments of the market, where extremely high quality but low batch sizes are required. Indeed, one automated

system can output hundreds of heterostructures per year at a fraction of the cost required to run a silicon foundry, which is enough to fulfil the need for specific high-end optoelectronic devices in aerospace, military, quantum computing and medical fields, and should not be overlooked.

Concluding remarks

At present, the technological side of the field is stagnating. Eliminating transfer-induced inhomogeneity (both strain and interlayer contamination) is essential to progress and access the full potential of 2D materials. When such problems plague even bespoke research devices fabricated by leading experts in sophisticated cleanroom environments using ‘clean’ mechanically exfoliated 2D crystals, it is superficially challenging to see how these may be eliminated in an industrial setting.

A paradigm shift in the way 2D crystals are transferred is therefore required, with a transition away from polymeric carriers towards more mechanically, thermally, and chemically stable carrier surfaces. Ultra-high vacuum or fluid environments are a promising way forward [156], but the current reliance on polymeric support films must be overcome to enable their full potential.

Acknowledgments

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9. Electronics of twisted 2D materials

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Status

Some of the most exciting and enigmatic phases of matter result from strong electron-electron interactions or topological electronic bands. Recently, moiré systems have become key platforms for studying the interplay between these effects, drawing from a wide range of 2D vdW materials, which include single and multilayers of graphene and various semiconducting TMDCs.

A unique aspect of 2D materials lies in the ability to directly modify their electronic properties by layering one atomically thin crystal atop another, which allows for their surface-exposed electronic wavefunctions to strongly overlap. When stacked vdW crystals have a small lattice mismatch or relative twist angle, a ‘moiré pattern’ arises, creating a tuneable artificial superlattice potential many times larger than the constituent atomic lattices (figure 10). Under suitable conditions this can generate extremely flat electronic bands with quenched kinetic energy, leading to the emergence of strongly correlated phases with broken symmetries including correlated insulators, generalized ferromagnets, and unconventional superconductors. In addition, the moiré-induced mini-Brillouin zone can have inherently altered Berry curvature compared to its constituent materials, giving rise to nontrivial topology and quantum geometry.

Early work relied on scanning tunnelling microscopy to establish the existence of moiré patterns in twisted graphene structures and angle-aligned graphene on hBN [157]. In 2013, the graphene/hBN moiré lattice was shown to host Hofstadter butterfly physics in a magnetic field, arising due to the interplay between comparable electronic and magnetic length scales [158]. The field was subsequently supercharged by the 2018 discovery of unconventional superconductivity and correlated insulating states in ‘magic-angle’ twisted bilayer graphene (MA-TBG) [13, 159], comprising two sheets of monolayer graphene twisted by the so-called ‘magic’ angle of approximately 1.1° (resulting in a superlattice period of ≈ 10 nm). Since then, interest in moiré materials has grown rapidly. Researchers from around the world remain fascinated by the countless new quantum states of matter arising in moiré materials, and the field has grown to encompass well over a dozen distinct moiré platforms

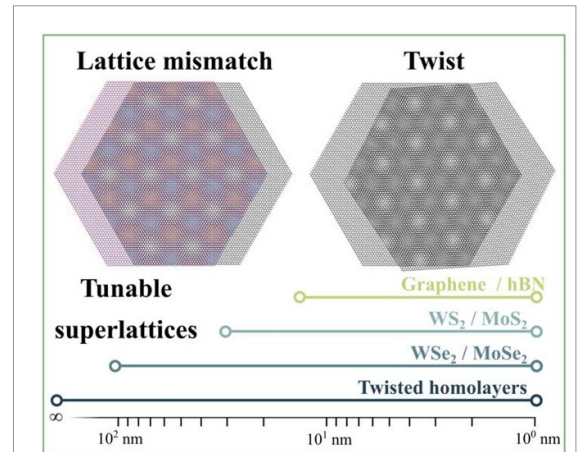


Figure 10. Cartoon schematic of moiré pattern formed by stacking atomically thin crystals with either a lattice mismatch or a relative twist angle. The characteristic length scales of different types of moiré materials are shown below, varying depending on the relative twist angle. ‘Homolayers’ indicate structures in which the same material is twisted upon itself (e.g. twisted bilayer graphene).

featuring a wide range of exciting physics and unexpected new discoveries each year.

Current and future challenges

A vast array of exotic quantum states are possible within the framework of moiré quantum matter, and many current and future challenges lie in discovering, cataloguing, understanding, and manipulating these states. A notable example is superconductivity, which was first discovered in magic-angle twisted bilayer graphene but has since been found in a larger family of twisted graphene multilayers, and in twisted bilayer WSe₂. Numerous experiments have probed these superconducting phases, including studies of potential rotational symmetry breaking, electrostatic Coulomb interaction screening, macroscopic quantum coherence in Josephson junctions and SQUID devices, and microscopic studies of the superconducting gap [160]. These experiments collectively point to unconventional superconductivity in twisted graphene, with signatures of nematicity and anisotropic pairing symmetries. However, key open questions remain, including the roles of electron-phonon and electron-electron interactions in Cooper pair formation, and whether common mechanisms underlie superconductivity across various twisted graphene and TMD moiré systems.

Many other fingerprints of strong correlations have been observed, including ‘strange-metal’ behaviour in magic-angle graphene and signatures of tuneable Kondo lattice formation in aligned MoTe₂/WSe₂ heterostructures. Gapped states at commensurate moiré band dopings, typically associated with a spontaneous lifting of spin/valley degeneracies or broken discrete translational symmetry, are also common. Accurately predicting these phases across different moiré platforms, and unambiguously

determining their ground state ordering, often remain as outstanding challenges. For example, many of the features seen in MA-TBG are captured within a topological heavy fermion description, characterized by the coexistence of itinerant and localized charge carriers within the flat band. However, developing a complete understanding of the resulting correlated states and their connection to superconductivity is currently work in progress.

The combination of intrinsic Berry curvature and spontaneously broken time-reversal symmetry leads to new forms of electronic ordering with intertwined topological and correlated properties. Numerous twisted graphene and TMD moiré systems support the integer quantum anomalous Hall (QAH) effect, driven by interaction-induced spin and orbital magnetism that opens a gap between otherwise degenerate Chern bands. Remarkably, the fractional QAH effect has recently been discovered in twisted MoTe₂ and in moiré lattices of rhombohedral-stacked multilayer graphene aligned with hBN [161, 162]. The nature of these fractional QAH states and their connection to fractional quantum Hall states in Landau levels is a topic of intense interest.

Alongside the emerging physics, several overarching challenges face the field. A major experimental hurdle is reliably reproducing states sometimes seen in only a single sample [151], and scaling these effects to wafer-scale device arrays. Key issues include the extreme sensitivity of many-body ground states to precise twist angles, dielectric environments, and unintentional strains formed during the mechanical device assembly [160]. Theoretically, several challenges persist in modelling strongly correlated systems. These include accurately calculating band structures for moiré materials with thousands of atoms per unit cell, distinguishing between nearly degenerate ground states of strongly interacting systems, and developing new paradigms for understanding correlation-driven topological phases of matter.

Advances in science and technology to meet challenges

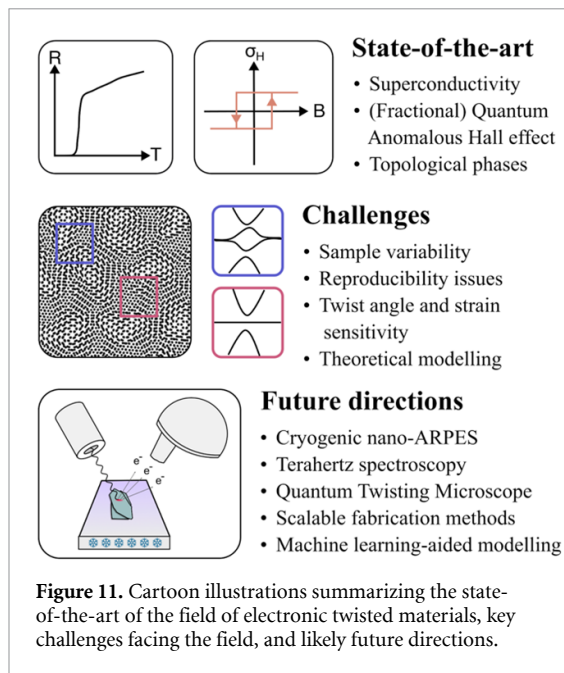
Currently, state-of-the-art moiré devices are made by exfoliating bulk crystals down to atomically thin layers with Scotch tape, then stacking flakes at controlled twist angles using a dry transfer technique. However, this strategy yields only a single micrometre-scale sample at a time, and is susceptible to introducing large in-plane strains that can substantially change the desired physics of the structure. The development of robotic exfoliation and stacking systems equipped with machine-learning-enabled flake detection and control may provide a pathway towards increasing the yield of this fabrication technique. Additionally, further development of techniques to directly manipulate the stacking of 2D vdW flakes by pushing them with an atomic force microscopic (AFM) tip may be useful for constructing strain-free devices with

on-demand twist angles [163]. Efforts to scale these systems to wafer scale will likely require new synthesis and transfer techniques based on chemical vapour transport or molecular beam epitaxial growth of large-area single crystals, paired with advanced robotic transfer and device assembly technology.

In parallel, the ongoing development of advanced characterization and modelling techniques will be critical for future progress. Experimentally, the field would benefit from further development of cryogenic nano-ARPES to probe the evolution of the spectral weight of moiré systems as a function of doping and other key tuning parameters. Advanced terahertz spectroscopy techniques are also valuable for probing the low-energy physics of the flat moiré bands. Microscopic probes operating at millikelvin temperatures will be informative, enabling direct connections between the atomic- and moiré-scale properties of these materials with their mesoscopic phenomena. These will likely include advances in scanning techniques including tunnelling, compressibility, magnetization, and optical spectroscopy. The quantum twisting microscope represents an emerging frontier in the study of moiré quantum matter [164], in which vdW layers adhered to an AFM tip can be deterministically rastered across and twisted upon a separate vdW stack, all while various quantities are measured.

Additionally, it will be fruitful to further develop techniques for directly controlling the properties of moiré materials, including the use of pressure and uniaxial strain to control the effective Hamiltonian of the system, and the integration of metallic screening layers near the moiré interface to control the strength of Coulomb interactions. Fabricating lateral junctions between different emergent phases presents new opportunities for deterministically engineering exotic quantum states of matter. For example, interfacing superconductivity with integer or fractional QAH states is predicted to generate Majorana or parafermion modes carrying non-Abelian excitations, which may be useful for the development of topological qubits. Further manipulating the resulting topological boundary modes with electrostatic gates and quantum point contacts will be needed in order to detect and braid these exotic quasiparticles.

Lastly, new theoretical paradigms are needed for improving the modelling of strongly correlated and topological states of matter, and for answering key open questions facing the field. Understanding the critical role of quantum geometry in setting the properties of strongly correlated and unconventional superconducting phases lies at the frontier of condensed matter theory. Additionally, fractional Chern insulator states arising at zero magnetic field present new opportunities to understand the microscopic properties of quasiparticles with fractionalized charge excitations and anyonic quantum exchange statistics.



Concluding remarks

Moiré materials are currently at the forefront of the study of intermixed correlations, topology, and superconductivity in condensed matter physics owing to their extraordinary versatility. Future progress in this field necessitates a multifaceted

approach to improving and scaling sample fabrication, developing new techniques for characterizing and directly controlling their properties, and advancing theoretical capabilities for better understanding and more efficiently predicting new physics in existing and emerging moiré materials (figure 11). Beyond fundamental discoveries, these designer quantum materials hold promise for the development of future electronics, including as ultra-sensitive quantum detectors and in various forms of quantum information storage and processing devices.

Acknowledgments

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10. Moiré nano-optoelectronics

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Status

Advent of moiré materials. The possibility to stack 2D crystalline layers with nearly perfect interfaces has revolutionized the design of electronic and nanophotonic materials. vdW heterostructures offer virtually limitless possibilities for materials creation as, unlike traditional growth techniques, material selection is free from constraints imposed by lattice mismatch. Such freedom allows for the creation of electronic and photonic phases through modulation of spin-orbit coupling, exciton amplitudes, energy shifts or scattering rates. The range of achievable quantum phases expands with additional tuning routes offered by electrostatic gating, electric or magnetic fields, temperature, strain engineering, etc. As 2D heterostructures fabrication grew, rotational stages were developed to align crystallographic axes of two different crystals, resulting in superlattice potentials with length scales of 10–20 nm and observations of phenomena such as replica of Dirac fermions, Hofstadter gaps and Brown-Zak fermions. This technique could later be used for precise control over the twist angle between two or more homolayers. In that case, the twist angle defines the size of the band-folding Brillouin zone and possible inter-layer hybridization, enabling control of the ratio between interaction strength and electronic bandwidth. Such ‘moiré’ materials stand out for their exceptionally tuneable band structures and their ability to host a wealth of novel physical phases, including correlated insulators, superconductors, orbital ferromagnets, Wigner crystal states, strip phases, topological multiferroic orders, moiré excitons, and bosonic exciton crystals to name a few [160, 165, 166]. These unique properties make twisted moiré materials ideal candidates for easy-to-fabricate quantum simulators, with all known correlation-induced symmetry-broken phases identified in these materials. However, their exact nature and underlying mechanism remain elusive.

Optoelectronic probes of moiré materials. Since the early days of graphene research, optical probes have been used for characterization: Raman spectroscopy, for example, allows for identification of stacking order and layer number of various 2D materials. Over time, both free space and near-field techniques were incorporated to gain insights into e.g. carrier energy relaxation dynamics, carrier transport, bandgap, exciton energy, Berry curvature and heat transport [166, 167]. For example, scanning photocurrent experiments, achieved using near-field optical microscopes (SNOM), allow for the

observation of the plasmonic response in moiré systems, for the extraction of parameters such as the local Seebeck coefficient or for visualization of plasmons. For example, near-field photocurrent studies of minimally twisted graphene bilayers revealed that plasmons reflect at domain boundaries, shedding light on the local strain profile and displacement of the graphene layers [167]. Similarly, photocurrent nanoscopy experiments revealed inter-band plasmons [168] in graphene bilayers or correlated insulating states in twisted trilayers [167]. Notably, the plasmons in graphene can also be leveraged to observe phenomena in proximity layers such as moiré ferroelectricity [169].

By probing the current response of a moiré material exposed to light, photocurrent measurements are another versatile tool to sense the properties of electronic states, Bloch band quantum geometry, quantum kinetic processes and device characteristics [167]. Two prominent quantum geometric photocurrents arise from inter-band transitions: injection and shift photocurrents. These exhibit a sensitive dependence on the crystalline symmetries, parameters that are readily controlled within moiré heterostructures. With their exceptional tunability, large unit cells, topological properties and large density of states, moiré systems represent an ideal system to study large quantum geometric photocurrents. Their unique symmetries allow for advanced polarisation sensing in the infrared (IR) [170] and THz ranges [171].

Moiré optoelectronic devices. In terms of optoelectronic device design, moiré materials present strong light-matter interactions and large photo-response, positioning them as prime candidates for photodetection and photoconversion applications. For these applications, the exceptional tunability of their spectrum as well as the energy scale of relevant optical transitions present advantages. By simply adjusting the twist angle, it becomes possible to control the wavelength from ultraviolet down to the THz range. For twist angles above 1° , bandgaps of 50–100 meV facilitate photo-induced transitions throughout the IR range [172], opening possibilities for IR detection or spectroscopy applications. For smaller twist angles, the formation of flat minibands with a high density of states significantly enhances the dynamical conductivity, leading to a strong photo-response. In this regime, correlated insulating gaps and bandwidths are typically between 10 and 100 meV, leading to resonant inter-band transitions with detection capabilities in the far-IR and THz energy ranges. Specifically, the narrow bandwidths enabled by moiré materials enable superconductivity at ultra-low carrier densities with sharp superconducting transitions and ultra-low heat capacity, effects that can be utilized for single-photon detection in the mid-IR and THz range with exceptionally fast response times and high energy resolutions [173].

Equally, their narrow and tuneable energy ranges allow for supercritical shifts of the Fermi surface, where a sharp transition combined with negative differential conductance can be exploited for broadband single-photon detection [174]. In addition, the ability to engineer symmetry breaking in twisted 2D materials opens doors for symmetry breaking optoelectronics, where groundbreaking effects like the BPGE and opto-valley Hall effects can be engineered with potential applications in chiral light-emitting diodes or moiré quantum emitters [166, 167].

Beyond optoelectronics: moiré nanophotonics.

Besides their potential for optoelectronic devices, moiré materials are sparking significant interest due to the possibility of engineering entirely new types of photonic excitations, including non-reciprocal plasmons, quantum geometric plasmons, moiré excitons, resonantly hybridized excitons, and other reconstructed collective excitations [165, 166]. Near-field techniques, in particular, offer promising avenues for exploring various light-matter coupling mechanisms within these materials. Since the properties of excitons are directly linked to the underlying Bloch states, they can serve as sensitive probes for the potential landscape of twisted materials. For example, in twisted TMDCs, the spatially displaced wave functions of electron-hole pairs forming excitons (at K and K' moiré sites) allow for optical transitions with properties similar to conventional bilayer excitons but tuneable energies, and spin-layer selectivity [165]. Moiré materials can also host more complex excitonic states such as moiré-trapped interlayer trions, satellite moiré exciton peaks and non-trivial many-body states involving interlayer charge transfer excitons and interlayer moiré excitons with, e.g. a hole wavefunction surrounded by three electron wavefunctions. The long lifetimes and strong dipolar interactions in moiré materials can also lead to the formation of correlated excitonic states. These states hold promise as sensitive probes for the correlated phases observed in neighbouring systems. They also offer a tuneable platform to access various exotic quantum phases, including non-interacting Bose gases, superfluid phases, quadrupole and dipolar excitations, and electron-hole plasmas.

Current and future challenges

Despite significant research, fundamental challenges remain in moiré optoelectronics. Understanding the nature of moiré correlated phases is one of them, which requires the combination on various techniques. Optoelectronic techniques hold promise to reveal properties invisible to conventional electron transport and scanning probes. However, extending purely optical methods across

a wide frequency range would face hurdles like low signal-to-noise ratio and substrate contributions as moiré materials are smaller than IR and THz wavelengths. It then becomes crucial to upscaling moiré materials for practical photodetection applications. In basic science, photocurrent measurements offer a potential alternative to circumvent these limitations.

Additional challenges in practical devices originate from unwanted reflections from gates and need for careful integration with existing technology to avoid compromising performance. Going further, integration with waveguides, cavities, plasmonic structures or ring resonators could create a vast array of high-performance optoelectronic devices such as single-photon emitters or optical modulators.

Unlocking new functionalities also presents exciting possibilities. Trapping interlayer excitons using periodic strain profiles or electrostatics could lead to tuneable quantum emission of single photons, photon-induced gating and Purcell enhancement for enhanced light-matter interactions. Promising tuning knobs could include ultrafast optical excitations, electric and magnetic fields, pressure and Floquet engineering, although not yet demonstrated.

Advances in science and technology to meet challenges

An important challenge lies in the improved fabrication methods. Both device applications and fundamental research calls for the necessity to fabricate large, clean and reproducible moiré devices. Assembling atomically thin crystals on top of one another in unfavourable stacking configurations has proved a challenging task, and naturally places severe doubts on the upscaling potential. Nonetheless, researchers have already demonstrated the capabilities to grow twisted heterostructures using CVD, which marks an important milestone towards device applications based on moiré materials [175]. However, SC domains so far remain small (10 μm). In addition, one should be able to stack different layers similar to tandem solar cells to improve low-power photodetectors (PDs) while maintaining the desired properties.

Concluding remarks

The study of moiré materials at the interface between condensed matter physics and photonic techniques presents a fertile ground for fundamental advances. Probing the band structure, their interactions with valleys and quantum metrics through advanced techniques hold immense potential to unlocking

novel functionalities. The unique combination of ultra-strong optoelectronic response and precise control over energy scales in moiré materials represents a paradigm shift and promises a future brimming with groundbreaking applications and transformative technologies.

Acknowledgments

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11. Polaritonics of 2D materials

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Status

A polariton is a quantum mechanical superposition of a photon with a matter excitation: plasmons, phonons, excitons, magnons, to name a few examples. The hybridized character of polaritons renders them uniquely advantageous for investigating complex material phenomena while preserving the experimental versatility of photons. In the context of applications, the photonic component lends compatibility with photonic device architectures, whereas the matter excitation component imparts access to substantially enhanced optical nonlinearities and rich electro-optical and magneto-optical responses, far exceeding those achievable in conventional optical media.

These unique attributes of polaritons are greatly extended in vdW materials because these materials can be easily transferred onto patterned substrates and integrated with a variety of cavities, photonic crystals, and metastructures to promote strong and even ultra-strong light-matter interaction. Early examples include integrating TMDC monolayers with planar cavities to create exciton-polaritons at room temperature with interesting valley properties.

An exciting opportunity arises from creating polariton systems with non-trivial topologies by design. Integrating a TMDC monolayer on spin Hall photonic crystals (figure 12(a)), spin Hall polaritons were formed, supporting edge modes between two spin Hall domains with helical far field emission (figures 12(b) and (c)) [176]. Recent theoretical work suggests that polariton Chern bands can be formed by using hexagonal photonic lattices and introducing time reversal symmetry via the 2D materials; a THz topological gap can be opened, which is a few orders of magnitude larger than in other systems.

A fertile ground is to integrate moiré superlattices, consisting of twisted vdW layers, into polaritonic systems. In moiré superlattices, supercell sizes, electronic band structures, optical resonances, and their dynamics are readily tunable by the twist angle between two stacked layers. Each moiré supercell may confine excitons on the nanometre scale as illustrated in figure 12(d) [177], effectively forming a regular array of quantum dots beyond the reach of any other material platform. When the moiré superlattice is

integrated into a cavity, the resulting moiré polaritons retain the large oscillator strength of 2D excitons while acquiring strong nonlinearity typical of 0D excitons (figures 12(d) and (e)), thus circumventing the conditional trade-off between light-matter coupling strength and polariton nonlinearity. Charged polaron-polariton and dipolar polaritons have also been shown to feature enhanced nonlinearity resulting from stronger Coulomb interactions and static dipole interactions, respectively.

Another emerging frontier takes advantage of the rapidly expanding functionality of vdW materials, for example, the growing family of vdW magnets such as NiPS₃ and CrSBr. In these materials, excitons are coupled to the magnetic order. Consequently, the coupling between excitons and cavity optical modes gives rise to polaritons whose properties are also correlated with magnetization (figure 12(f)) [178]. Similarly, molecular materials with demonstrated strong coupling between light and vibrational modes extend the family of polaritons [179].

Current and future challenges

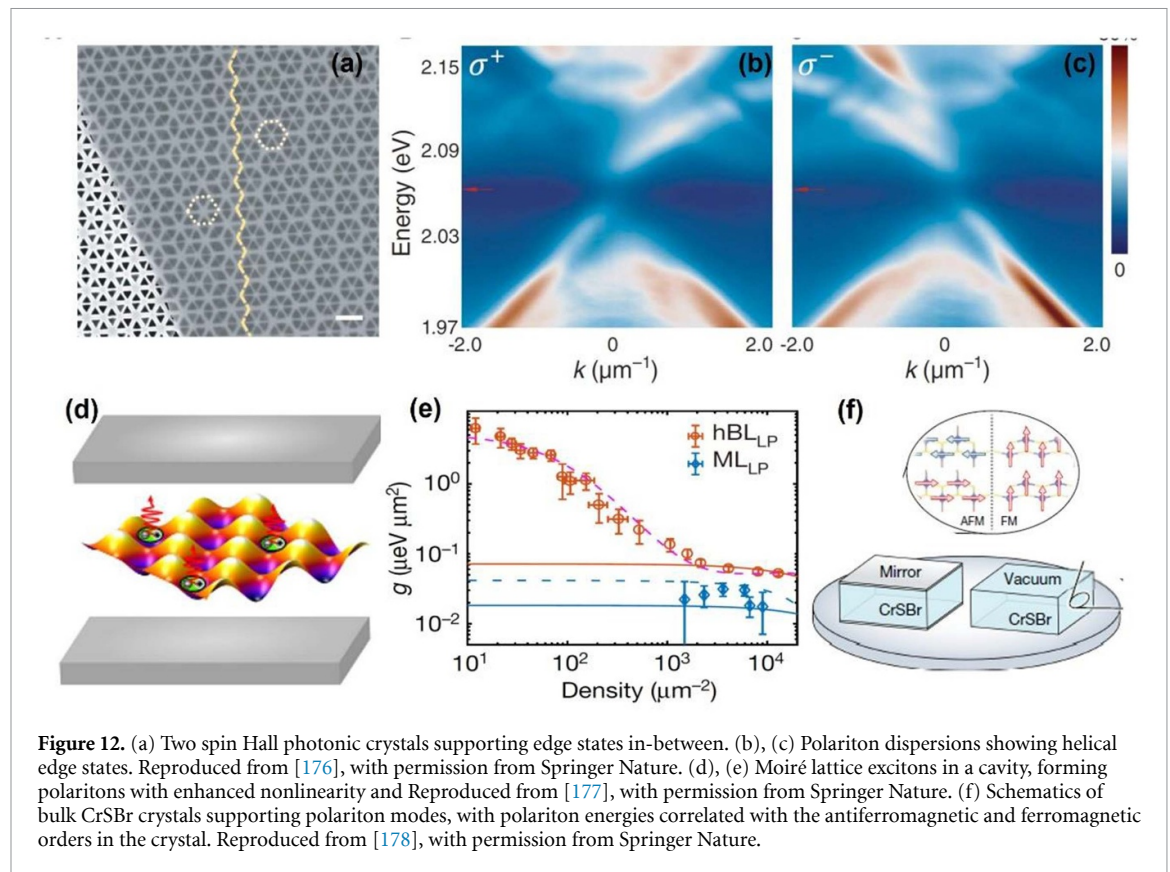
Integrating advanced photonic structures with high-quality 2D optical materials and heterostructures in a scalable fashion is a major challenge. Demonstrations of high optical quantum yield, long coherence length, or coherence time of the matter excitations integrated with cavities have mainly been achieved with manually prepared 2D heterostructures with lateral dimensions of a few microns. Polariton nonlinearity, though enhanced through new mechanisms unique to vdW systems, remains below the polariton blockade limit.

Polariton propagation loss has hampered a range of applications, such as ultralow-threshold polariton lasers, topological and quantum polaritonics, and nano-sized polariton sensors. Reducing propagation loss further will enable practical applications by allowing precise, on-demand control of polariton wavefronts and dispersion. This capability is essential for effective nano-light manipulation and paves the way for nano-optical computation and information-processing circuits, analogous to the role of electrons in conventional electronics.

Advances in science and technology to meet challenges

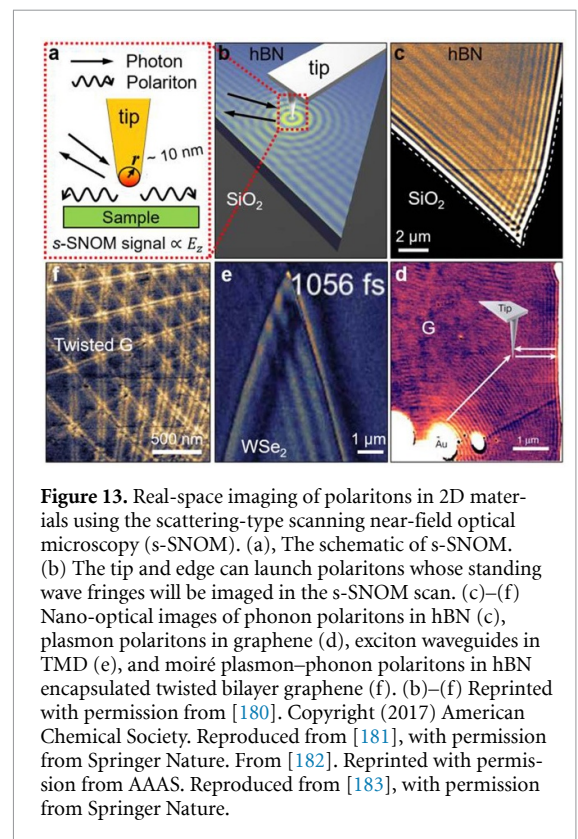
While new methods for growing and assembling 2D materials and heterostructures with improved interfaces and uniformity continue to emerge, characterization techniques for resolving polariton modes and their propagation are also advancing rapidly.

A series of propagating polaritons in 2D materials have been imaged in real space using scattering-scanning near-field optical microscopy (s-SNOM, figure 13). The nanoscale sharp metallic tip in the s-SNOM experiments (figures 13(a) and (b)) transfer the energy and bridge the momentum mismatch between photons (straight arrow) and



polaritons (wave arrow), thereby launching the polariton waves whose standing wave interferences can be imaged as fringes. Representative works include imaging phonon polaritons in hBN (figure 13(c)) [180], surface plasmon polaritons in graphene (figure 13(d)) [181], excitons in TMDs along waveguides (figure 13(e)) [182], and moiré plasmon–phonon polaritons in twisted bilayer graphene encapsulated by hBN (figure 13(f)) [183]. Imaging these polaritons and their hybrids in vdW heterostructures relies on nanophotonic advances such as high-quality resonators, phase-change dynamics, charge-transfer control, and bandgap engineering.

Additional progress has been driven by exploiting low-symmetry crystals for anisotropic propagation and by using isotopic engineering to create novel energy–momentum dispersions. More recently, twisted heterostructures have been shown to generate polaritonic nano-light crystals and to enable wavefront engineering, nano-light canalization, and topological transitions in unprecedented ways. Another notable advance is the development of cryogenic s-SNOM, [184] where low temperatures enhance quantum and correlated responses in materials. In parallel, progress in advanced THz sources and microscopy has extended polaritonics into the long-wavelength regime, enabling direct studies of collective low-energy responses in carriers, spins, charge-density waves, and moiré superlattices.



Because polaritons are excited states, theoretical predictions and analyses of their properties are particularly challenging. Different theoretical methods have

been utilized to explain polariton-assisted energy transfer, polariton-polariton interaction, Bose-Einstein condensation, group velocity normalization, and photonic crystal polaritons, to name a few examples. More recently, *ab initio* quantum electrodynamics [185] and multiscale molecular dynamic simulation methods have been advanced, in particular, to describe molecular systems. Additional theoretical developments are essential to accurately describe vacuum properties within the ultra-strong coupling regimes, to model collective phenomena arising from long-range Coulomb interactions in hybrid polaritonic systems, and to explore the simultaneous strong coupling of light with various types of excitations.

Concluding remarks

Recent progress with polaritons in 2D materials is encouraging and will likely lead to the creation of entirely new types of polaritons hosted by advanced vdW materials and heterostructures. The field will

rapidly evolve with an improved understanding of the new vdW heterostructures and superlattices. Future research with these 2D material polariton systems will leverage their novel properties to explore quantum and collective phenomena previously difficult to access, such as polariton quantum blockade, fractional quantum hall states of polaritons, and integrated polariton circuits of polaritons—in device configurations and at operating temperatures that are suitable for practical technological applications.

Acknowledgments

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12. Quantum photonics and lightwave electronics

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Status

Optoelectronics stands on the cusp of a major transformation through the integration of LMs [186–189]. These herald a new era of solutions to pressing issues, including the quest for energy sustainability. They can significantly boost the efficiency of both information and communication technology (ICT) and light harvesting, as well as providing energy-efficient resources for AI. Concurrently, LMs are poised to thrust quantum information science and engineering (QISE) into a realm of practical usability, offering unprecedented performance advantages over classical options. Here, we highlight recent ideas and advances for energy solutions, AI, and QISE based on graphene, semiconducting LMs, and their heterostructures (LMHs).

Graphene can provide advanced functionalities in key technological devices and is the most mature of the LMH technologies. It already has delivered competitive energy efficiency and speed for devices such as low-power and hyperspectral PDs useful for autonomous driving, and modulators integrated in silicon-photonics, outperforming the state of the art [187]. Emerging applications include photosynthetic devices, LiDAR, security, and ultrasensitive physical and chemical sensors for industrial, environmental, and medical technologies.

Twisted LMs have provided promising new directions for AI devices. Asymmetric potential and ferromagnetic switching in twisted bilayer graphene were used to achieve synaptic behaviours for neuromorphic computing functions [190, 191]. By leveraging tuneable quantum geometric properties of twisted bilayer graphene and advanced AI algorithms, intelligent sensing of high-dimensional optical information with a single on-chip sensor was demonstrated [170]. Recently, LMs have been configured to mimic the dynamics of biological synapses

[192], heralding a new generation of energy-efficient AI hardware.

Semiconducting LMs are currently evolving fast as a new platform for quantum technology (see figure 14). They have already shown potential as scalable components, such as quantum light sources, photon detectors and nanoscale sensors, and enabled new materials discovery within the broader field of quantum simulations. Yet, harnessing quantum information within semiconducting LMs has remained challenging when operating at GHz clock speeds because each electron scattering event—occurring roughly 10 000 times per GHz cycle—terminates quantum operations.

Lightwave electronics addresses this critical QISE barrier by using the oscillating electric field of intense optical carrier waves as ultrafast biasing fields, enabling quantum operations that outpace the oscillation cycle of light [189]. As illustrated in figure 15, lightwave electronics can transport electrons coherently at petahertz (PHz) clock speeds—one million times faster than conventional electronics and 100 times faster than scattering occurs—and flip quantum states within a few fs [193, 194] under ambient conditions. Utilizing a quasiparticle-collider setup shown in figure 15, such quantum operations have been timed with attosecond precision to access delicate multi-electron interactions and correlations within LMs [195], providing direct access to electronic entanglement states. These breakthroughs have set the stage for meaningful QISE advancements that will enable quantum sensing, communication, and transduction applications, and augment classical electronic and photonic devices with entanglement capabilities.

Current and future challenges

The intrinsic confinement of electrons within LMs leads to minimally screened interactions that synergistically enhance the coupling between light, charge, lattice vibrations, and spin states. By crafting LMHs, electrons can be confined, transported, and topologically altered across desired layers—unlocking new functionalities and broadening the design landscape. However, many demonstrations are still based on manually constructed, micro-scale materials. Wafer-scale growth of LMs and LMHs is the next challenge.

Realizing PHz and entanglement electronics (figure 15) requires overcoming several escalating challenges: conducting single operations swiftly enough (1-fs timescale) to surpass electron scattering events; generating a sequence of such operations, ensuring high-precision timing and control (100-as timescale); chaining multiple operations to leverage coherent, correlated, or entangled electrons for QISE

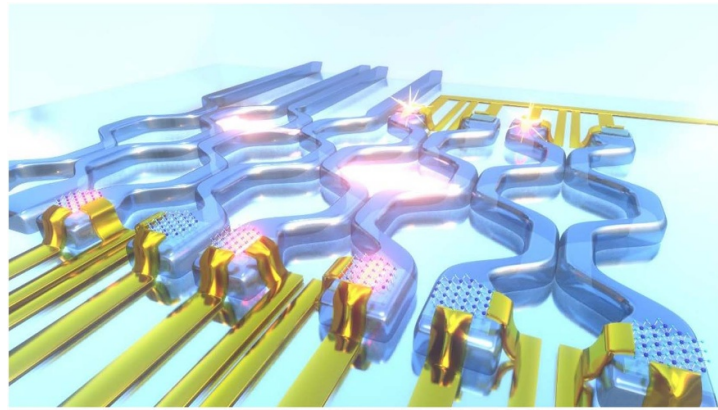


Figure 14. Scalable integrated photonics. Scalable integrated photonic circuits built from on-chip quantum devices using critically coupled LMHs. Reproduced from [188], with permission from Springer Nature.

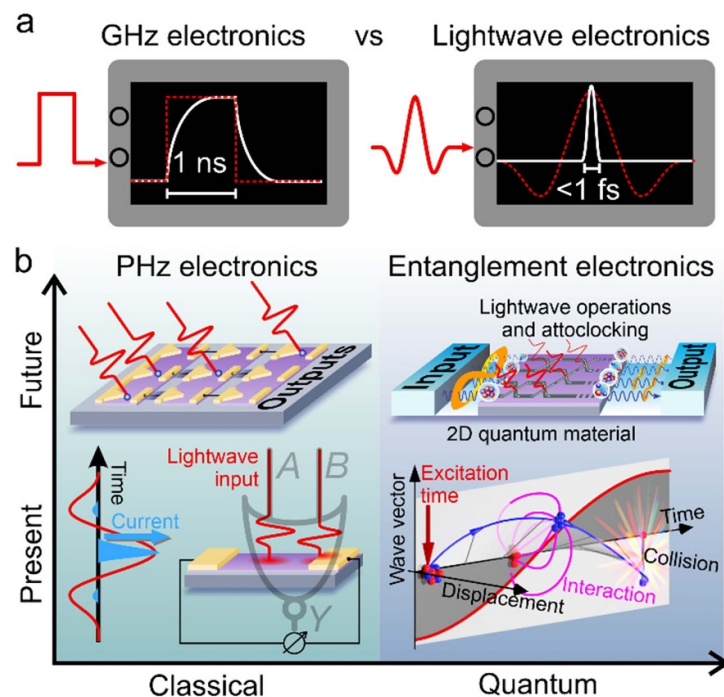


Figure 15. Vision of lightwave electronics. (a) Conventional electronic components (left) respond to an input signal (red line) with electronic response (white line) on nanosecond timescales, reaching only GHz frequencies—much slower than the intrinsic electronic scattering timescales. In contrast, a lightwave input (red line, right) can induce quantum response synchronized with its field peaks, enabling subcycle switching on attosecond timescales. As a result, lightwave electronics can operate significantly faster than electronic scattering processes, making quantum-coherent operations at petahertz (PHz) rates possible. (b) Strong lightwaves can nonlinearly and coherently excite directional currents, following the main peak of few-cycle pulses (inset, lower left). This principle has enabled basic logic-gate operations (lower left, schematic; Reproduced from [194], with permission from Springer Nature) using the carrier-envelope phase of two pulses as inputs (A and B) and the output (Y) encoded in the current between electrodes, laying the groundwork for PHz electronics. Future directions could include building an entire PHz processor (top left) by integrating hybrid multi-electrode–lightwave arrays. Lightwave-operated quasiparticle colliders can directly detect and drive multi-electron correlations (spheres) by attoclocking excitation-to-collision timing (lower right; Reproduced from [195], with permission from Springer Nature). Advances could improve excitation, control, timing, and readout of multi-electron correlations in LMs (top right; Reproduced from [189], with permission from Springer Nature) by chaining multiple quantum-state operations within the lifetime of coherences for entanglement electronics.

applications; and integrating and connecting to existing photonic or electronic platforms. Although significant progress has been made, further innovations, particularly in sequencing and chaining operations, are necessary. To achieve these stringent goals, lightwave electronics could utilize short, asymmetric lightwaves that impart net, directional momentum onto

electrons. This necessitates the development of flexible and stable methods to generate arbitrary waveforms, akin to DC pulses. To transition this technology from the laboratory to practical applications, lightwave-electronic components could be integrated with nanophotonic or plasmonic structures to locally drive and connect individual LMH components (see

figure 14) with conventional optoelectronics circuits, without relying on free-space optics. This integration is also critical for improving efficiency and reducing costs.

A combination of theoretical investigations and advanced quantum spectroscopic tools will be essential for directly accessing QISE-relevant correlations. At present, both theory and experiment face significant challenges. Multi-electron predictions are computationally prohibitive, and flexible and robust sources and detectors for complex quantum states of light remain elusive. Developing such predictive tools and technologies would be crucial for leveraging quantum states for various applications.

Advances in science and technology to meet challenges

While promising progress has been made for wafer-scale synthesis of graphene, hBN, and TMDCs, many applications in energy, AI, and QISE demand LMHs consisting of a variety of LMs with diverse physical properties. Since different LMs can require distinctive synthesis conditions, it is challenging to directly synthesize the desirable LMHs on demand. As a result, future technologies will require both wafer-scale synthesis and autonomous/robotic and AI-assisted transfer techniques [154] for the preparations of wafer-scale LMHs on demand. Successful integration of LMs into existing electronic and silicon-photonics platforms is also paramount.

Lightwave electronics has also been extended to the videography of single-electron dynamics [189] by combining near-field techniques with attosecond science. Extending this capability to visualize multi-electron correlation dynamics—capturing the temporal evolution of interactions among multiple electrons—remains an elusive goal. Understanding how many-body correlations and decoherence influence emergent phenomena is equally challenging, yet addressing these challenges could lead to fascinating quantum effects, with implications ranging from entanglement electronics to exploring the fundamental properties of quantum phases.

For QISE advances, achieving a reliable readout via quantum transduction—which converts quantum information in solids to different modes—is essential. Current developments are promising but require significant improvements to minimize losses detrimental to quantum-information applications. This underscores the need for further exploration into LMHs, digital alloys, highly efficient high-harmonic generation sources, and sophisticated quantum transduction techniques.

Concluding remarks

With their unique electronic properties and reconfigurability, LMs and their heterostructures offer numerous opportunities in energy efficient ICT, neuromorphic computing, intelligent sensing, and QISE. Future AI systems will greatly benefit from large-scale synaptic circuits based on LMHs. As one of the fastest-growing electricity consumers globally, ICT can markedly improve its energy efficiency through integrating LMH optoelectronics and silicon-photonics. By integrating sensing systems with synaptic circuits, it becomes possible to directly process sensed information with AI algorithms, substantially mitigating information transmission bottlenecks.

This ongoing integration promises reduced production costs through simpler designs, while delivering higher data rates at lower power consumption, critical for advancing 5G, 6G, ubiquitous sensor networks, and AI. The capability of LMs to transmit and receive multiple wavelengths provides a cost-effective solution to achieve necessary data rates beyond the year 2025. Additionally, LMs used as broadband PDs are pivotal for mid-IR detection—the fingerprint region for many gases and molecules—where conventional silicon-photonics PDs are unsuitable. This is crucial for a range of applications in healthcare, security, and environmental monitoring.

For QISE, lightwave electronics presents unique opportunities to control and measure the dynamics of electronic quantum states and their correlations at natural time and length scales. The integration of LMs is essential in enhancing existing optoelectronics with entanglement processing capabilities. This could revolutionize classical technologies by increasing clock rates into the PHz regime, and quantum technologies by unlocking the full quantum potential of semiconducting LMs.

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13. 2D Semiconductor FET and 3D integration

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Status

The atomically thin channels of 2D semiconductors (in particular, TMDCs) enable ideal switching behaviour at nanometre channel length and provide the ultimate material solution for device miniaturization. The weak vdW interaction allows for seamless monolithic 3D (M3D) integration with Si and other materials to address the limitation silicon-based approaches in terms of density, interconnection and multi-function. With their exceptional advantages such as ultimate device scaling, M3D integration, and heterogeneous integration potential, 2D semiconductors represent the most promising pathway for extending Moore's Law and enabling beyond-Moore's-Law technologies.

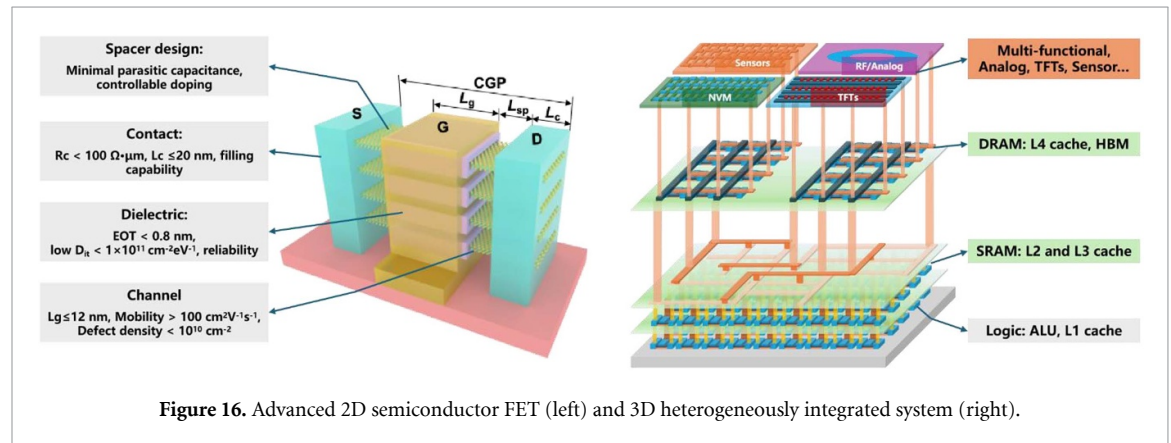
Since the first MoS₂ FET, 2D semiconductor transistors have achieved remarkable progress over the past decade [196–198]. At device level, developing technologies that simultaneously satisfy performance, power, and area (PPA) requirements is crucial, which demands co-optimizations of contacts, gate

dielectrics, doping and parasitic capacitance while scaling down device dimensions. Effective switching behaviour at gate lengths as short as 0.3 nm has been demonstrated [199], showcasing the scaling potential of 2D semiconductor. However, in advanced nodes, contacted gate pitch (CGP) is scaled all together, and both channel and contact length need to meet stringent requirements. Recently, several semimetals such as bismuth and antimony have been shown to form an atomically sharp interface with MoS₂, yielding a specific contact resistivity of $42 \Omega \cdot \mu\text{m}$ [200, 201]. Building on this and orbital hybridization, state-of-the-art semi-metallic Sb (01 $\bar{1}$ 2) contact now achieves $R_c = 85 \Omega \cdot \mu\text{m}$ at $L_c = 20 \text{ nm}$, lower than Si transistors [202, 203]. By simultaneous scaling channel and contact, the first 1 nm node FET with CGP = 40 nm was successfully demonstrated whose key PPA metrics meet the International Roadmap for Devices and Systems (IRDS) target [203] (see table 1).

Achieving small effective oxide thickness (EOT) is essential to suppress short-channel effects in scaled transistors, regardless of architecture. Due to the absence of dangling bonds, direct ALD is challenging. By introducing organic or inorganic buffer layers, sub-1 nm EOT and 60 mV dec^{−1} switching have been demonstrated in 2D semiconductor FETs by ALD [204–208]. vdW stacking is another interesting approach. By transferring high-k dielectric nanosheets—such as SC Al₂O₃, SrTiO₃, and GaF₂—on to 2D semiconductor channel, transistors with scaled EOT and pristine interface have also been demonstrated [209, 210]. Beyond planar devices, the industry has been placing significant emphasis on advancing technologies for 2D semiconductor GAA devices. Leading organizations such as IMEC, TSMC, and Intel have unveiled their manufacturing process flows for GAA devices and conducted systematic simulations [211–213]. A critical challenge remains achieving uniform deposition of the surrounding dielectric layer. TSMC presented the first Demonstration of a GAA Monolayer-MoS₂ Nanosheet nFET, achieving $410 \mu\text{A} \mu\text{m}^{-1} I_D$ at 1 V V_{DD} with a 40 nm gate length [212]. In advanced process devices, doping plays a critical role in reducing contact resistance, the series resistance in spacer regions, and parasitic capacitance. However, due to their atomically thin bodies, 2D semiconductors cannot be doped via ion implantation. Their relatively large ionization energies also make it difficult to effectively activate dopants introduced directly, rendering doping technology for 2D semiconductors a significant ongoing challenge. Recently, researchers have achieved a substantial reduction in parasitic capacitance by introducing air-gaps, enabling devices to reach a gate delay of less than 37 ps-comparable to that of silicon-based devices at the same technology node [213].

Table 1. Key performance benchmark of state-of-the-art silicon and 2D technology with IRDS requirements.

	3 nm Fin-FET(HP)	IRDS 2028(HP)	IRDS 2028(HD)	2D (At present)	2D (Requirements)
I_{on} ($\mu A \mu m^{-1}$)	874	759	546	1200	2000
I_{off} ($nA \mu m^{-1}$)	10	10	0.1	$<10^{-3}$	$<10^{-3}$
SS($mV dec^{-1}$)	82	70	67	60	60
CGP (nm)	48	42	42	40	≤ 40
R_c ($\Omega \mu m$)	271	245	245	42	<100
EOT (nm)	1	0.9	0.9	0.5	0.8
D_{it} ($cm^{-2} eV^{-1}$)	$<1 \times 10^{10}$	$<1 \times 10^{10}$	$<1 \times 10^{10}$	$<1 \times 10^{12}$	$<1 \times 10^{11}$
Mobility ($cm^2 V^{-1} s^{-1}$)	125	80	80	>100	>100
Defect density (cm^{-2})	$<10^6$	$<10^6$	$<10^6$	$<1 \times 10^{12}$	$<1 \times 10^{10}$

**Figure 16.** Advanced 2D semiconductor FET (left) and 3D heterogeneously integrated system (right).

2D semiconductors naturally exhibit a layered vdW stacked structure. Due to the absence of covalent bonding between the 2D material layers and the underlying materials or substrate, they can be integrated with back-end-of-line (BEOL) circuits on a front-end-of-line substrate using low-temperature transfer or growth techniques. Therefore, 2D semiconductors are recognized by the IRDS as one of the most promising materials for M3D integration. Furthermore, M3D integration (see figure 16) offers significant advantages over traditional packaging approaches by enabling seamless vertical stacking of devices on a single substrate without the use of through-silicon vias or microbumps [214]. Unlike packaging methods, which rely on stacking pre-fabricated chips and introduce parasitic capacitances and interconnect delays, monolithic integration employs ultra-dense inter-tier vias and low-temperature processes to achieve higher vertical interconnect density and reduced signal delay. This approach not only minimizes the physical footprint but also enhances energy efficiency and performance by allowing transistor-level partitioning and closer proximity of stacked layers. Furthermore, monolithic integration supports the incorporation of diverse materials and functionalities—such as logic, memory, and sensing—within a unified 3D architecture, making it ideal for advanced computing applications and energy-efficient systems.

Recent advancements in M3D have achieved remarkable progress, including wafer-scale fabrication of 2D material-based FETs using MoS_2 and WSe_2 [215, 216]. These breakthroughs feature multi-tier stacking with low thermal budgets ($<200^\circ C$), preserving the integrity of lower layers while enabling diverse functionalities such as logic operations, memory, and sensing. CMOS circuits, such as inverters and NAND gates, have been successfully realized using complementary n- and p-type FETs in vertically stacked configurations [217]. Additionally, heterogeneous M3D integration of graphene-based sensors with MoS_2 memtransistors has enabled near-sensor computing, supported by ultra-dense interconnects with 62 500 I/O per mm^2 . Expanding this paradigm further, a six-layer 3D nanosystem integrating transistors and memristors has demonstrated AI task execution [218]. Collectively, these advancements highlight the scalability and versatility of 2D materials in redefining semiconductor architectures and capabilities.

Current and future challenges

For M3D integration, the inter-tier challenges such as electrical isolation, topography management, and thermal dissipation become increasingly critical as the number of stacked layers grows [219]. Heat buildup in dense 3D architectures poses a significant risk to performance and reliability, necessitating innovative solutions like heat spreaders (HS),

thermal vias, and materials with high thermal conductivity. Graphene's exceptionally high in-plane thermal conductivity—up to $5000 \text{ W (m}\cdot\text{K)}^{-1}$ at room temperature—allows it to serve as an effective HS between tiers in 3D stacks, significantly reducing localized hotspots. Simulations show that incorporating graphene layers can lower peak temperatures by as much as 68 K compared to stacks without graphene. Additionally, h-BN provides excellent thermal conduction with low interfacial thermal resistance, enhancing electrical isolation and thermal coupling between layers. Additionally, achieving a smooth planarized surface is essential to reduce topography-related impacts on top-tier device fabrication, ensuring layer uniformity and alignment. Device-to-device variability further exacerbates these issues, particularly in high-density circuits where precision is paramount. Finally, achieving dense and reliable interconnects while maintaining structural integrity and ensuring compatibility with BEOL processes adds to the complexity of scaling efforts, requiring holistic solutions across material, process, and architectural dimensions.

Advances in science and technology to meet challenges

On the design side, reliable technology computer aided design model, process design kit (PDK) and electronic design automation (EDA) tools for 2D semiconductors are needed to transition from individual device and small-scale systems to very-large-scale integration [220–222], [28]. We need to better control material defects and process variations and come up with variation-aware design methodology to bridge this gap. The EDA tools for 3D integration of 2D materials include multi-PDK support for hybrid CMOS and 2D material processes, advanced multi-physics simulation for electrical, thermal, and mechanical effects, and

precise interface modelling to optimize 2D material-silicon contacts. For 3D architectures, tools must handle high-aspect-ratio structures, ensure uniform deposition, and extract parasitic in complex interconnects. System-level co-simulation is critical to integrate analogue, digital, and RF components with 2D material-based devices. Additionally, tools must enable modular design, efficient thermal management, and robust reliability analysis to support scalable, high-performance 3D heterogeneous integration.

Concluding remarks

To realize the vision of commercial-scale M3D integration of 2D materials, research and development efforts must prioritize scalable and reliable fabrication processes. Immediate goals include refining synthesis methods to produce defect-free, uniform 2D materials at 6–8 inch wafer scale and developing transfer techniques that preserve material quality and ensure clean interfaces and low strain across the entire wafer. Innovations in BEOL-compatible processes will be crucial for seamless integration into existing silicon-based manufacturing workflows. Mid-term objectives involve the realization of unified 3D architecture that integrate diverse functionalities, such as logic, memory, and sensing, within a single chip. Achieving inter-tier electrical isolation and mitigating thermal effects will be essential for robust, high-performance systems. Long-term aspirations include the commercialization of multifunctional 3D chips that leverage the unique properties of 2D materials for applications in neuromorphic, quantum, and AI computing. The integration of 2D materials into 3D architecture offers transformative potential, enabling task-specific, energy-efficient, and versatile electronics. By addressing these challenges, the semiconductor industry stands poised to usher in a new era of sustainable and advanced computing technologies.

14. 2D materials for energy storage

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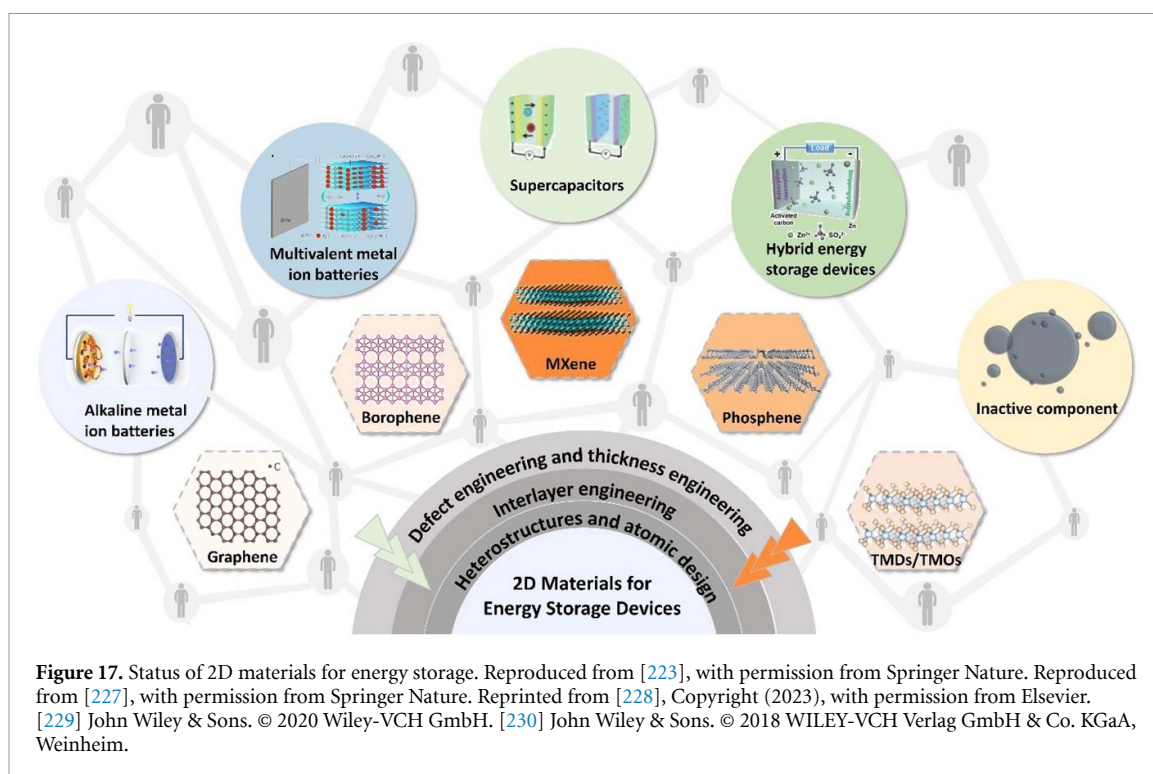
Status

Energy storage, particularly batteries and supercapacitors, has garnered overwhelming interest in the last few decades to overcome the issue of intermittency of sustainable green energy due to the geographical and seasonal dependence for impending energy crisis and CO₂ emission reduction [223–226]. As essential components of batteries or supercapacitors, electrode materials greatly determine the key electrochemical performance and practicality for applications. Unlike bulk materials, which suffer from limited ionic adsorption sites and violent volume changes, 2D materials have emerged as promising electrode materials, having made a monumental leap since the discovery of graphene in 2004 (figure 17). For energy storage devices, most researchers focus on inorganic 2D materials, such as graphene and their derivatives, TMDCs, transition metal oxides, layered double hydroxides, metal carbides/nitrides, hBN, black phosphorus, etc. Presently, 2D materials could perform as different components in energy storage devices with fast ionic transport and adjustable physicochemical characteristics. (i) *Electrodes materials*. With tuning of morphology, framework and charge transport properties through doping, alloy composition,

hybridization, and surface functionalization, heterostructures through vdW, especially for combination of conductive and active components, are prone to high capacity, high power/energy density and long cyclability [227–230]. (ii) *Inactive components*. Some 2D materials could perform as conductive additives for constructing conductive cross-linked network, depending on the full contact among points, lines and surfaces. Remarkably, holey 2D materials with adjustable and customized framework hold promise for filtration or selective ion transport as separators or electrode|electrolyte interface. For improving the potential of 2D materials in present and future applications, it is important to tune the properties of 2D materials when it comes to interlayer interaction, in-plane bonding configuration, Fermi energy level, electronic band structure and spin–orbit coupling [231].

Current and future challenges

Some issues must be addressed before the properties of 2D materials could be used to the fullest extent [232, 233]: (i) *instability of nanosheets morphology and limited electrochemical performance of single 2D materials for electrode materials*. Due to the high surface free energy of 2D materials, tendency to restack in no order restricts the utilization rate of edge and in-plane active sites. Additionally, although 2D materials with expanded interlayer distance contribute to the improved electrochemical performance for electrode materials, the larger interlayer distance means the decrease of volumetric energy density of batteries. (ii) *Unclear specific mechanisms for energy storage devices*. Previous investigations report that graphene and other 2D materials could be combined to improve the energy storage performance via different methods, such as ample geometric defects, surface wrinkles/corrugations, but most of them rarely clarify clearly the synergistic effect. (iii) *Lack of precise application-driven design*. Notably, the general permutations and combinations of different 2D materials cannot meet the requirements from different scenarios. The greater the complexity and multifunctionality demanded by the intended applications, the more sophisticated the synthesis strategies should be to exercise control over the structure, atomic arrangement and morphology [234]. Specially, the atomic-level microstructure and electrochemical performance for energy storage devices, such as catalysts for metal-air batteries, needs further explorations. (iv) *Difficult scalability and reproducibility* [235]. It is still difficult to control dimensions and structures of 2D nanosheets with high quality and high production rate, considering the high cost and environmental



concerns. Future generations of printable energy storage devices require the processability of the hybrid materials.

Advances in science and technology to meet challenges

To deal with the above challenges, ingenious strategies and technologies need to be explored to enable accurate synthesis of 2D materials and deep understanding of structure-property relationships. Recent advances in fabrication technologies, such as solid lithiation and exfoliation, ALD and molecular beam epitaxy, allow precise control over thickness and composition, especially for the scalable production. To improve the electrochemical performance for energy storage devices, surface chemistry of 2D materials is adjusted through chemical doping and surface functionalization for pseudocapacitance and charge carrier concentration improvement, interlayer enlargement for large ion storage and fast kinetics, Janus structure for improving binding energy with electrolyte ions and metals and other controlling methods. Since Janus structure is not cost-effective, alternative 2D materials-based heterostructures with amorphous architecture could alleviate structural stress in charging/discharging process, devoting to the high-rate capability and long cyclability. From this point of view, defect engineering and interface engineering are promising to modulate the physicochemical characteristics of 2D materials-based heterostructures. Furthermore, regulation of chemical affinity of 2D interfaces associated with the surface charge density and distribution could be an interesting topic for metal-air batteries. To further figure out the

synergistic effects, specific model system and further DFT investigations are supposed to be carried out. Unique technologies that go beyond conventional characterization techniques, such as scanning electrochemical microscopy or EQCM, appropriately supplement our understanding of such systems by offering direct insights into the reaction behaviour of samples at the nanoscale level, including the interfacial charge transfer and ionic transfer. Furthermore, advanced computational techniques like high-throughput computational screening and ML to guide more accurate and efficient synthesis is a promising solution.

Concluding remarks

Since it is in the early stage of 2D materials development and their industrialization, the promising pathways of 2D materials in the future could be considered in the following aspects. (1) *Cost-effective and precise synthesis technologies with high performance.* To overcome the traditional methods with cumbersome and complex feature, solution-based methods, such as solid lithiation and exfoliation, become alternatively innovative method, which provide a way of modifying the characteristics of 2D materials during the growth process. Specifically, interlayer engineering could be a complement way to host the ions with large radii. (2) *Advanced characterization and computational simulation.* To ensure quality control and clarify the material growth mechanisms, it is essential to record real-time observations during the growth of 2D materials and device fabrication processes. Additionally, comprehensive understanding of the promotion mechanisms in energy

storage devices (e.g. binding ability, charge transfer number) would require further developments on the *in-situ* probe techniques and DFT approaches. (3) *All-2D system construction*. Capitalizing on the advantages of 2D materials in terms of size reduction, planar electrochemical energy storage systems are of great importance for further practical application and model system for characterization, which have been achieved through complete integration of electronics and energy storage on a single substrate. (4) *Selective and specific applications*. For all-solid-state batteries and future generation of printable energy storage devices, 2D materials provides a feasible way for constructing a highly conductive

network or highly ion conductive interphase. Close collaboration and coordination among different fields could facilitate smooth development of 2D materials for next-generation energy storage.

Acknowledgments

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15. 2D materials for electrocatalysis

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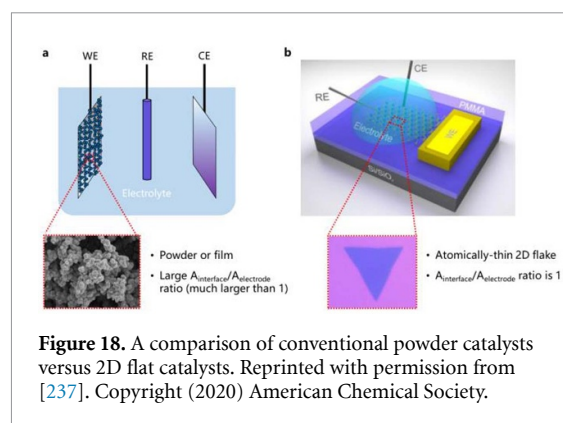
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Status

Electrochemically converting a chemical into another more value added one via electrocatalysis is a promising technology, especially when the reaction is driven by green electricity from solar, wind, hydro-power, etc, which can realize the goal of 'kill two birds with one stone'. On one hand, it starts with cheap resource like water or even unwanted harmful reactants like carbon dioxide, contaminates in water, etc. On the other hand, it can produce valuable products without consumes much fossil resource. Different types of electrocatalysis reactions have been studied extensively, from water electrolysis which produces hydrogen and oxygen discovered in 1800, to other reactions including electrochemical carbon oxide reduction, nitrogen reduction, oxygen reduction, water oxidation, organic molecule oxidation, organic electrosynthesis, and different coupled reactions. The field is becoming increasingly important and urgent these years due to global mission of carbon neutrality.

The use of an efficient electrocatalyst is key for industrial implementation of these techniques, because a suitable electrocatalyst can decrease reaction barrier and consequently electricity consumption during reaction. This in turn will reduce the cost of the conversion process to make it economically competitive over traditional conversion process like thermal catalysis. Among various catalysts, 2D materials including single-element ones like graphene, thin layer metal (metallene) or non-metals (e.g. phosphorus, silicene), as well as compounds represented by TMDCs/carbides/nitrides/phosphides, carbon nitrides, are particularly promising [1, 236]. First, they have large surface area which will help adsorb reactants and catalytic reaction. Second, 2D materials have a flat and well-defined structure without surface reconstructions, making them ideal model catalysts for mechanism studies (figure 18). For example, MoS₂ is a well-known electrocatalyst for HER, and monolayer MoS₂ is widely used for mechanism study because of its well-defined structure [237]. Third, there are many types of 2D materials with widely tunable compositions and electronic structures, and 2D materials can feasibly assemble into a whole structure with finely engineerable micro- and macro-structures. For example, Luo *et al* reported the synthesis of 2D MoS₂/Mo₂C heterostructures for hydrogen evolution at high-current-density



(HCD), in which MoS₂ nanosheets help mass transfer and Mo₂C decorates improve catalytic activity [238]. Other advantages of 2D materials include low-cost mass production capability, thin thickness induced easier charge separation, etc. All these features suggest that 2D materials are promising in various electrochemical conversion technologies, as witnessed by the achievement of using 2D material electrocatalysts in the past two decades. Due to large amount of 2D materials as well as different types of electrocatalysis processes, this section will mainly focus on 2D metal compound catalysts especially transition metal sulphides/nitrides/carbides, and their uses in water electrolysis to narrow down the topic.

Current and future challenges

Despite with great success, there are several challenges in 2D material electrocatalysis. The first challenge is about the structure of real active site. Of course, one needs a catalytic active site with the best intrinsic activity, meaning suitable and balanced adsorption energy to different intermediate species. In reality, several factors may affect the structure of real active site, including electrolyte environment, pH, pressure, voltage, etc. Meanwhile, catalyst usually undergoes surface and sub-surface reconstruction, especially at oxidative potential, making accurate identification of real catalytic active site under operation conditions challenging [239]. The second challenge is about HCD performance over a long period. To make various electrocatalysis technologies practical useful, it is a must to go to HCD. The overall performance of a catalyst at HCD are jointed determined by many factors including intrinsic activity of active site, amount of active site and their exposure, mass transport, electron transport, microstructure of catalysts, etc. In addition, when translocate the performance of an electrocatalyst from three-electrode cell to a membrane electrode assembly device, other factors will play roles, for example, interface between catalyst and support, chemical and mechanical robustness of the electrode, etc. The third challenge is about selectivity to a certain product. For some electrocatalytic conversion processes like carbon dioxide reduction and organic electrosynthesis, there are multiple

products generated simultaneously, including C1, C2, C3, and higher, as well as different enantiomers [240]. Separation of different products could be energy and time extensive, and therefore, developing catalyst which show high selectivity to certain products and can operate with a high partial current is important. The fourth challenge is about economic considerations, including electricity cost and catalyst cost.

Advances in science and technology to meet challenges

New techniques and understandings are needed to address the above challenges. First, among all types of catalysts, 2D materials might be the ideal platform to identify the real active site, mainly because the dangling bond free and surface reconstruction free feature of 2D materials. As a comparison, nanoparticle catalysts may have surface reconstruction, which becomes more complicated when putting into liquid electrolyte and applying a voltage. From this angle, researchers can pay more attention to use 2D materials as model catalysts for mechanism studies, including compare intrinsic activity of different sites, dopants, point defects, edge configurations, etc [241, 242]. *In situ* techniques like spectroscopy and high-resolution imaging will be necessary. Note that micro-cell devices are interesting to study 2D material electrocatalysis and correlate activity with material structures. It is also noteworthy that there is still interest to explore new 2D material catalyst, as witnessed by a recent work reporting synthesis of 2D tungsten MXene ($\text{W}_2\text{TiC}_2\text{T}_x$) for hydrogen evolution [243]. Second, 2D materials can assemble into a monolith with engineerable structures. By selecting 2D materials with high activity, and optimizing macro- and micro-structures, one can obtain catalysts with high performance at HCD. Besides that, for such high performance monolithic catalytic electrodes, one needs to pay attention to their stability, mainly including chemical stability and mechanical stability, which is a prerequisite for long term use under extensive bubble bombardment. For chemical stability, the formation of a stable reconstructed layer may be important. For mechanical stability, a strong covalent or metallic or ionic bonding at interface of catalyst and support is important. Meanwhile, such a strong bonding should not induce a large charge transfer resistance across the catalyst-support interface, as demonstrated in a recent work showing the preparation of a family of homologous metal heteromaterials with chemically bonded metallic interface for very stable electrolysis [244]. Third, the selectivity of hydrogen or oxygen production in water electrolysis under pure, alkaline, or acidic water is high enough. Meanwhile, the selectivity of C1 or certain C2 products in carbon oxide reduction is also high

to meet applications. However, for water electrolysis in complicated electrolyte like contaminated water or sea water, selectively generation of hydrogen and oxygen against other products like chlorine still needs to be improved. For carbon dioxide reduction, obtaining C3 or higher carbon products with high selectivity and Faraday efficiency are important tasks, which can be solved by using highly active and selective catalysts well positioned on a stable support. Also, there are various new electrochemical reactions aiming for synthesizing products by electricity, in which selectivity towards one certain produce is important. Fourth, increasing energy efficiency, i.e. produce more target products under certain electricity is an important criterium for economic considerations, which calls for high performance and highly selective catalysts. Reducing amount of noble metals by alloying, single atom catalysis, functionalization, defect engineering, strain modulation, exposing as many as possible noble metals to reactants, are useful ways to reduce catalysts cost. Meanwhile, using earth abundant resources especially minerals like molybdenite made of 2D MoS_2 [245], is promising to pursue further.

Concluding remarks

To conclude, 2D materials have shown promising as high-performance durable catalysts for various electrochemical reactions. Several 2D materials-based water electrolysis catalysts have shown potential to run at HCD over long period in three-electrode cells and membrane electrode assembly electrolyzers, while more efforts are needed to move forward for large scale industrial implementation. The use of 2D materials in other electrochemical reactions beyond water electrolysis and carbon oxide reduction are mostly in the fundamental study stage, in which more efforts are needed to elucidate the reaction active site, improve selectivity, and make it works robust over long-term operation at industrial required current density conditions.

Acknowledgments

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16. Filtration and separation with 2D materials

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Status

Membranes are key components in systems as diverse as batteries, fuel cells, controlled delivery devices, solar cells and large-scale energy-efficient separation and purification systems. Wherein the membranes act as a selective barrier that selectively lets some components (e.g. gases, liquids and ions) transport while restricts the movement of others. Current membranes, especially polymeric membranes, generally suffer from the trade-off relationship between permeability and selectivity. New membrane materials are developing to surpass the limitation.

The discovery of graphene opens a new era of 2D materials [1]. Featuring with unique atomic thickness and micro-metre lateral dimensions, 2D materials offer new opportunities for the next generation of high-performance (high permeability, high selectivity, and stability) separation membranes. There are two main types of 2D materials membranes (2DMMs): single-layer (porous nanosheet) membrane and laminar membrane. The former one is composed of monolayer or a few layers of 2D materials with intrinsic or perforated in-plane nanopores. The latter one is fabricated by assembling nanosheets.

2DMMs represented by graphene and graphene-derived materials have driven rapid progress in the past decade. Figure 19 displays a historic timeline and highlights some breakthrough in 2DMMs field. The first 2DMMs were produced between 2008 and 2012 with single layer graphene [246] and laminar GO membranes [247], respectively. In the following years, more attention is paid to the theoretical study of molecular transport [248], the precise construction and regulation of nanochannels in 2DMMs (e.g. tuning interlayer spacing [249] and intrinsic pore size [250], creating in-plane pores [251]), and the improvement of stability [252]. The booming of graphene membranes also inspires researchers developing other 2DMMs, such as MXene, transition-metal phosphorus trichalcogenides nanosheets [253], MoS₂ [254] membranes. To meet the standard of industrial application, the scale-up in 2DMMs [252] is underway.

Current and future challenges

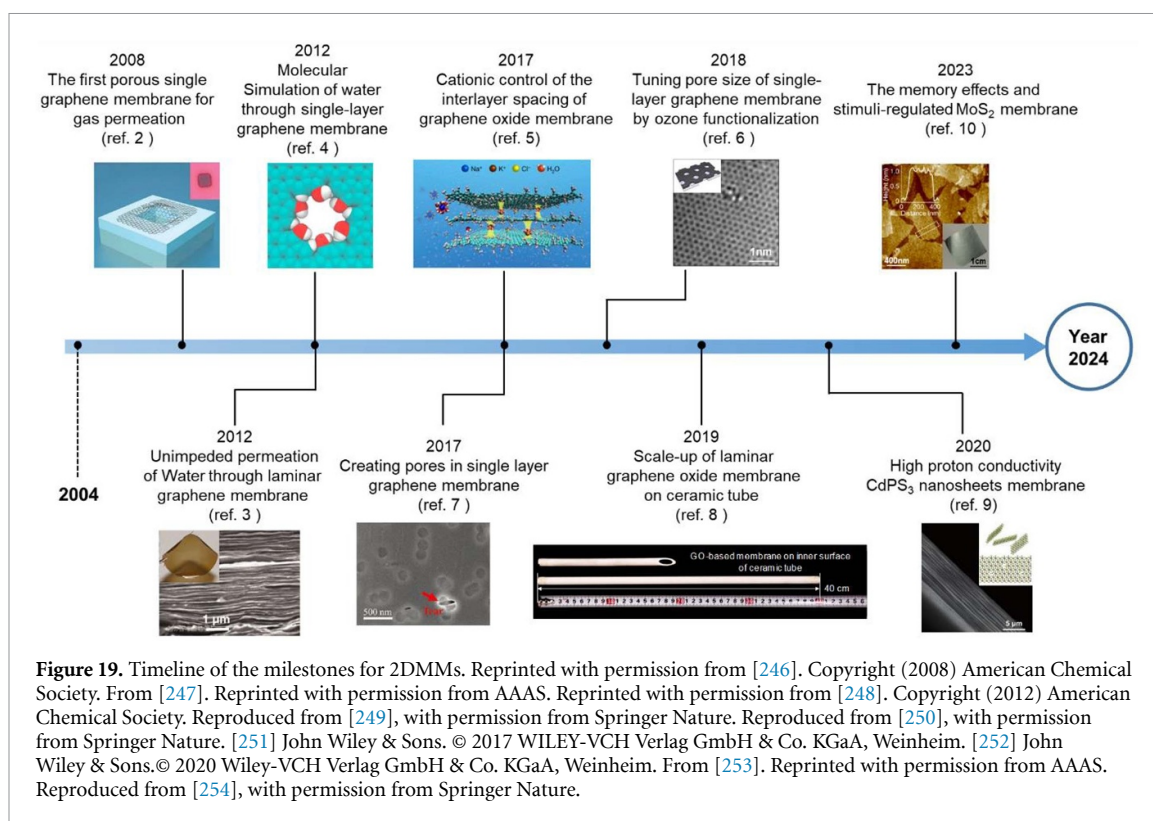
Since the discovery of graphene in 2004, a great success for 2DMMs has been achieved. Nevertheless, there are still some issues and challenges to be

addressed. For the single-layer (porous nanosheet) membrane, the major challenge lies in that it is hard to synthesize high-quality single or few layer with controllable features (e.g. pore size, in-plane porosity, and functionalization degree) and the reproducibility of nanosheets is insufficient, which generally are essential to unlock the potential of scale-up of 2DMMs towards practical application. For laminar membrane, the key point lies in how to precisely control the interlayer spacing especially at the angstrom scale. The stability for real-world applications is another concern. The membrane swelling easily generates especially in aqueous solution that will enlarge the interlayer channels and decrease the size-sieving property, thereby leading to the membrane disintegration. At present, it remains challenging to accurately characterize the subnanometre transport channels and there is a lack of theoretical models for the description of mass-transfer behaviour within these channels of 2DMMs. The application of 2DMMs towards challenging mixtures separation (e.g. olefin/paraffin, xylene separations) has not been fully demonstrated yet. More importantly, the 2DMMs synthesis is only on the laboratory scale, more efforts should be devoted on the scale-up of defect-free 2DMMs to meet the requirement of real industry applications.

Advances in science and technology to meet challenges

To meet the above-mentioned challenges, the following aspects should be considered:

- (i) *Nanochannel construction and application for challenging separation.* Owing to the uneven distribution of functional groups or intercalators in 2DMMs, the interlayer nanochannels or in-plane pores are undesirable for separating challenging mixtures with very close molecular sizes, such as olefin/paraffin, O₂/N₂, and xylene separations. Thus, it needs to develop novel 2D materials with uniform functional groups and well-defined pore apertures and novel strategies to regulate the nanochannels to sub-angstrom-scale precision are also highly necessary.
- (ii) *Nanochannel characterization and transport mechanism.* Advanced characterization techniques at atomic-scale resolution, such as positron annihilation lifetime spectra and *in situ* high-resolution transmission electron microscopy, need to be developed to reveal the structures of the nanochannels of 2DMMs and probe the real-time molecular/ionic transport behaviours in nanochannels, which can be combined with theoretical calculation to establish the theoretical model for guiding the rational



structural design and performance optimization of 2DMMs.

- (iii) *Large-scale fabrication and performance evaluation under practical conditions.* Novel synthesis methods for 2D materials and defect-free, large-scale 2DMMs need to be developed, and the yield of high-quality nanosheets needs to be enhanced to satisfy production demands. The performance evaluation should consider the real application conditions, such as high temperature, high pressure, and the possible contaminants-containing feed.

Concluding remarks

The field of 2DMMs is rapidly growing, high-quality single and few-layered nanosheets with different nan-

omaterials have been developed for high performance separation membranes. In the future the atomic-scale characterizations and mass transport mechanism should be strengthened. More efforts can be devoted to new construction strategies with integration of mathematics, physics, chemistry, materials and AI and meanwhile the scale-up for real industry application.

Acknowledgments

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17. 2D materials for thermal management

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Status

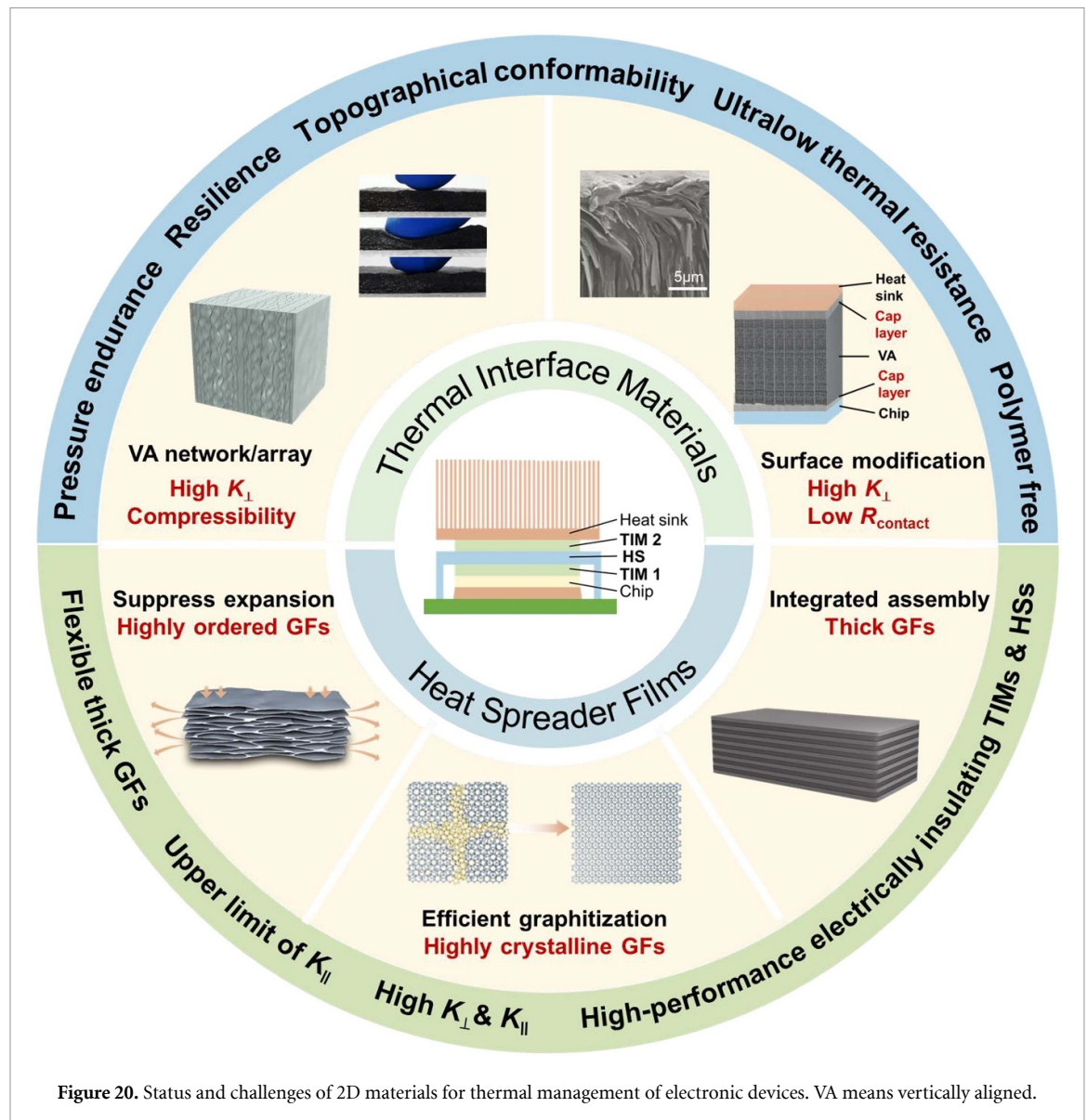
The integration of chiplets into system-level packaging, driven by advancements in AI, high-performance computing, the Internet of Things, and 5G/6G communications, has been formally incorporated into the IRDS. However, the high degree of integration leads to significant overheating issues, which have become a primary factor limiting the performance, reliability and longevity of electronic devices. This urgently calls for the development of efficient thermal management materials and technologies to ensure the optimal performance and reliability of electronic devices. A typical thermal management system in integrated circuit (IC) chips, as illustrated in figure 20, consists of a heat sink, an integrated HS, and two thermal interface materials (TIMs), designated as TIM 1 and TIM 2 [255]. TIMs reduce thermal resistance by filling air gaps between the IC and heat sink, while the HS dissipate heat from hotspots to broader areas.

2D materials, characterized by atomic-scale thickness and extended lateral dimensions, exhibit exceptional in-plane thermal conductivity due to their highly ordered lattice structures and strong covalent bonds, offering promising solutions for next-generation thermal management challenges. For instance, graphene demonstrates an ultrahigh in-plane thermal conductivity of up to $5300 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, while h-BN, an electrical insulator, also exhibits high in-plane thermal conductivity up to $700 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ [255, 256]. However, 2D materials (nanosheets) typically need to be assembled into macroscopic assemblies for thermal management applications, such as films for HS and arrays or networks for TIMs. The thermal conductivity of these 3D assemblies is influenced not only by lattice defects in the nanosheets, such as vacancies, heteroatoms, and GBs, but also by macroscopic structural disorders like disordered nanosheet arrangements [257]. These challenges can be effectively mitigated through high-temperature treatments and alignment assembly techniques that orient the nanosheets along a specific direction [257, 258]. In addition, these 3D assemblies must also meet stringent requirements for mechanical properties and stability to ensure their practical applicability in thermal management systems.

Advanced TIMs must simultaneously exhibit high through-plane thermal conductivity and excel-

lent compressibility. The mostly widely used TIMs are polymer-based composites, which are fabricated by incorporating highly thermally conductive fillers, such as graphene and h-BN, into polymer matrices [226]. However, a trade-off exists between thermal conductivity and compressibility. While higher filler content enhances thermal conductivity, it often compromises compressibility, making the composite less effective at accommodating assembly tolerances. To meet practical application requirements, TIMs should demonstrate good compressibility under low pressure, specifically achieving a thickness reduction of 30%–60% under pressures ranging from 0.2 to 0.5 MPa. To fully utilize the intrinsic thermal properties of 2D materials, researchers are focusing on creating continuous and efficient thermal pathways, such as constructing high-crystalline vertically aligned graphene and h-BN networks or arrays [259–261]. Furthermore, to optimize heat dissipation efficiency, surface structure optimization of these vertically aligned 3D assemblies is crucial for minimizing interface thermal resistance. This can be achieved by applying a cap layer to the surface of TIMs in contact with the chip/heat sink to match the rough topography of heat sinks and increase the effective heat transfer area. Strategies include modifying the surface with low-melting-point metals [262] and constructing arc-like arrangements on vertically aligned networks or arrays [263].

Compared to traditional HS technologies, including metal foils, heat pipes, and vapour chambers, GF offers superior advantages, including high thermal conductivity, tunable thickness, good flexibility, remarkable stability, low density, and exceptional tolerance to extreme environmental. These properties make GF highly promising for applications in portable electronics and spacecraft. For these applications, achieving an in-plane thermal conductivity as high as possible is crucial, which requires GFs with ultra-low defect density, large grain size, and highly ordered crystalline structures. Current strategies to enhance the thermal conductivity of GFs focus on two key areas (1): suppression of structural expansion. GO is a widely used precursor for fabricating GFs owing to its exceptional processability. However, during thermal annealing, the decomposition of functional groups into gaseous products causes structural expansion in the film, disrupting the ordered structure. Strategies such as pre-reduction of GO precursors [264], construction of gas escape channels within GO films [265], and multi-step hot pressing [266] have proven effective in fabricating compact and ordered GFs. (2) Efficient graphitization strategies. Based on in-depth studies of the structural evolution and graphitization behaviour of GFs, strategies such as introducing high-temperature lattice defects can significantly boost



their graphitization [267]. In addition, thick GFs are necessary to ensure superior thermal transfer capabilities. Advanced integrated assembly methods, such as continuous centrifugal casting [268] and water-induced self-fusion [269], can produce highly aligned thick GFs. Stacking and adhering thin GFs through metal welding or binders has also been demonstrated as an effective approach [270]. The rapid development of fabrication technologies of GFs has also facilitated the development of h-BN films [271, 272]. Both films now have been commercialized and are now used in various high-tech fields such as smartphones and satellites.

Current and future challenges

The development of high-performance TIMs still faces several technical challenges. First, considering that the gap between the heatsink and IC can increase by several tens of micrometres at elevated temperatures, TIMs need exhibit self-recovery properties with

a recovery ratio exceeding 50% to maintain optimal thermal contact and prevent interface delamination. Second, compression in vertically aligned 2D materials-based TIMs might cause sheet tilting and interface separation, reducing thermal conductivity under high packaging pressures. Consequently, the fabrication of high-performance TIMs with resilience and pressure endurance capabilities represents an essential technical requirement. Third, traditional thermally conductive silicone greases, which are widely used as TIMs for CPU cooling due to their adequate compressibility and topographical conformability, face limitations such as volatility, poor thermal shock resistance, and inadequate long-term durability. Addressing these challenges is crucial for developing TIMs that meet the demands of diverse and extreme application scenarios.

Significant opportunities remain for advancing 2D materials-based HS. First, the upper limit of thermal conductivity for GFs is still unclear

from both fundamental and technological perspectives. Key challenges include achieving high thermal conductivity at large film thicknesses while maintaining good flexibility. It is also highly desired to improve the out-of-plane thermal conductivity of the film without significantly compromising in-plane performance. Moreover, the currently used high-temperature graphitization (2500 °C–3200 °C) results in significantly elevated equipment maintenance requirements and substantially increased energy consumption levels. Second, the progress in thermally conductive yet electrically insulating h-BN based HS significantly lags behind that of GFs, primarily due to the difficulties in mass-production of h-BN nanosheets and their chemically inert surface. A stable, additive-free h-BN dispersion is still lacking. Further research is needed to explore the potential of heat treatment to enhance the thermal conductivity of h-BN film and to understand h-BN's high-temperature fusion and recrystallization behaviour.

Advances in science and technology to meet challenges

Advances in 2D materials-based TIMs are fundamentally dependent on the rational structural design of 3D assemblies. The construction of interlocking architectures is crucial for stabilizing vertically aligned graphene arrays. Optimization of the polymer matrix and the interfacial characteristics between 2D materials and the polymer matrix is also needed. Furthermore, designing vertically aligned crumpled graphene arrays or networks would be helpful for achieving excellent resilience capability. As a high-performance alternative to traditional thermally conductive silicone greases, polymer-free all-graphene or h-BN-based 3D assemblies can be strategically designed to fully exploit their unique advantages, including good flexibility, low thermal expansion coefficient, and outstanding thermochemical stability, to function simultaneously as both an efficient thermal filler and a flexible matrix. AI is anticipated to play an important role in the design of 3D assemblies for TIMs.

To approach the limit of thermal conductivity in GFs, a comprehensive understanding of the structural and property evolution throughout the whole fabrication process from graphene into GF is crucial. This includes systematic investigation of precursor material, film fabrication process, and graphitization parameters, particularly through advanced *in situ* characterization techniques combined with theoretical simulations. The formation of multiple covalent bonds between adjacent graphene layers would be essential

for achieving high out-of-plane thermal conductivities. To address the challenges of high-temperature graphitization, developing efficient catalysts to reduce graphitization temperatures below 2000 °C represents a critical research direction with broad implications. For practical applications, low-cost and high-yield fabrication methods of 2D materials-based films and their integration with electronic components need to be developed.

The realization of thermally conductive yet electrically insulating TIMs or HSs requires more research on h-BN, including the scalable production, surface functionalization, uniform dispersion, and controlled assembly. The chemical conversion from graphene to h-BN, together with exploration of other thermally conductive yet electrically insulating 2D materials, offers a promising alternative approach.

Concluding remarks

In summary, 2D materials including graphene and h-BN have emerged as pivotal components in TIMs and HS for advanced thermal management applications. By leveraging the assemblability and scalability of 2D materials, structural designs such as vertically aligned graphene networks or arrays and highly ordered GFs have been developed to achieve optimal thermal conductivity. Although significant efforts are still needed to approach the upper limit of the thermal conductivity, practical applications require a careful balance between thermal conductivity and mechanical properties, including tensile strength, flexibility, compressibility, and resilience. Additionally, the structural and performance stability of these materials needs to be further evaluated under extreme conditions, such as high temperature, high humidity, vacuum, and strongly corrosive environments, to ensure reliability in some real-world scenarios. Furthermore, the adaptability of these materials for seamless integration with other components remains a critical consideration for their widespread adoption in next-generation electronic devices. Last but not least, cost-effectiveness is a key factor that must be prioritized for large-scale applications.

Acknowledgments

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18. Flexible electronics with 2D materials

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Status

Since the discovery of the world's first transistor in 1947, solid-state electronics has undergone remarkable development and currently achieved tremendous success. However, the next generation of everyday electronic gadgets and wearable healthcare devices is aiming for a light-weight design with mechanical flexibility, which is hard to achieve with conventional bulk semiconductors. Originally, flexible devices were created using soft organic materials or by using unconventional device architectures, where rigid bulk semiconductors were embedded into an elastomer with stretchable interconnects. However, the rigid nature of bulk semiconductors, combined with the weak biological compatibility and poor stability of organic materials, impeded further advancements and led to a need for alternative ultra-thin functional materials that are cost-effective and energy-efficient.

After the experimental demonstration of graphene flakes two decades ago, 2D materials attracted significant research attention and have been extensively explored for use in flexible electronics. The exceptional electrical, optical and sensing characteristics of 2D materials make them a suitable choice for developing high-performance electronics. Particularly, their mechanical superiorities associated with ultrathin nature and thickness controllability, make them excellent candidates for developing flexible devices on soft substrates. Various 2D materials such as graphene, TMDCs, black phosphorus, hBN, MXenes, transition-metal oxides, and 2D perovskites have been explored so far and used according to their characteristics and target applications [273]. The 2D materials-based ultrathin devices possess specific mechanical capabilities, such as bendability, flexibility, conformability, and stretchability, which arise due to their low stiffness associated with the ultralow cross-sectional area despite having a high Young's modulus. The strong intra-layer covalent bonding in layered 2D materials provides an incredibly high strain limit, high in-plane mechanical strength, and high Young's modulus. For example, graphene exhibits excellent flexibility with low stiffness, a large Young's modulus (~ 1 TPa), and high fracture strain limit ($\sim 25\%$). Whereas TMDs also exhibit large Young's modulus (120–400 GPa) with breaking strain limits in the range of 6%–11% (figure 21) [273]. Exploiting these features, 2D materials-based flexible devices have demonstrated several applications, including smart wrist bands [274], bendable

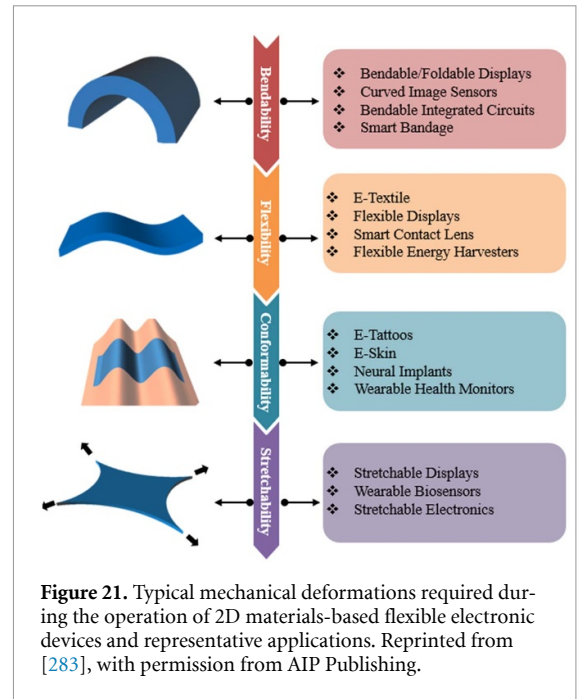
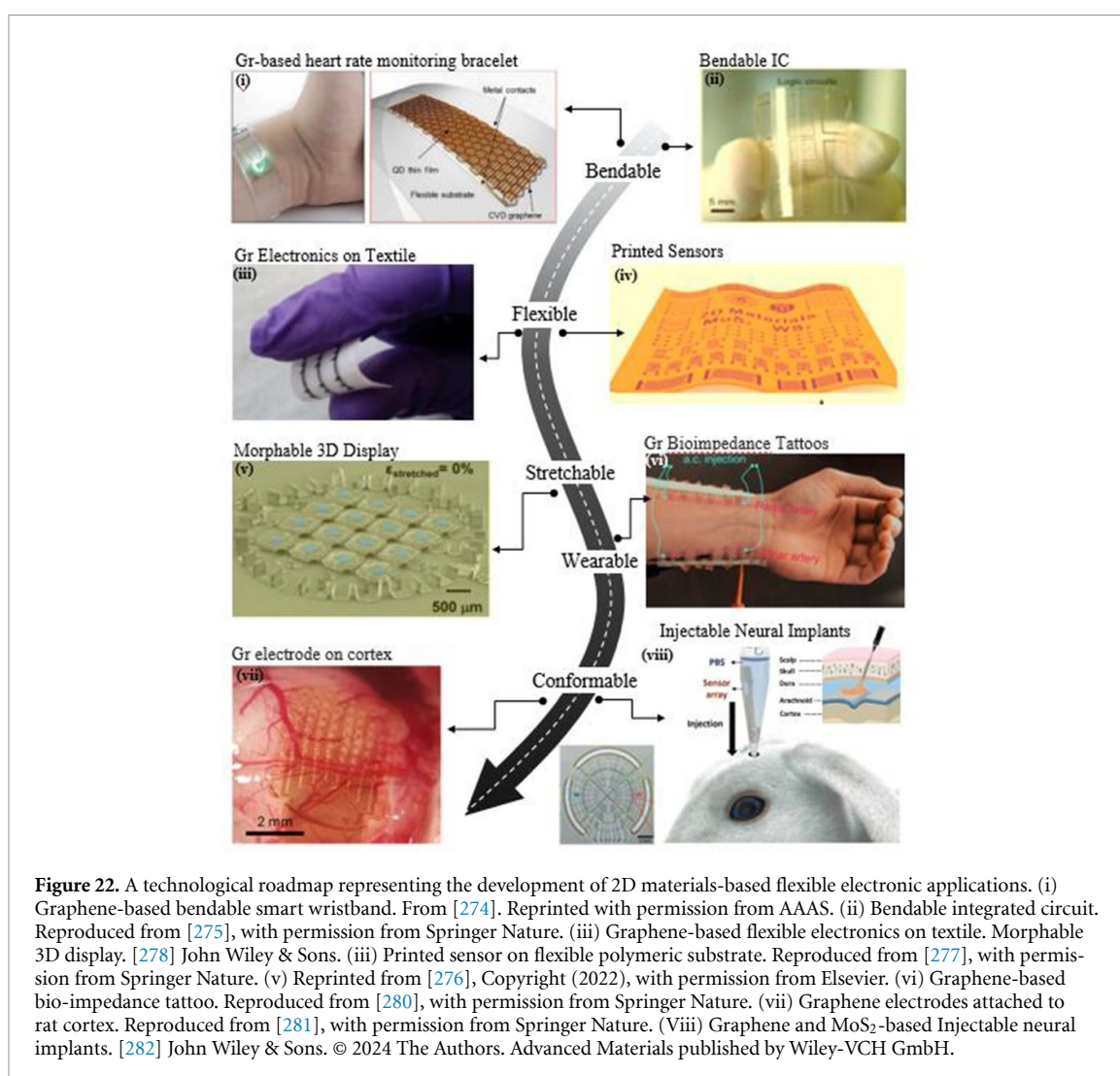


Figure 21. Typical mechanical deformations required during the operation of 2D materials-based flexible electronic devices and representative applications. Reprinted from [283], with permission from AIP Publishing.

ICs [275], flexible/stretchable displays [276], printed flexible electronics [277, 278], and sensors for use in extreme environmental conditions [279]. In addition, origami-inspired unconventional devices [276], flexible bioelectronics [280], conformable and implantable healthcare devices [281–283] have also been demonstrated (figure 22).

Current and future challenges

Due to ultralow thickness and dangling bonds-free surfaces, 2D materials hold significant potential for developing high-performance flexible electronics. However, 2D materials face several inherent limitations and challenges that hinder their deployment at commercial level. For example, the existence of high contact resistance, difficult deposition of high-quality dielectric material on dangling bonds-free 2D material's surface and complicated selective doping for local p-or n-type conversion are the major challenges of 2D electronics. Additionally, the defect-free 2D materials are desirable to develop high performance electronic devices, but the production of ultrapure large-area 2D materials is still a challenge. Apart from the aforementioned intrinsic issues, the flexible devices developed with 2D materials experience several additional challenges. For example, the high surface roughness and low thermal budget (the total amount of heat a material can withstand before degradation) of the commonly employed flexible polymeric substrates are the detrimental issues. Additionally, the poor water vapour transmission ratio of the polymeric substrates can accelerate the oxidation-induced degradation of 2D materials and subsequently leads to



instability and performance deprivation in the fabricated devices. The 2D materials-based large area flexible electronic devices, such as flexible/stretchable micro-displays, flexible image sensors, and wearable/attachable healthcare devices usually consist of a multitasked structure including a substrate, backplane electronics, a front plane of active units, and the encapsulation layer. During the function, these devices repeatedly experience various mechanical deformations such as bending, twisting, shearing, and stretching which incorporate an unsolicited strain into the device components leading to performance degradation and even mechanical failure. The recurrent mechanical deformations can cause sliding, buckling or delamination in the device layers, resulting in a loss of mechanical integrity and device functionality. Additionally, applied strain can alter the intrinsic properties of 2D materials, which can affect the device's performance and stability. Therefore, to effectively integrate 2D materials into practical flexible applications, the material-related intrinsic issues along with other challenges associated with flexibility such as limited processing

temperature, strain-induced failure, and inferior performance must be addressed appropriately.

Advances in science and technology to meet challenges

Significant advances via extensive research and investigations have been made aiming to establish the appropriate solutions to existing challenges. To tackle the most common issue of doping in 2D materials, various nonconventional surface doping strategies have been developed to obtain the desired tuning in charge carrier polarity while preserving the lattice structure and other intrinsic features. Treating 2D material's surface with specific organic compounds and chemicals offers an easy way of tuning the doping type through electronic charge transfer. However, these methods have a serious limitation of unstable doping. Depositing a thin layer of an oxide dielectric on 2D material's surface, particularly on TMDs, is another strategy to achieve stable doping and p-/n-type conversion via oxygen vacancies-mediated electronic charge transfer at the interface. Advancements in local doping techniques for 2D materials not only

enabled the fabrication of electronic circuits but also helped in mitigating contact resistance issues. For example, the existence of an ultra-thin oxide layer between the metal electrode and 2D materials helps to decrease contact resistance by preventing physical damage associated with the Fermi level pinning issue that occurs in the 2D materials during the metal deposition. To address the high contact resistance issue in 2D materials, several other approaches, such as the use of transferred metal electrodes, the use of metallic or semi-metallic phases of 2D materials, edge contacts, and the use of semi-metals such as Bi and Sb have also been attempted. Depositing a thin oxide buffer layer on top of the polymeric substrates not only extends device lifespan by reducing moisture permeation but also mitigates performance degradation caused by high surface roughness. The numerous advantages of the ALD method, including low-temperature processing, conformal surface coverage, uniform thickness, and precise thickness control over large areas, make ALD the most preferred technique to deposit high- k dielectrics, such as Al_2O_3 and HfO_2 on the 2D material's surfaces as a gate dielectric or as a buffer layer for reducing surface roughness and moisture permeation of flexible polymeric substrates. The limited temperature tolerance and huge mismatch in the thermal expansion coefficients of commonly employed polymeric substrates lead to the search for alternative substrates. To this end, mica and ultrathin glass (UTG) (UTG $\sim 400^\circ\text{C}$, mica $\sim 700^\circ\text{C}$) have been explored as non-polymeric alternatives. However, their brittleness and limited strain tolerance provide only modest mechanical advantages. To fabricate flexible devices, 2D materials are typically synthesized on a hard SiO_2/Si or sapphire substrate followed by transferring them to the desired polymeric substrates via solution- or laminator/hot press-based dry transfer method for the device fabrication. These transfer processes usually incorporate several defects including surface contaminations, wrinkles, tears and micro-cracks, leading to degradation in material quality and thereby device performance. The recently developed adhesive wafer bonding-based large area dry transfer method can be a possible alternative to the conventional methods.

Advancing the low-temperature synthesis of 2D materials would revolutionize the development of 2D material-based flexible devices on polymeric substrates. Additionally, the low-temperature synthesis can enable the M3D hetero-integration of various 2D materials on flexible platforms, paving the way for novel flexible 3D electronics with high integration density and unparalleled multifunctionality. Recent research has demonstrated a substantial achievement with the wafer-scale synthesis of high-quality MoS_2

monolayers at a temperature as low as 150°C on the UTG and polymer substrate [284]. An alternative approach is the all-solution-based processing of device fabrication, which includes the synthesis and printing of 2D materials and other device components on flexible substrates at low temperatures. Although 2D materials with ultrathin thickness exhibit high flexibility and are ideal for flexible electronic applications, they are also susceptible to strain-induced damage. Therefore, to avoid mechanical failure in 2D materials-based flexible devices, it is crucial to adopt a suitable device architecture with proper strain management. Integrating the active 2D materials near the neutral mechanical plane (NMP) in the device architecture substantially decreases the risk of mechanical failure. Furthermore, ensuring consistent performance under repeated deformations is crucial, particularly for the applications of wearable healthcare devices, which require stretchability comparable to that of human skin ($\sim 60\%$). To achieve such mechanical virtues in the devices, several non-conventional architectures, such as serpentine, buckling, origami, and kirigami, have been employed in interconnects and active 2D materials. As the field advances, 2D materials-based flexible devices have been integrated with wireless communication capability, particularly flexible healthcare devices for efficient data recording and transfer while maintaining human comfort. Additionally, with the rapid advancement in AI technology, ML-based data analysis techniques can dramatically decrease the time required for analysing physiological data and can provide real-time clinical information to users.

Concluding remarks

The advent of 2D materials as alternatives to traditionally brittle materials marked a pivotal moment for the field of flexible electronics. Although substantial progress has been made toward the utilization of 2D materials in flexible electronics at the laboratory scale, their commercial implementation is still at the early stages, and an in-depth understanding and technological development to overcome various challenges associated with 2D technology are needed. Specially, it is essential to establish a production and fabrication line specifically designed for the manufacturing of devices utilizing 2D materials similar to that of conventional Si foundry.

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19. 2D materials for sensing technologies

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Status

Since its discovery in 2004, graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has marked a breakthrough, and paved the way for research in the emerging field of 2D materials (2DMs). Due to their unique electronic, optical, and mechanical properties, the 2DM systems, such as TMDCs, black phosphorene (BP), and MXene, have been extensively studied from material properties to emerging applications. Notably, 2DM exhibits high surface-to-volume ratios, excellent mechanical flexibility, and remarkable sensitivity to external stimuli, making them highly suitable for sensing applications [235, 285]. 2DM sensors offer exceptional capabilities in detecting a wide range of signals, including temperature, humidity, light, strain, gas, and biomolecules. Moreover, their atomic thinness enables the development of flexible and transparent sensors that can be seamlessly integrated on diverse substrates. Table 2 presents a comparative summary of performance metrics of 2D material-based sensors and their 3D counterparts.

Over the past decade, significant progress has been made in the emerging field of 2DM sensors. Graphene and other 2D materials, ranging from MXene to h-BN (figure 23(a)), have been extensively investigated in sensing applications. Such new LMs, including metallic, semiconducting, and insulating types, have been utilized as active sensing elements. For instance, graphene-based thermometers have been developed for sensing temperature, MXene-based PDs for sensing IR light, BP-based gas sensors for detecting volatile organic compounds, MoS₂-based strain sensors for monitoring human blood pressure, and rGO-based biosensors for sweat diagnostics [235, 285–287]. Specifically, the sensing mechanisms in 2DM sensors rely on the interaction between the analytes or target molecules and the 2DM itself, affecting sensor design and optimization [235]. Common sensing mechanisms include piezoelectric, electrical, optical, or electrochemical effects (figure 23(b)). The piezoelectric mechanism involves changes in the band structure and electrical conductivity of 2DM (e.g. MoS₂) under strain, enabling tactile sensing. The electrical mechanism relies on modifications in charge carrier concentration, mobility, or bandgap of 2DM (e.g. semiconducting TMDs) in FETs [294] due to the presence of analyte molecules in the channel region. The optical mechanism exploits changes in

the absorption, emission, or scattering properties of 2DM when analyte molecules bind, facilitating sensitive and label-free detection. The electrochemical mechanism involves the quantitative detection of electron transfer or oxidation/reduction reactions between the 2DM-modified electrode surfaces and analytes for environmental or health monitoring [285]. Ongoing research aims to uncover new mechanisms and refine sensor designs to enhance the sensitivity, selectivity, and reliability of 2DM sensors.

As FET being the fundamental sensor structure, 2DM FET sensors have the capability of converting physical, chemical, or biological quantities into electrical signals and can modulate performance using diverse gates (figure 24(c)), enabling fast and sensitive detection [235]. To parallel and simultaneous monitor multiple analytes or parameters, 2DM sensor arrays have been developed, offering enhanced selectivity, sensitivity, and multiplexing capabilities. In addition, the associated circuit is designed to allow for on-chip signal processing, calibration, and data analysis. With the integration of 2DM sensors and CMOS peripheral circuits (figure 23(d)), the 2DM sensor arrays and circuits offer promising avenues for advanced sensing technologies. Moreover, multifunctionalities in sensor array systems can be implemented by a M3D integration of 2DMs and Si or III–V layers via vdW growth and transfer techniques [295]. Figure 23(e) illustrates the M3D architecture, which enables vertically stacking multiple chiplets in 3D packaging. This stacking integration allows for the combination of various layers, such as transmitters, 2DM sensors, memory, and Si CMOS, thereby providing additional functionality. Incorporating AI algorithms, such as artificial neural networks, enhances the performance of 2DM sensors, addressing challenges related to cost, speed, and power consumption [296]. Additionally, in contrast to rigid substrate-based sensor chips, flexible and stretchable sensors based on 2DMs can offer disruptive solutions for emerging applications such as healthcare monitoring, humanoid robotics, and human-machine interface technologies [297].

Current and future challenges

While 2DM sensors offer great promise, there are several challenges that researchers are currently addressing and will continue to face in the future.

Material quality and scalability: achieving large-scale, high-quality production of wafer-scale 2DMs with consistent properties is essential to ensure uniformity and reproducibility across specific sensor devices. Controlling the growth, synthesis, and transfer processes is crucial in this regard. vdW integration of 2DM in both n-type and p-type configurations is

Table 2. Performance metrics of 2D material-based sensors and their 3D counterparts [235, 285–293].

Sensor type	Key metrics	2D materials & sensor performance		3D materials & sensor performance	
Gas Sensor	Limit of detection	MoS ₂	0.1 ppb (NO ₂)	ZnO	1 ppm (NO ₂)
Strain Sensor	Gauge factor	Graphene/ MoS ₂	>10000	Silicon	~100
Photodetector	Responsivity & detectivity	MoS ₂ /BP/MoS ₂	>10 ⁶ A W ⁻¹ , >10 ¹⁶ Jones	Ge/Si	0.5–1 A W ⁻¹ , ~10 ¹² Jones
Pressure Sensor	Detection limit & sensitivity	Graphene/MXene composites	<6 Pa, >600 kPa ⁻¹	Bulk metal films	>10 Pa, <50 kPa ⁻¹
Biosensor	Limit of detection	MoS ₂ /GO	10 nM (glucose)	Pt-based electrode	10 μM (glucose)
Temperature Sensor	Temperature coefficient (TCR)	Graphene, CNT composites	High TCR, flexible, fast response	Metal film/silicon diode	Lower TCR, rigid
Humidity Sensor	RH resolution	MXene	<1% RH	Polymer or ceramic	~5% RH

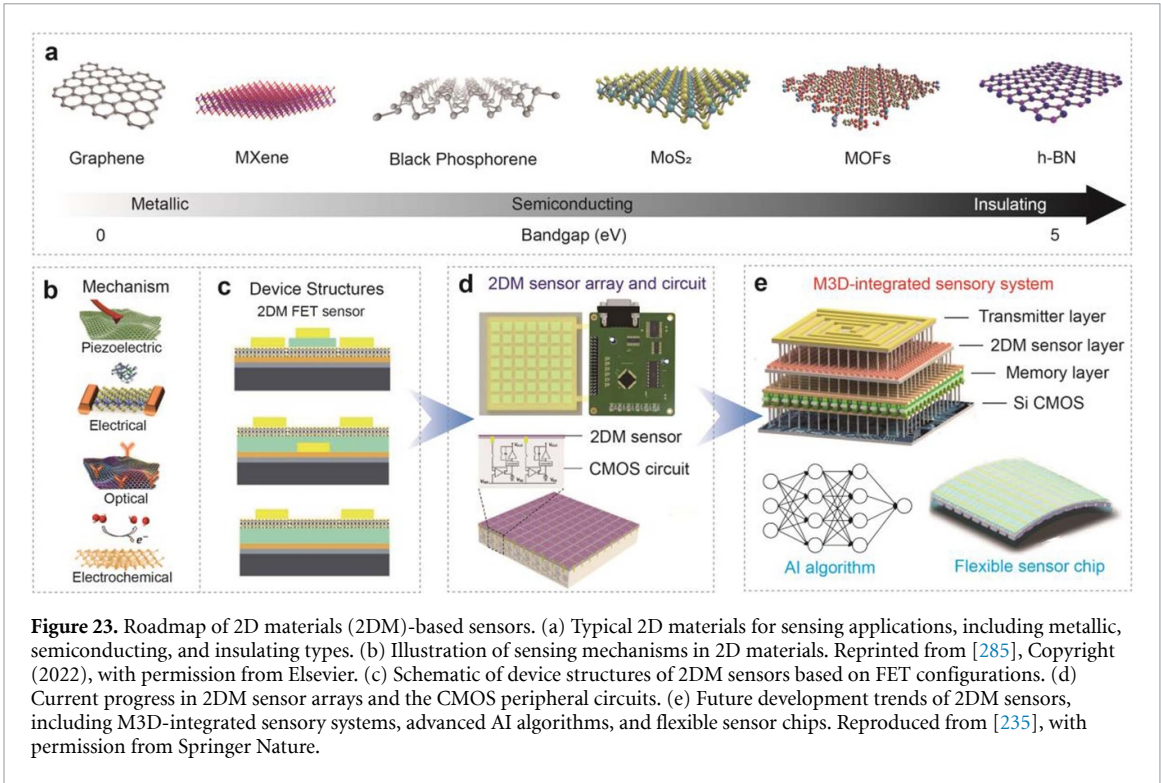


Figure 23. Roadmap of 2D materials (2DM)-based sensors. (a) Typical 2D materials for sensing applications, including metallic, semiconducting, and insulating types. (b) Illustration of sensing mechanisms in 2D materials. Reprinted from [285], Copyright (2022), with permission from Elsevier. (c) Schematic of device structures of 2DM sensors based on FET configurations. (d) Current progress in 2DM sensor arrays and the CMOS peripheral circuits. (e) Future development trends of 2DM sensors, including M3D-integrated sensory systems, advanced AI algorithms, and flexible sensor chips. Reproduced from [235], with permission from Springer Nature.

highly desirable for extending functionalized sensing capabilities.

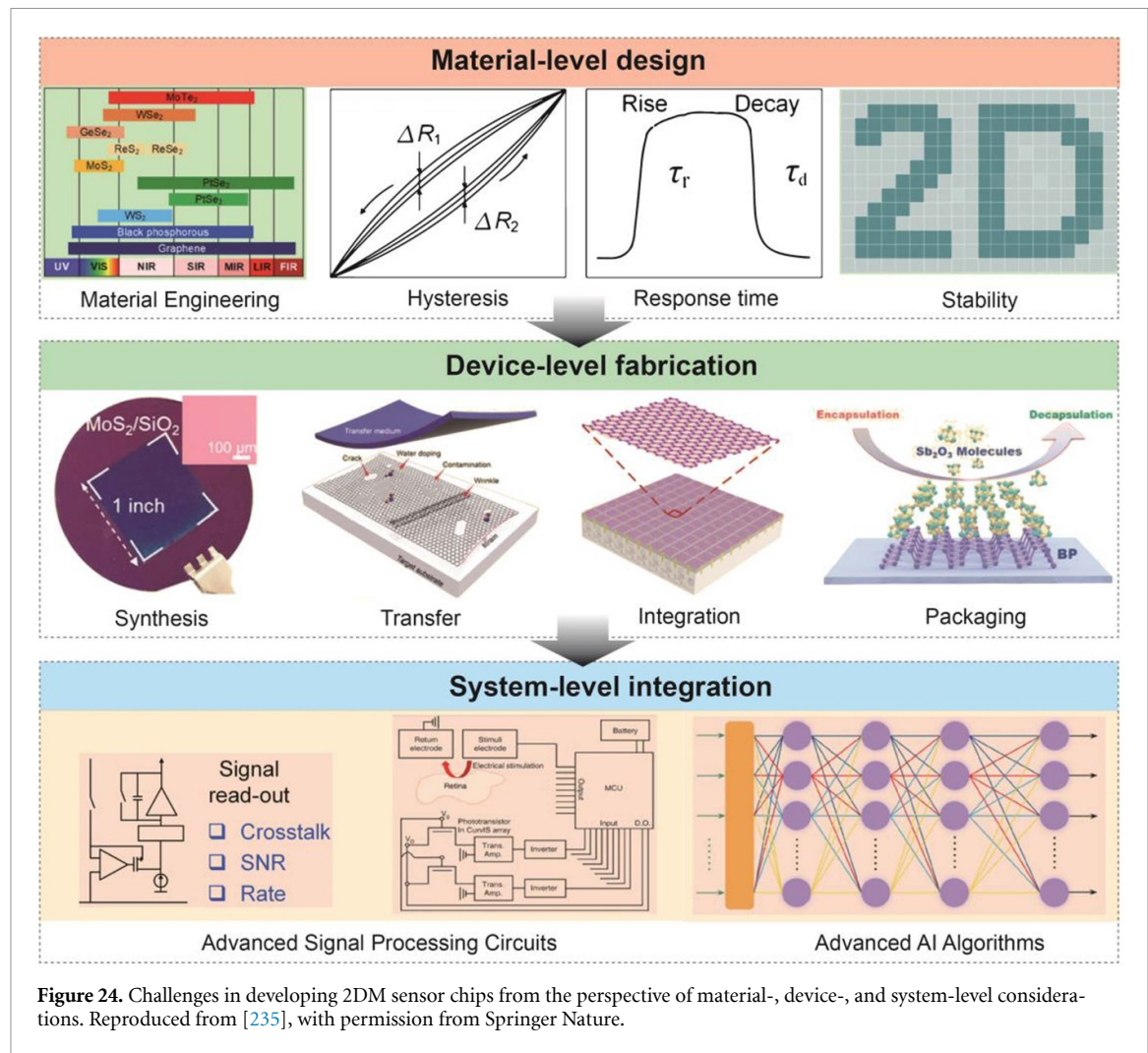
Sensing performance: a deep understanding sensing mechanisms at the atomic and molecular level is essential for optimizing 2DM sensor design. Enhancing the sensor’s ability to accurately discriminate between different substances or stimuli (i.e. selectivity) is crucial for accurate and reliable sensing. Strategies to mitigate degradation caused by environmental factors such as humidity, temperature, and chemical exposure are necessary to ensure long-term stability. Additionally, integrating multiple sensing modalities or functionalities into a single 2DM sensory system presents a complex task.

Integration and compatibility: seamless integration with existing Si-based electronics and systems necessitates compatibility with substrates,

encapsulation materials, and fabrication processes. Addressing challenges related to coordinating different sensing elements, signal processing, and data fusion in system-level integration is crucial for implementing advanced multimodal sensing systems.

Power efficiency: striking a balance between high performance and low power consumption is crucial for battery-powered applications. Strategies such as reducing power requirements, enhancing energy efficiency, or exploring self-powered configurations are necessary to optimize power efficiency in 2DM sensors.

Cost-effectiveness: advancements in manufacturing processes, material synthesis techniques, and economies of scale are needed to reduce the cost of 2DM sensors. Improving cost-effectiveness enhances



accessibility and commercial viability, making 2DM sensors more widely available.

Advances in science and technology to meet challenges

To address the challenges in 2DM sensors, a range of key techniques and methodologies are presented, encompassing material-level design, device-level fabrication, and system-level integration, as shown in figure 24.

- (1) **Material-level design.** Advanced techniques in LM synthesis, such as optimized growth recipes, substrate engineering, and doping, are being developed to enable large-scale and high-quality production of wafer-scale 2DMs with uniform and defect-free attributes. In addition, advanced techniques in materials characterization, such as high-resolution *in-situ* electron microscopy and spectroscopy, would provide insights into the structure, composition, and properties of 2DMs, facilitating material quality control and optimization. Advancements in theoretical modelling, computational simulations, and experimental

techniques are essential to deepen the understanding of sensing mechanisms in 2DM sensors. By studying the interactions between analytes or stimuli and 2DMs at different length and time scales, valuable insights into the electronic and chemical processes involved in sensing can be obtained. Theoretical analysis with techniques such as atomistic simulations, DFT calculations, and quantum mechanical modelling contribute to this understanding and verification. Overcoming challenges related to selectivity, stability, and integration of 2DM sensors requires innovative sensor designs. Exploring novel architectures like heterostructures and hybrids enhances sensing performance, while integration with complementary materials (e.g. polymers or nanoparticles) can add functionalities and improve selectivity. Additionally, strategies, including encapsulation techniques, protective coatings, and interface engineering, play a crucial role in enhancing the stability and reliability of 2DM sensors.

- (2) **Device-level fabrication.** Leveraging their compatibility with CMOS technology, 2DM sensors can adopt micro-electro-mechanical system

processes that are highly desirable for making the integration of sensing and processing functions on a single chip. To ensure seamless integration of 2DM sensors into system-level architectures, compatible fabrication processes, interconnectivity strategies, and interface engineering are crucial to achieve excellent compatibility with existing electronics. Advancements in material synthesis methods, such as CVD, and solution-based preparation are essential for enhancing the quality and scalability of 2DM sensors. Scalable manufacturing processes like R2R or large-area fabrication techniques enable high-throughput production at reduced costs, facilitating the widespread adoption of 2DM sensors. Furthermore, the utilization of reliable interfacial materials and flexible manufacturing approaches (e.g. 3D printing and deformation techniques) enable the integration of 2DMs, including vdW heterostructures, into flexible and wearable sensory electronics.

- (3) **System-level integration.** Optimizing the power efficiency of 2DM sensors can be achieved through energy-efficient sensor designs and low-power peripheral circuits. The utilizing of piezoelectric, thermoelectric, or triboelectric materials enables the development of self-powered sensory systems, while advanced signal processing methodologies enhance power efficiency for high-performance sensing applications. Moreover, as the complexity and volume of data generated by sensors increase, the development of advanced AI algorithms becomes crucial to improve the reliability and accuracy for real-time data processing, pattern recognition, and data fusion in 2DM sensory systems. AI-based approaches enable autonomous sensor operation, adaptive calibration, and intelligent decision-making. Leveraging the inherent parallelism and low-power operation of 2DMs, novel

architectures [298, 299], such as neuromorphic computing or in-sensor computing, enable real-time processing of sensor data and the implementation of deep learning algorithms directly within the sensory system. These advancements revolutionize data processing and analysis, leading to more efficient, intelligent, and autonomous sensing applications.

Concluding remarks

In the post-Moore era, as chip manufacturing approaches physical size limits, the 'More than Moore' paradigm has emerged. 2DMs, possessing high surface-to-volume ratios, excellent mechanical flexibility, and remarkable sensitivity to external stimuli, have highlighted significant progress in transformative sensing applications. The ongoing development of 2DM sensors with unique characteristics focuses on enhancing sensitivity, selectivity, response time, stability, and scalability through extensive studies in material engineering, integration techniques, and data analysis. These advancements will unlock novel intelligent applications, improve existing sensor technologies, and contribute to the development of energy-efficient advanced sensory systems (even in M3D architecture) for diverse fields such as healthcare, environmental monitoring, industrial process control, and beyond.

Acknowledgments

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20. Neuromorphic, quantum, and spintronic computing with 2D materials

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Status

The design of vdW heterostructures, integrating 2D materials (2DMs), offers fascinating opportunities for material innovation and the integration of novel charge, spin and optical features in functional devices. Thanks to a large 2DMs family portfolio, including metallic, magnetic, superconducting, semiconducting and insulating structures, unprecedented possibilities for material design in computing architectures are made possible, especially in the fields of neuromorphic computing, spintronics and quantum information processing. Particularly important is their atomically thin nature which paves the way for ground-breaking band-structure engineering through ‘proximity’ effects, opening new avenues for exploration in nanotechnology and ultracompact device design.

The recent proliferation of AI and ML has led to significant demands on conventional von Neumann computing architectures. In particular, the need for training on massive datasets for AI/ML results in uncomfortably high-power consumption due to the need to move large amounts of data between spatially separated memory and logic blocks. To overcome this von Neumann bottleneck, alternative neuromorphic (i.e. brain-like) computing concepts are being explored. Neuromorphic computing draws inspiration from the brain (figure 25) such as the co-location of memory and information processing, thus minimizing the movement of data and reducing power consumption by orders of magnitude compared to a digital computer. Other neuromorphic characteristics include highly nonlinear spiking voltage profiles that are analogous to the action potentials in biological neurons and hyper-interconnectivity that attempts to mimic the thousands of synaptic connections per neuron in the brain. With high gate-tunability that facilitates nonlinear charge transport and unconstrained vdW bonding that enables integration into complex geometries, 2DMs have emerged as leading candidates for next-generation neuromorphic computing [300].

In what concerns quantum technologies, 2D materials and various heterostructures have emerged in full force. Vital components of scalable quantum

chips such as quantum light sources, photon detectors and nanoscale sensors have been realized. In addition, availability of myriad of strong excitonic systems, coupled with the ability to optically select the valley state, may pave the way towards many body physics and exploration of exotic phases of matter through quantum simulations.

In a more detailed approach, realisation of quantum technologies from layered 2D vdW systems can stem from either exploring excitonic phenomena (limited to TMDCs, phosphorene, and related 2D semiconductors) or defects in wide band gap systems (hBN) [301]. The final application will dictate the hardware selection. As an example, valleytronics and many body exciton physics would be pursued with the former, while quantum sensing might be realized with the latter. It is important to add that both TMDCs and hBN can be interfaced with traditional cavities and photonic components—fabricated both from the host crystal, as well as from an external material (e.g. silicon nitride). This diversity of structures and properties truly makes the library of 2D materials a unique and rich playground for quantum information technologies for years to come [188].

In the realm of spintronics, the demonstration of proximity effects between graphene and strong spin-orbit coupling materials or magnetic materials have revealed ground-breaking phenomena, such as the room-temperature manipulation of pure spin currents through the spin Hall effect [302], or the imprinted exchange coupling in graphene from layered antiferromagnets that have achieved values on the order of 170 Tesla on length scales of hundreds of nanometres [303]. In a recent roadmap, scientific leaders and representatives from large industries such as Samsung, Global Foundry, and Thales have established the main advantages of 2DMs for spintronic applications and discussed the way for the further development of 2DM-based non-volatile memory technologies [129]. Furthermore, horizons for developing topological spintronics have been proposed theoretically [304].

Current and future challenges

Due to weak dielectric screening in 2DMs, nearly any 2D device can be made gate-tunable, thus presenting opportunities for achieving highly nonlinear charge transport characteristics that mimic biological neurons and synapses. For example, the carrier concentration on each side of 2DM p-n heterojunctions can be tailored with applied gate potentials, enabling nonlinear anti-ambipolar characteristics that can be harnessed for voltage spiking in addition to energy-efficient platforms for AI/ML classification [305]. While early demonstrations have achieved voltage spiking on biologically relevant timescales (i.e. kHz frequencies), opportunities remain for significantly

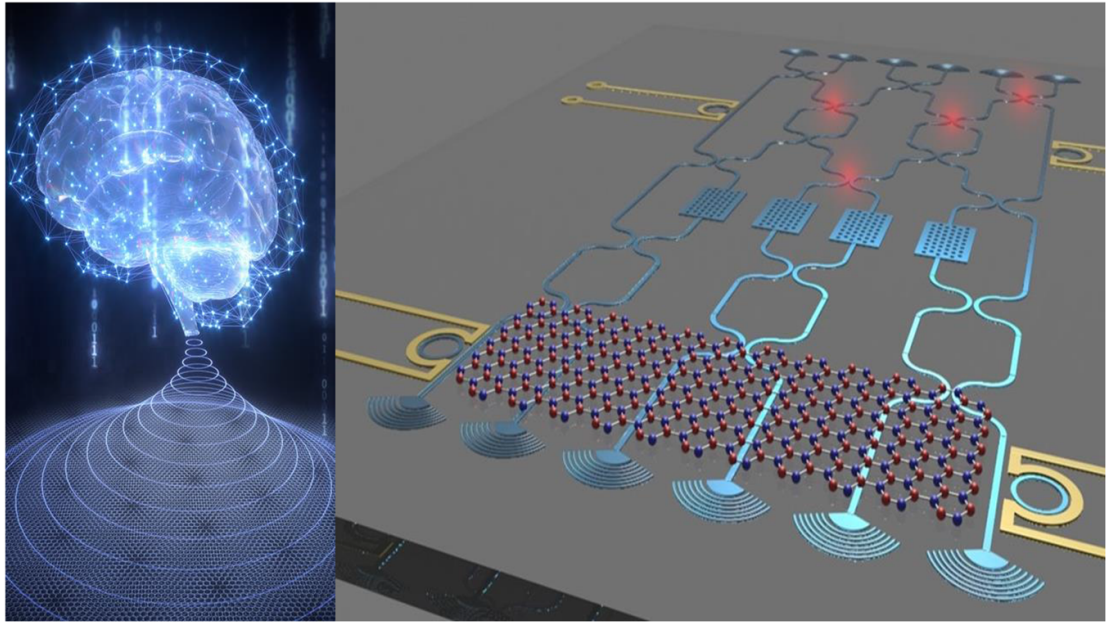


Figure 25. Left panel: with high gate tunability and unconstrained vdW integration possibilities, 2DMs are leading candidates for next-generation neuromorphic (i.e. brain-like) computing. Right panel: Schematics of a coupled cavity–emitter system using hexagonal boron nitride two-dimensional materials.

increasing the frequency response to timescales characteristic of modern digital computers (i.e. GHz frequencies). In another example, by exploiting the low barrier to defect motion at GBs in polycrystalline 2DMs, doping profiles can be reconfigured laterally with modest electric fields. These reconfigurable doping profiles provide non-volatile changes in conductance (i.e. memristor responses) that are analogous to synaptic responses in biological neural networks. By combining this memristive behaviour with gate-tunability of the overall carrier concentration (i.e. transistor responses), memory and information processing can be achieved at the same point in space in a hybrid memristor/transistor device that is referred to as a memtransistor. Moreover, the planar geometry of memtransistors implies that multiple contacts can be applied to the channel region to realize high degrees of interconnectivity in addition to bio-realistic heterosynaptic phenomena [306]. While 2DM memtransistors achieve many desirable neuromorphic features, their reliance on defective, polycrystalline materials presents challenges for realizing device-to-device uniformity over large areas, especially as the individual device sizes are scaled to nanometre dimensions. Most recently, the unique physics of twisted moiré heterostructures has presented additional opportunities for 2DM neuromorphic computing including room-temperature excitonic ferroelectricity and ratcheting charge transport that enable hardware implementation of higher order cognitive function such as associative learning with input-specific adaptation (figure 26) [191]. However, these moiré synaptic devices have only been realized through exquisite micromechanical exfoliation and

sequential stamping at the single flake level, which presents significant challenges for scalable manufacturing. In this regard, direct growth and/or large-area sequential transfer with precise angular control will be required to fully exploit moiré phenomena in practical neuromorphic computing systems.

For spintronics, as discussed in [129], there are many avenues for reducing the write current for practical magnetic random-access memory (MRAM) technologies (especially the STT and SOT-MRAM devices) while largely improving compactness of the technology and lowering power consumption. However, many challenges remain to be tackled. The main hurdle lies in the co-integration of 2DMs in heterostructures in a scalable way, limiting the use of dry or wet transfer and stacking by material assembly. Direct growth of heterostacks using CVD or molecular beam epitaxy (MBE) methods would be ideal, but it requires ultimate control of gas flow, substrate quality, and homogeneous temperature monitoring. On the other side, if advanced modelling is essential to anticipate on the upper limits of device performance, the variety of structural properties (number of layers in the stack, twist angle, substrate or encapsulation materials, disorder forms, etc) is too large for realistic modelling to be implemented through ‘human’ action. Consequently, AI-based approaches have become a cornerstone to accelerate material design and access to predictive modelling of their properties.

In the realm of quantum technologies, a key outstanding issue is understanding the photophysical properties of the quantum light source. Within the TMDC communities, there is a growing debate

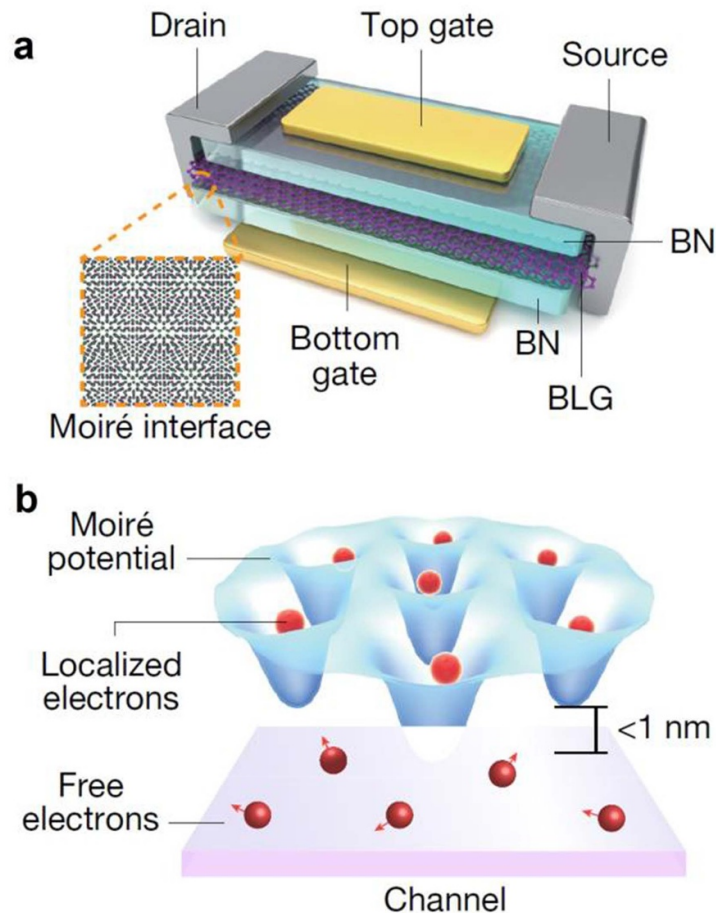


Figure 26. (a) Schematic of a moiré synaptic transistor produced from a twisted vdW heterostructure based on hexagonal boron nitride (BN) and bilayer graphene (BLG). (b) The moiré potential between the top BN and top BLG graphene results in a localized electron layer in direct proximity to a free electron channel, thus enabling ratcheting charge transport for advanced neuromorphic functionality. Panels (a) and (b) Reproduced from [191]. © The Author(s). Published by IOP Publishing Ltd. CC BY 4.0.

whether these are strain induced or localized to a particular defect. On the other hand, within the hBN community, the crystallographic nature of the majority of the visible emitters is still unknown, with a growing proposition that these are originating from donor–acceptor pairs or a unique localisation within the N antibonding orbitals [307]. In addition, it is yet to be seen what the most promising architecture is to combine quantum light sources based on 2D systems with integrated photonics on chip. One can envision a fully integrated, wafer-scale vdW quantum photonic chip, given the high refractive index of some of the TMDCs, and the ability to grow those over large areas.

Advances in science and technology to meet challenges

Advances in material fabrication and integration are definitely at the core of future improvement and commercialization of emerging technologies integrating 2DMs in neuromorphic computing, quantum technologies and spintronics. Possible twist angle

control would enlarge the possibility for optimizing a given property but that would also require robotic assembling to be operational at wafer scale. Despite proof-of-principle demonstrations, significant efforts are needed to develop more systematic approaches and tools able to upscale device fabrication in a manner compatible with industrial-scale manufacturing.

2D spintronics will also need to benchmark the best combination of materials for targeted metrics (e.g. larger spin-orbit torque efficiency with free field switching operation at the lowest possible current for magnetization switching). Again, this quest will demand the massive use of AI tools for material fabrication and exploitation of measurement data.

Concluding remarks

After twenty years of intense research following the discovery of graphene, the enlarged family of 2DMs has brought high value for active control of charge and spin degrees of freedom, opening possibilities for more energy efficient and compact technologies

able to solve current limitations of standard technologies in computing. However, despite the large investment and efforts worldwide, the lack of synergies between industry and academia and a suitable platform to network the concerned partners is a limiting factor for faster transfer from fundamental research to applications and commercialization, especially in the deep tech sector. International collaboration and large-scale public programs (such as the Graphene and Quantum Flagships in Europe) have initiated incubators and accelerators of knowledge-to-technology developments, but challenges remain in proper alliance design for overcoming the great challenges of implementation and deployment of breakthroughs to society as a whole.

Acknowledgments

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21. 2D materials for EMI shielding

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Status

EMI occurs when electromagnetic waves cause interference among various circuits and devices operating in proximity. With the proliferation of telecommunication devices and microelectronics, the detrimental effects of EMI have become more serious, necessitating stringent solutions. EMI shielding materials are employed to protect sensitive electronic devices and components from undesirable electromagnetic radiation through reflection, absorption, and multiple reflection mechanisms, which are primarily defined by the electrical conductivity, magnetic permeability, frequency and thickness and structural makeup of the materials, described by Simon's formulae shown in equation (1) and figure 27(a) [308],

$$SE_T = 50 + 10 \log \left(\frac{\sigma}{f} \right) + 1.7t\sqrt{\sigma f} + SE_M \quad (1)$$

where σ ($S \cdot cm^{-1}$), t (cm), and f (MHz), and SE_M refer to electrical conductivity, sample thickness, frequency, and shielding due to multiple reflection, respectively. Therefore, advanced EMI shielding materials with high conductivity, magnetic permeability, and controlled structural design are needed for efficient EMI shielding in applications such as electronic communication, consumer electronics, flexible and wearable devices, autonomous vehicles, medical equipment, and aerospace.

The emergence of 2D nanomaterials, especially graphene and 2D transition carbides/nitrides (MXenes), presents tremendous opportunities for EMI shielding material research and applications due to excellent electrical conductivity, 2D structural feature, and microstructure designability through solution-processability [309–311]. Since the pioneering work on graphene EMI shielding materials, studies on 2D nanomaterial and their related EMI shielding composites have attracted great interest from both academic and industrial communities. The number of research papers on 2D materials-based EMI shielding has surged, with graphene-based materials showing an overwhelming contribution compared to

other competing materials (figure 27(b)). In 2016, MXenes emerged as state-of-the-art EMI shielding materials, outperforming other synthetic materials of comparable thickness due to their superb metallic conductivity, tunable composition and surface chemistry, and solution processability. This triggered another wave of EMI shielding research into 2D nanomaterials [311]. The unique combination of high electrical conductivity, large surface area, high aspect ratio, and abundant surface functional groups allows for the production of efficient EMI shielding polymer composites/additives at low filler loadings, particularly when compared to traditional metal- and carbon-based shielding materials. Additionally, their nanometre-thick 2D structure enables them to assemble into ultrathin films, lightweight 3D architectures, and high-performance fibres/fabrics, adapting to various application scenarios (figure 27(c)). While some graphene-based products are being commercialized, and their potential for scalable applications is optimistically expected, further in-depth and systematic research is still required to replace traditional EMI shielding materials fully.

Current and future challenges

The research advances in 2D nanomaterials, notably Graphene and MXenes, have leveraged their intriguing physical characteristics and EMI shielding performances, positioning them as leaders in current and future lightweight EMI shielding applications. However, several challenges impede their practical applications, summarized as follows: (i) developing controllable synthesis methods for 2D nanomaterials with well-defined nanostructures and intrinsic properties are demanded. Understanding the intrinsic electrical, dielectric, and electromagnetic characteristics of 2D nanomaterials is essential to meet various application requirements. While some scalable production methods have been developed for graphene-based EMI shielding materials, the precise fabrication of diverse MXene materials still requires significant efforts. (ii) The general and scalable production methods of 2D nanomaterial-based polymer composites and macroscopic assemblies with customized microstructures and performances are needed. Rational microstructure design of 2D materials can modulate EMI shielding performance and other characteristics, such as lightweight feature, mechanical flexibility/stretchability, visible transparency, and required mechanical properties, making 2D nanomaterial-based shielding materials suitable for various specific applications. (iii) The fundamental interaction mechanisms of electromagnetic waves with 2D nanomaterials and their macroscopic structures/composites are still not well understood. It is essential to explore how the hierarchical structures of macroscopic shielding materials affect

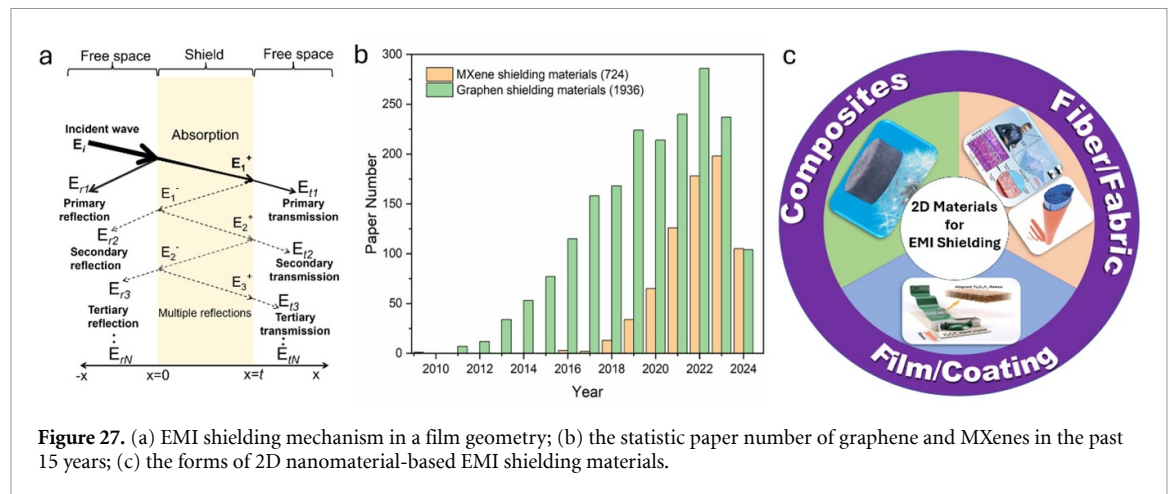


Figure 27. (a) EMI shielding mechanism in a film geometry; (b) the statistic paper number of graphene and MXenes in the past 15 years; (c) the forms of 2D nanomaterial-based EMI shielding materials.

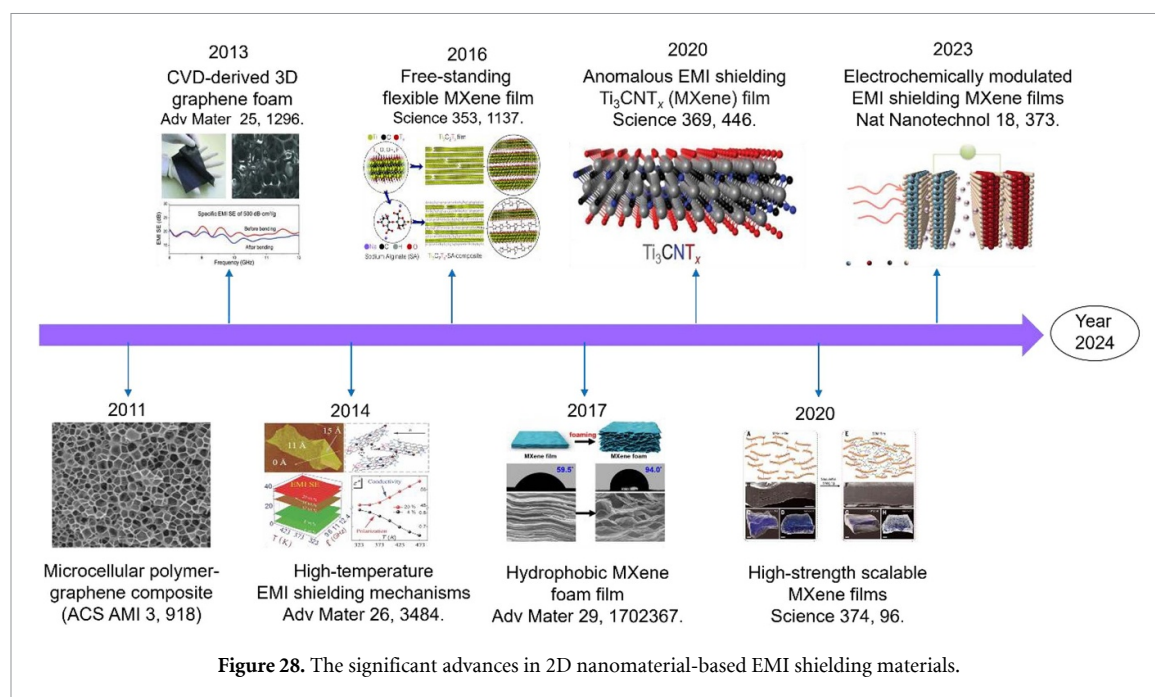
the electromagnetic parameters, internal multiple reflections, attenuation mechanisms and broadband EMI shielding performances. Understanding the performance stability and evolution mechanisms under extreme conditions (e.g. high/low temperatures, moisture, UV exposure, and environmental oxygen) is crucial for the practical applications in complex scenarios. (iv) The relatively higher costs of 2D materials may be a significant obstacle to their practical applications compared to that of currently dominant metallic shielding materials. Scalable and cost-effective production technologies for 2D nanomaterial-based shielding materials are needed. Alternatively, identifying critical and irreplaceable applications for 2D materials could justify their use over the conventional EMI shielding materials. (iv) The reflection-dominant EMI shielding mechanism of current 2D materials, due to their high electrical conductivity, leads to undesirable secondary EM pollution. Developing absorption-dominant EMI shielding materials requires significant attention. (v) Current 2D EMI shielding materials are mostly investigated within a narrow frequency range. However, the operating frequency of highly integrated electronic systems is continuously increasing. Therefore, it is essential to explore these materials across a broader frequency spectrum, including terahertz, IR, and beyond.

Advances in science and technology to meet challenges

Significant progress in the fabrication, property modulation, and applications of graphene- and MXene-based shielding materials has provided valuable insights for the research of 2D nanomaterials (figure 28). However, further advancements are still needed to address current and future challenges.

The EMI shielding research initially focused on polymer composites of conductive graphene, with tremendous efforts aimed at improving EMI shielding performance by optimizing matrix-filler interfaces, distribution/orientation, or forming efficient 3D networks. Importantly, free-standing 3D structures not only act as conductive networks for electron conductance in composites, but also serve as multifunctional lightweight aerogels, delivering both EMI shielding and thermal insulation. Techniques such as CVD, electrostatic assembly, emulsion-templated method, and 3D printing show great potentials for producing scalable and multifunctional EMI shielding materials.

MXenes offers versatile elemental compositions, nanolayer structures, surface terminations, and physical properties, presenting exciting opportunities for developing EMI shielding materials [311]. Among the available MXenes, $T_3C_2T_x$ is considered as the most promising candidate for EMI shielding applications [312]. The porous structure with rich interfaces in MXene foam significantly enhances EMI shielding capability [313]. Additionally, thermal annealing has been shown to enhance the microwave absorption properties of Ti_3CNT_x films [314]. Precise regulation of MXene terminations and flake size will help clarify the fundamental shielding mechanisms and enable the preparation of high-performance films and fibres [315]. The deliberate design of interfacial interactions integrates high tensile strength, electrical conductivity, and shielding performance in 2D nanomaterial films [316]. Furthermore, processing approaches including drop-casting, spray-coating, and scanning centrifugal casting facilitate the scalable production and practical applications of 2D nanomaterial EMI shielding materials.



Fabricating fibres and fabrics using 2D nanomaterial, either by loading them onto existing fabric substrates or through wet-spinning, is also a promising approach for developing efficient EMI shielding [317]. Although graphene-based fibres have exhibited high electrical, thermal, and mechanical performances, significant work remains to be done for MXene fibres, despite some encouraging advances.

Developing predictive models to understand the EMI shielding mechanism of millimetre-wavelength EM waves interacting with nanometre-thin 2D materials will aid in designing superior shielding material for next generation electronics. Traditional electromagnetic theories mainly address the EMI shielding properties and mechanisms of uniform materials, making them not perfectly suitable for 2D nanomaterial composites. ML methods and theoretical simulations can provide valuable insights and guidance for the rational design and mechanism understanding of 2D nanomaterial-based EMI shielding materials.

Developing magnetic MXenes will not only improve EMI shielding properties but also mitigate the secondary reflections and EMI pollution. Exploring novel precursors, including Cr, Mn, or other magnetic elements in single, bimetallic, or multi-metallic compositions, within ordered or solid-solution structures of MAX phases, could impart magnetic properties to the respective MXene structures. Currently, only Cr-based magnetic MXene has been reported at low temperatures, necessitating further developments to achieve room-temperature

magnetic properties for absorption dominant and multispectral EMI shielding.

Concluding remarks

Over the past 15 years, significant advancements have been made in the field of 2D nanomaterial-based electromagnetic shielding materials. This progress includes leveraging the intrinsic electromagnetic properties of 2D nanomaterials, developing polymer composites and hybrids, flexible films, and multifunctional fibres/fabrics, and understanding of EMI shielding properties and underlying mechanisms. However, critical issues and challenges remain, such as precisely modulating the structure and performance of 2D nanomaterials, integrating efficient electromagnetic shielding properties with other material characteristics, and developing large-scale production and application technologies for these materials. Future research should address these challenges to overcome barriers to the widespread adoption of 2D nanomaterials for EMI shielding applications in advanced electronics.

Acknowledgments

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22. 2D materials for composites

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Status

A range of 2D materials has been discovered over the past two decades that includes graphene, h-BN, TMDCs and transition metal carbides, nitrides or carbonitrides (i.e. MXenes) to name just a few. Such 2D materials are typically derived from 3D vdW solids and can be exfoliated from the bulk by mechanical, chemical or electrochemical methods to isolate their 2D form [318]. Table 3 lists the basic physical, mechanical, electrical and thermal properties of typical 2D materials. The values in the table are combination of both experimental and theoretical studies. A review of table 3 indicates that 2D materials such as graphene and 2D h-BN possess low densities and high specific surface areas, which maximizes interfacial contact with the matrix material into which these fillers are dispersed. In terms of elastic properties, 2D materials offer Young's moduli in the range of 133–1000 GPa, with graphene having the highest value. For fracture and impact properties, graphene offers the highest tensile strength (~ 130 GPa), h-BN displays the highest fracture toughness (~ 5.5 MPa $\sqrt{\text{m}}$), while MXenes exhibit exceptionally high strain-to-break (up to $\sim 25\%$). Graphene is by far the most electrically and thermally conductive member of the 2D materials family, while h-BN is electrically insulating. TMD materials such as MoS₂ have the highest dielectric constants. From the above discussion, it is evident that 2D materials offer an impressive range of physical, mechanical, electrical and thermal properties, and show outstanding potential to influence the properties of polymer, ceramic and metal matrix materials into which they are dispersed. The challenge is to what extent can this potential be exploited in nanocomposites.

Current and future challenges

Composites are materials that are constitute of at least two components and have properties superior to those of the component materials in isolation. The main properties of interest for nanocomposites are mechanical, thermal, electrical and barrier although perhaps the most exciting prospect is the ability of nanocomposites to excel in more than one of these properties, i.e. displaying multifunctionality. The addition of a filler with a high Young's modulus

to a matrix with a low modulus leads to a composite with a Young's modulus higher than that of the matrix [320]. Table 3 shows that 2D materials have very high levels of intrinsic stiffness and strength that were anticipated to lead to nanocomposites containing 2D materials reflecting these properties. In the event it has been shown [321] that the main factor limiting the improvement in mechanical properties is the aspect ratio (length/thickness) of the 2D material (figure 29(a)) along with its orientation, controlling stress transfer from the matrix to the reinforcement. Other factors controlling stiffness by maximizing the effective filler aspect ratio are the level of exfoliation and degree of dispersion of the nanofillers [321].

Figure 29(b) shows that there is an increase in Young's modulus upon adding graphene nanoplatelets (GNPs) to an epoxy resin and that the level of reinforcement increases with increasing s . Aspect ratio is found to have similar effect upon toughness, since higher levels of s lead to tougher nanocomposite materials through mechanisms such as interfacial debonding and pull-out [322]. On the other hand, the spectacular values of strength of 2D materials (table 3) are never realized in nanocomposites as the interface will generally fail before the 2D reinforcement undergoes fracture.

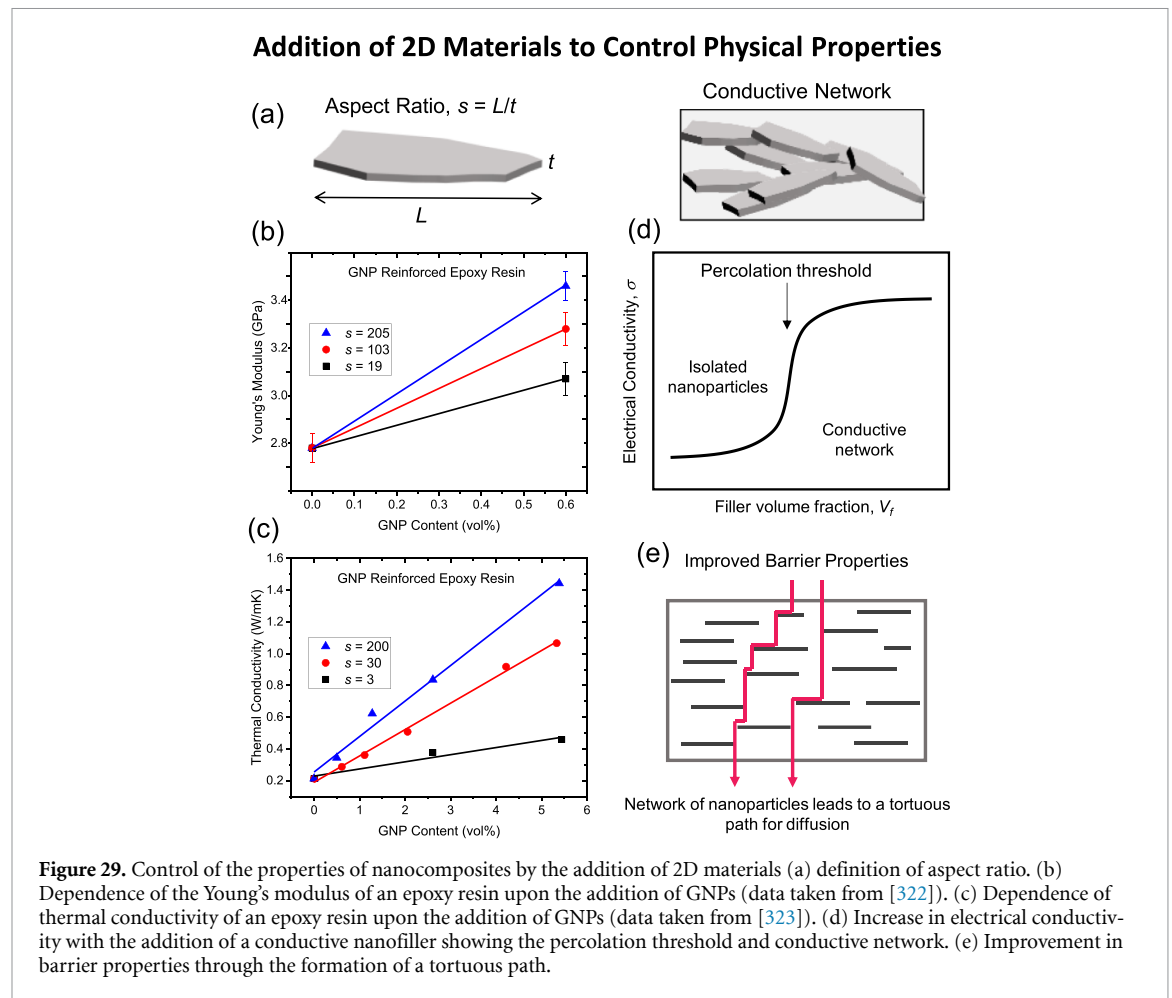
One general feature of the behaviour is that if the property of the nanofiller is orders of magnitude different from that of the matrix, the scope for improvement is limited as the result of the mechanisms involved. This is shown in figure 29(c) for the addition of GNPs to an epoxy resin where although a higher s leads to better enhancement of the thermal conductivity of the resin, there is only a factor of 5 improvement, despite the thermal conductivity of graphene being up to $10^4 \times$ higher (table 3). Although the values of Young's modulus and thermal conductivity generally increase linearly with nanofiller loading, electrical conductivity shows quite different behaviour as seen schematically in figure 29(d). The conductivity remains similar to that of the insulating matrix at low loadings and then undergoes a rapid rise by many orders of magnitude at the percolation threshold once a conductive network is formed. One advantage of 2D nanofillers, as opposed to nanoparticles or nanotubes, is that they have they have the potential of being used in barrier applications as they have the possibility of forming networks that lead to a tortuous path for the diffusion of a gas through a polymer matrix as shown in figure 29(e). 2D crystals also show excellent processibility in liquid or solid matrices.

Advances in science and technology to meet challenges

One of the main challenges in the development of nanocomposites reinforced with 2D materials is by

Table 3. Typical properties of two-dimensional (2D) materials that show promise as additives in nanocomposite materials [319].

	Physical properties		Mechanical properties				Electrical/thermal properties		
	Density (g cm^{-3})	Specific surface area ($\text{m}^2 \text{g}^{-1}$)	Young's Modulus (GPa)	Ultimate tensile strength (GPa)	Fracture Toughness ($\text{MPa } \sqrt{\text{m}}$)	Strain to failure (%)	Electrical conductivity (S cm^{-1}) at RT	Dielectric constant	Thermal conductivity ($\text{W m}^{-1} \cdot \text{K}$)
Graphene	2.267	2630	1000	130	4	13-19 (armchair) 6-11 (zigzag)	10^6	~ 1.8 (in plane) ~ 3 (out of plane)	1500-2500
Molybdenum disulphide	5.06	5.28-27.82	270 ± 100	23	1.8	6-11	10^4	15.5-15.9 (in plane) 6.2-6.9 (out of plane)	23.2-155
MXenes	2.6	49.5-61.4	133-517	14-70	—	9-24 (armchair) 11-23 (zigzag)	5000-15 000	—	55.8
Hexagonal Boron Nitride h-BN	2.1	198.41-964.3	~ 860	~ 70	5.25-5.76	12.5-13.3	10^{-13} - 10^{-6}	6.82-6.93 (in plane) 3.29-3.76 (out of plane)	340

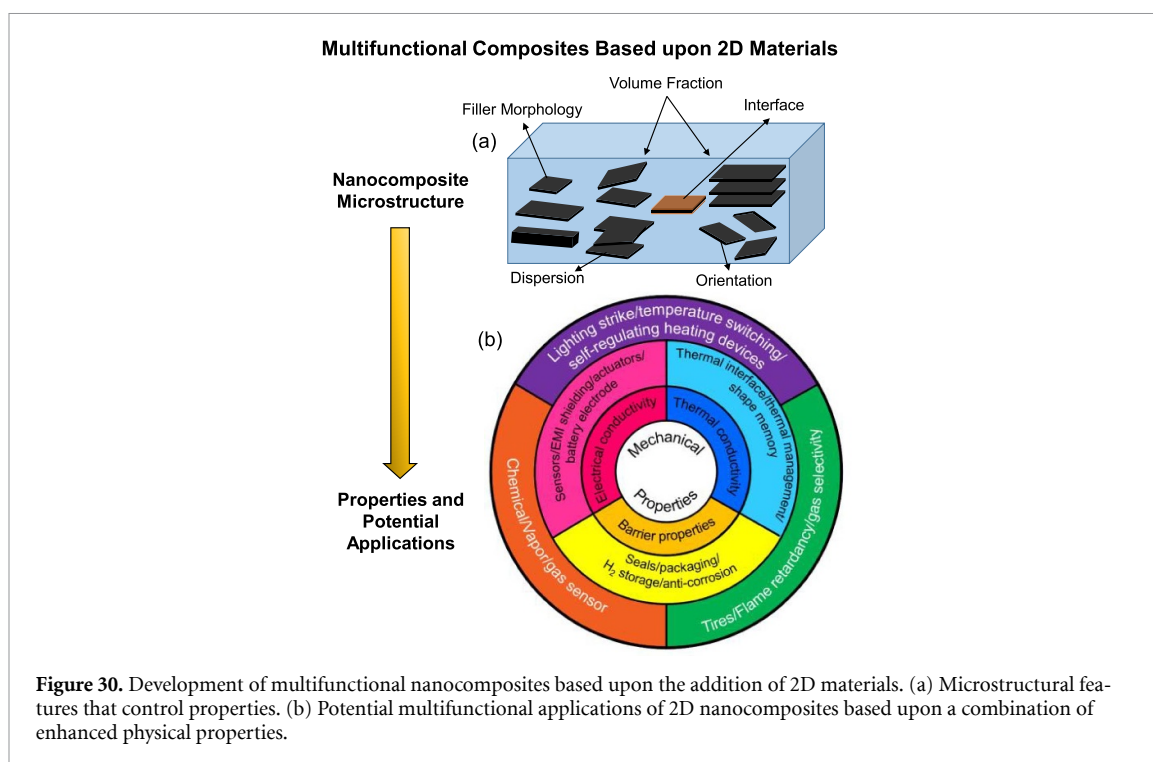


obtaining the nanofillers with good control of nanoparticle microstructure (size, shape and aspect ratio) and the ability to produce them reproducibly in large quantities at a reasonable cost [318]. On the other hand, there is little need to develop any new nanofillers as we now have a broad palette of materials available with a whole range of impressive physical properties (table 3).

One of the attractions of polymer-based nanocomposites is that they are generally easy to process and can be moulded into complex shapes using conventional techniques such as injection moulding. There is plenty of scope for developments in production processes such as additive manufacturing [324] and using inks based upon 2D materials for the ink-jet printing of components [325]. It is well established that the properties of nanocomposites depend strongly upon their microstructure [321] as shown in figure 30(a). The different processing techniques could be employed to control and optimize microstructure of nanocomposites. For example, the best mechanical properties are generally obtained with uniform distributions of nanofillers whereas recent studies have shown that improved barrier properties can be obtained with the 2D materials concentrated

near the surface [326]. In addition, processing methods such as fibre spinning can be used to align the 2D nanofillers in a particular direction that may again produce materials with both enhanced mechanical properties and anisotropic electrical and thermal conductivities.

Most of the original studies upon using 2D materials in nanocomposites have employed the nanofillers in their native states without any special surface treatments. As it is now well established that mechanical properties depend strongly upon stress transfer across the filler-matrix interface, there is scope for more systematic studies being undertaken of methods of functionalizing interfaces in 2D materials and employing surfactants to optimize dispersions and hence properties [325]. In particular, the filler-matrix interface strength must be carefully tuned to concurrently enhance both the elastic and fracture properties. One of the most exciting prospects for nanocomposites based upon 2D materials is being able to exploit their multifunctional properties [327] as shown schematically in figure 30(b). There is further scope to control multifunctionality through the use of hybrid systems with two or more types of 2D materials or the inclusion of other geometries of nanofiller.



Concluding remarks

It is clear that there have been spectacular developments in the field of 2D materials over the past 20 years. Such materials have been shown to have a whole spectrum of impressive intrinsic physical properties that could be exploited in nanocomposites. As the mechanisms whereby the properties of the composite matrix are enhanced are becoming better understood, we are also learning the limits for property modification. Nevertheless, there is plenty of scope for us to use our imagination to develop new

ways in which 2D materials can be employed in nanocomposites, particularly for exciting multifunctional applications.

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23. Commercialization and standardization

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Status

Possessing outstanding properties, graphene-related 2D materials (GR2Ms) and 2D materials (2DMs) more generally have demonstrated their potential in completely different application areas. There are now hundreds of companies reported to sell 'graphene' worldwide, with many able to offer large quantities of materials per annum or large-scale deposition machines. Alternatively, high-quality 2D materials can be grown on the wafer scale on microelectronics industry-compatible tools. This has been achieved after several years of the industry increasing the scale and quality of production. However, to make an economic impact with materials of such potential, the commercialization process is key, with more effort still required (see figure 31). Nevertheless, the 2DMs industry has made significant progress over the last 15 years, from a few companies attempting to convince mainstream end-users of a wonder material that would revolutionize their sector, to many companies working within different international supply chains for real-world products.

Currently, the word 'graphene' is informally used within the community as a generic name for a broad range of carbon-based 2DMs differing in structure, morphology and/or chemical composition, more accurately referred to as 'graphene-related 2D materials' or GR2Ms (as defined in ISO/TS 80004-13:2024). Some of these are being sold commercially, but are not actually 'graphene' or GR2Ms, instead being nano-graphite [329]. Therefore, setting accurate international standards for the various forms of GR2Ms is crucial for efficient communication across the supply chain. Both terminology and measurement standards are being developed or have been published by two international standardization bodies [330], the International Organization of Standardization (ISO) and the International Electrotechnical Commission (IEC), within their nanotechnology technical committees, ISO/TC229 and IEC/TC113 [329, 330]. In contrast, 2DMs for microelectronics applications are less standardized, although leading manufacturers are considering semiconducting 2DMs for ultimately scaled

transistors in logic circuits [212, 331]. In principle, their standardization can follow the example of GR2Ms: Through a holistic approach, different GR2Ms can be measured and defined using a set of published complementary international standards (see figure 32). These standards are based on verified processes as demonstrated through international interlaboratory studies [332] within the Versailles Project on Advanced Materials and Standards (VAMAS), established by the G7 in 1982 to promote global trade through innovation and adoption of advanced materials. There are also other standards published or under development within IEC/TC113 WG8, that are focused on more specific measurements taken from academic literature, for example, IEC/TS 62607-6-6: 'Graphene—strain uniformity: Raman spectroscopy'. However, there is an absence of reference materials or specific standards within the technological areas being targeted by graphene and 2DM-producing or -enabling companies.

Current and future challenges

The commercialization of such versatile materials typically begins with applications that are less technically challenging or belong to more mature areas. For example, some of the first commercial applications of GNPs are thermally conductive films, functional coatings, composite materials, and conductive additives in lithium-ion batteries (figure 31). These areas serve as useful examples for understanding the commercialization process and the challenges of transitioning new materials from the laboratory to real-world products. In thermally conductive films, GNPs are assembled into films for use in microchip cooling and in 2018, Huawei launched a high-performance cellphone, Mate 20X, claiming the world's first application equipped with such technology. Since then, many other cellphone manufacturers have adopted these films, for example, Xiaomi, Oppo, and OnePlus, with over 300 million devices sold. This early adoption of graphene was due to this industry's short supply chains, as well as the rapid feedback process from end users to materials producers.

Most other applications utilize GNPs as functional additives, for example to enhance electrical conductivity and/or protect against electrochemical corrosion. Functional coatings also have a relatively short supply chain to their final customers, and the industry has many tools, dispersing agents and experience in handling nanoparticles. However, the qualification time required is much longer than in consumer electronics, hindering progress. For example, salt spray tests according to the NORSOK M-501 standard require a 4200 h cyclic corrosion test.

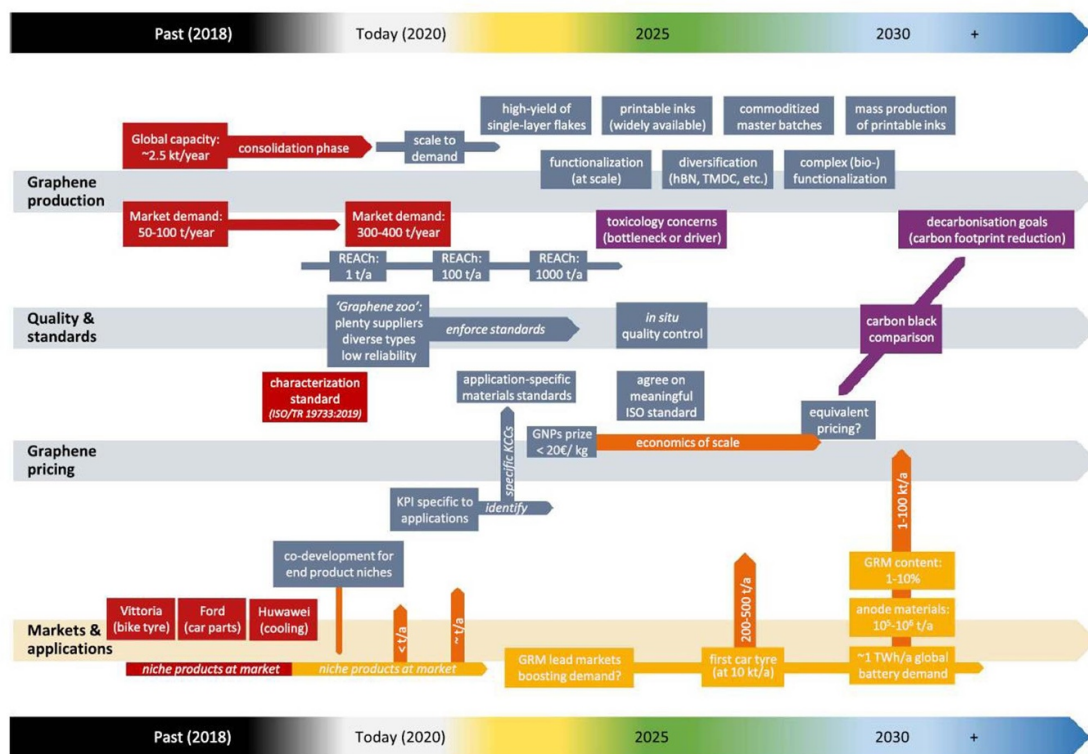


Figure 31. Graphene and related materials Roadmap 2020. Reproduced from [328]. © The Author(s). Published by IOP Publishing Ltd. CC BY 4.0.



International
Organization for
Standardization



International
Electrotechnical
Commission

Terminology Standard - ISO/TS 80004-13:2024

Measurement Technical Report - ISO/TR 19733:2019

Classification Framework - ISO/TS 9651:2025

**Structural Characterisation of Graphene
from powders and dispersions –
ISO/TS 21356-1:2021**

**Structural Characterisation of GO Flakes -
ISO/TS 23879**

**Chemical
Characterisation of
Graphene related
2D materials -
ISO/TS 23359:2025**

Structural Characterisation of Graphene Sheets - ISO/TS 21356-2

Figure 32. Current landscape of joint ISO and IEC 2DM standards published or under development and their associated designations (including publication date where applicable), enabling standards (red), as well as measurement standards for materials consisting of flakes or particles in a powder or liquid dispersion form (light blue) or produced as sheets, for example through chemical vapour deposition (CVD, dark blue).

This slows down development feedback cycles and the commercialization process. Additionally, coatings used in large construction projects, such as bridges, require significant regulation. Without standards and design guidelines, companies hesitate to use innovative materials. This can become a ‘chicken and egg’ problem, where standards that can be the basis of regulation require users and application cases to support their necessity.

Adding GNPs into polymers to improve their electrical and/or thermal conductivity has been a focus for many years. An example of an early commercial application of these nanocomposites involves modifying polyamide (PA6) fibre through the incorporation of GNPs in the organic compound caprolactam. Although graphene-modified PA6 did not have long testing periods nor standards as commercialization hurdles, it required developing many manufacturing steps; (1) dispersing GNPs into caprolactam, (2) the use of a PA6 polymerization plant to manufacture PA6 chips, (3) a spinning company to produce the fibre, (4) stock dyeing, (5) weaving the fibre into fabric and (6) tailoring products such as apparel or bed linens. Hence, it took more than 10 years of development until MLILY Inc. launched products with graphene-modified PA6, now available in over 73 countries.

As another example, GR2Ms have been of great interest for energy storage. Their conductivity and chemical stability offer advantages in various aspects of lithium-ion batteries, particularly when using GNPs as a conductive additive [333]. The supply chain in this application is very short. GNPs are dispersed into NMP (N-Methyl pyrrolidone), a common solvent in the production/supply of GNPs and in the coating of lithium-ion battery electrodes. Then, GNPs are added to a slurry (LiFePo₄) for cathode production. Today, lithium-ion battery manufacturers such as BYD and Gotion in China have one or more product lines that benefit from GNP additives.

The supply chain situation in the semiconductor industry is more complex. Here, factories cost billions to build and maintain, and the process lines cannot be easily adapted to new materials. Hence, tool manufacturers must be convinced of investing in new tools for the deposition, etching, encapsulation, and possibly transfer of 2DMs. Additionally, manufacturers must invest in setting up manufacturing sites that can handle new materials, which are often considered contaminants in the existing clean rooms, and then in extensive testing to assess variability, reliability, and yield. This will only happen if 2DM technology presents a performance-price advantage over the incumbent technology. Judging when that happens may be another ‘chicken and egg’ problem.

Advances in science and technology to meet challenges

Many aspects of standardisation still need to be addressed in the future, beyond the current ISO/IEC standards under development (figure 32). This will require the completion of VAMAS studies, as well as the continued revision of the standards already published. It will be key to include 2DMs as a whole into the current measurement standards, as well as to consider new measurement standards for these other 2D materials (for example, measuring chemical properties). Meanwhile, new international or sector-specific standards will likely be required for new products containing 2DMs, as they enter markets where no standards are in place. At the same time, standards will typically be required only for the final product and not be specific to any involved 2D materials. For example, standards exist for assessing the mechanical properties of composites, a mature area, so GR2M nanocomposites will not require a new standard. The use of GNPs as an additive in concrete for construction is a good example of standardization needs. Many benefits and substantial improvements such as improved mechanical properties have been demonstrated by companies, which would lead to less concrete used and therefore a significant benefit to net zero carbon emission targets. This material is already in use in the real world with hundreds of tons of product poured to date. However, there is understandably significant regulation in place in construction due to safety, which hinders use in load-bearing applications. Regulation is typically based on standards, which are in turn based on data and verification. Hence, more work is required for the commercialization of 2DM products to meet regulatory requirements.

Focusing on the beginning of the supply chain, achieving reproducible production of 2DMs requires well-defined procedures for mass production, taking into account application-specific requirements. Here, standardizing product definitions across different manufacturers would help avoid confusion for downstream users. This approach is being addressed within ISO and IEC through a Classification Framework (figure 32). A lack of knowledge about product characteristics has led to many inconsistent and even contradictory results in graphene and 2DM applications. Therefore, rapid and cost-effective quality control processes are required that are verified through accurate and precise quality control standards.

Concluding remarks

A coherent, hierarchical structure of international standards is required for industry, providing a comprehensive methodology for controlling materials

properties as well as the performance of the final products. Strong communication between academia and industry will be key to achieving a deeper scientific understanding of the roles of 2DMs in particular products, evolving beyond 'graphene' being used as a gimmick in consumer products. Forming an ecosystem involving the scientific community, business community, government and the general public will lead to a significant contribution of these 2DMs to the development of human civilization, as many other materials have in the past, creating a step change in technology.

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Data availability statement

No new data were created or analysed in this study.

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