

Two-Dimensional Materials: Properties, Synthesis, Applications and Future Prospects

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Abstract

Two-dimensional (2D) materials have emerged as one of the most significant areas of contemporary materials science because of their exceptional structural, electronic, optical, mechanical, thermal, and chemical properties. Unlike conventional bulk materials, 2D materials consist of atomically thin layers in which strong in-plane bonding is combined with relatively weak interlayer interactions. This unique structure enables properties that can be controlled through thickness, composition, defects, strain, surface functionalization, and heterostructure formation. Graphene was the first widely recognized member of this modern class, stimulating extensive research into other 2D systems such as transition-metal dichalcogenides, hexagonal boron nitride, MXenes, black phosphorus, layered oxides, and van der Waals heterostructures. These materials have demonstrated considerable potential in electronics, optoelectronics, sensors, energy storage, catalysis, environmental remediation, flexible devices, and biomedical technologies. Their large surface area and tunable interfaces are particularly attractive for electrochemical and catalytic applications. At the same time, challenges associated with large-scale synthesis, defect control, environmental stability, reproducibility, toxicity, cost, and integration with existing technologies continue to restrict widespread commercialization. Recent developments in artificial intelligence, computational materials science, scalable deposition methods, and heterostructure engineering are creating new opportunities for overcoming these limitations. This paper examines the fundamental characteristics of two-dimensional materials, major synthesis techniques, important material classes, technological applications, challenges, and future research directions. It argues that the transition from laboratory-scale demonstrations to practical applications will depend on scalable manufacturing, sustainable synthesis, standardized characterization, and interdisciplinary research.

Keywords: Two-Dimensional Materials, Graphene, MXenes, Transition-Metal Dichalcogenides, Nanotechnology, Heterostructures, Energy Storage, Sensors, Electronics, Materials Science

1. Introduction

The development of two-dimensional materials represents a major transformation in modern materials science. Conventional materials research has traditionally concentrated on bulk materials whose properties arise from three-dimensional structures. The discovery and subsequent study of atomically thin materials demonstrated that reducing a material to one or a few atomic layers can dramatically alter its physical and chemical characteristics. At this scale, surface effects, quantum confinement, interfacial interactions, and defects become particularly important.

Graphene became the most prominent example of this phenomenon after its experimental isolation and characterization. Its exceptional mechanical strength, electrical conductivity, thermal conductivity, optical transparency, and flexibility stimulated enormous scientific interest. More importantly, graphene demonstrated that a single atomic layer could possess technologically useful properties rather than merely being a simplified form of a bulk material. The field subsequently expanded rapidly. Researchers identified and engineered numerous other 2D materials with distinct properties. Transition-metal dichalcogenides can exhibit semiconducting behavior, hexagonal boron nitride provides electrical insulation and chemical stability, black phosphorus offers thickness-dependent electronic properties, and MXenes combine high conductivity with hydrophilic surfaces and tunable chemistry. The emergence of van der Waals heterostructures has further expanded the field by allowing different atomically thin materials to be stacked without conventional lattice matching requirements.

Two-dimensional materials are now investigated across almost every major area of materials science. Their applications range from transistors and photodetectors to batteries, supercapacitors, sensors, membranes, catalysts, biomedical systems, and flexible electronics. However, technological potential must be balanced against manufacturing challenges. The ability to synthesize high-quality 2D materials in laboratories does not necessarily guarantee inexpensive, reliable, and environmentally responsible industrial production.

2. Structural Characteristics of Two-Dimensional Materials

The defining feature of a 2D material is its extremely small thickness, often approaching the atomic scale. Strong chemical bonding generally exists within the plane, while weaker interactions may occur between individual layers. This structural arrangement produces strong anisotropy, meaning that physical and chemical behavior can differ substantially between directions parallel and perpendicular to the layer.

The high surface-to-volume ratio is another important characteristic. In bulk materials, most atoms are located inside the material and have limited direct interaction with the environment. In atomically thin materials, a much larger fraction of atoms is exposed at or near the surface. This can increase chemical reactivity, adsorption capacity, sensing sensitivity, and catalytic activity.

Electronic properties can also change dramatically with thickness. Some materials exhibit transitions between direct and indirect band gaps as the number of layers changes. This makes thickness control an important tool for designing optical and electronic devices.

Defects are equally significant. Vacancies, substitutions, grain boundaries, wrinkles, and edge sites can alter conductivity, catalytic activity, magnetism, and mechanical properties. Although defects may be undesirable in some electronic applications, they can be beneficial for catalysis, sensing, and energy storage. Thus, modern 2D materials research increasingly focuses on controlled defect engineering rather than simply eliminating all imperfections.

3. Graphene and Its Scientific Importance

Graphene is a single layer of carbon atoms arranged in a hexagonal lattice. Its discovery generated enormous interest because of its combination of mechanical, electrical, thermal, and optical properties.

The mechanical strength of graphene makes it attractive for reinforcement in polymer and ceramic composites. Even relatively small quantities can modify stiffness, strength, electrical

conductivity, barrier properties, and thermal behavior. Graphene-based composites have consequently been investigated for aerospace components, automotive structures, coatings, packaging, conductive materials, and flexible devices.

Graphene also has excellent electrical conductivity. This has encouraged research into transparent conductive films, sensors, electromagnetic shielding, flexible electronics, and energy-storage electrodes. However, pristine graphene lacks a conventional band gap, which limits its direct use in some digital transistor applications. Researchers have therefore explored chemical functionalization, nanoribbon formation, defect engineering, and heterostructure approaches to modify its electronic characteristics.

Graphene's thermal conductivity is another attractive feature. It has been studied for thermal management in electronic devices where heat dissipation is increasingly important.

Despite these advantages, commercialization has been complicated by production costs, quality variations, differences between synthesis methods, and difficulties in achieving consistent properties at industrial scale. The term “graphene” can refer to materials with substantially different numbers of layers, defect densities, and functional groups, making standardized characterization particularly important.

4. Transition-Metal Dichalcogenides

Transition-metal dichalcogenides (TMDs) represent another important family of 2D materials. Materials such as molybdenum disulfide (MoS_2), tungsten disulfide (WS_2), and related compounds have attracted attention because of their semiconducting, optical, catalytic, and mechanical properties.

Unlike graphene, several TMDs possess band gaps suitable for electronic and optoelectronic applications. This has generated interest in atomically thin transistors, photodetectors, light-emitting devices, and flexible electronics.

The optical properties of TMDs are particularly interesting because strong excitonic effects can occur in atomically thin layers. Their response to light can be adjusted by controlling layer number, strain, defects, and chemical environment.

TMDs are also studied as catalysts. Edge sites and engineered defects can provide active locations for chemical reactions. MoS_2 , for example, has been extensively investigated for hydrogen evolution and other electrochemical reactions.

Nevertheless, challenges remain in producing large-area TMD films with uniform thickness, controlled defects, and reproducible electronic properties. Integration with conventional semiconductor manufacturing also requires compatible processing temperatures and fabrication methods.

5. MXenes: A Rapidly Developing Family

MXenes are a relatively new family of two-dimensional transition-metal carbides and nitrides. They generally exhibit high electrical conductivity, large surface areas, hydrophilic surfaces, and chemically tunable compositions. These characteristics have made MXenes particularly attractive for energy storage, electromagnetic shielding, sensors, catalysis, and flexible electronics.

The surface chemistry of MXenes is especially important. Their surfaces can contain functional groups that influence electrical properties, hydrophilicity, ion transport, and interactions with

other materials. This makes them highly adaptable for composite and electrochemical applications.

MXenes have attracted considerable attention in supercapacitors because their conductivity and layered structure can facilitate charge storage and transport. They have also been explored in batteries, where ion insertion and surface reactions contribute to electrochemical behavior.

Sensors represent another major application. MXene-based systems can respond to mechanical deformation, gases, chemicals, humidity, biological molecules, and temperature. Their flexibility and conductivity make them attractive for wearable sensing platforms.

However, MXenes also face important stability challenges. Some compositions can undergo oxidation or degradation under environmental conditions. Improving storage stability, processing methods, and large-scale synthesis remains essential for practical implementation.

6. Synthesis Methods

The performance of a 2D material depends strongly on the synthesis route. Methods are commonly divided into top-down and bottom-up approaches.

Top-down methods begin with a bulk layered material and separate it into thinner layers. Mechanical exfoliation can produce exceptionally high-quality flakes but usually has low yield and limited scalability. Liquid-phase exfoliation can produce larger quantities and is useful for inks and composite processing, although controlling thickness and defect concentration can be difficult.

Chemical exfoliation can also produce substantial quantities but may involve reactive chemicals and generate structural or surface modifications. For industrial applications, the environmental impact of solvents and chemical reagents must therefore be considered.

Bottom-up methods construct materials from atoms, molecules, or chemical precursors. Chemical vapor deposition (CVD) is particularly important because it can produce relatively large-area films. Molecular beam epitaxy and related deposition techniques can provide precise control over growth conditions but may require expensive equipment.

Physical vapor deposition and atomic layer deposition are also being investigated for specific material systems. These methods can offer control over thickness and composition, making them potentially valuable for electronics and coatings.

The choice of synthesis technique depends on the intended application. High-quality flakes may be suitable for fundamental research, whereas large-area uniform films are more important for industrial electronics. Therefore, synthesis must be considered in conjunction with device requirements.

7. Two-Dimensional Heterostructures

One of the most exciting developments in 2D materials research is the creation of van der Waals heterostructures. These structures are formed by stacking different atomically thin materials together. Because the layers can be held together through van der Waals interactions, researchers can combine materials with different properties without requiring conventional epitaxial lattice matching.

A heterostructure may combine a semiconductor, conductor, and insulator into an atomically thin architecture. Such structures can provide new opportunities for transistors, photodetectors, tunneling devices, quantum systems, and energy technologies.

The relative rotational orientation between layers can also produce important phenomena. Small rotational misalignments can generate moiré patterns that modify electronic behavior. In selected systems, these structures have been associated with unusual correlated electronic phenomena.

Heterostructure engineering therefore represents a transition from discovering individual materials toward designing material systems. Researchers can select individual layers according to their electrical, optical, magnetic, or chemical characteristics and combine them to obtain emergent properties.

8. Applications in Electronics and Optoelectronics

The electronics industry continuously seeks materials that can support smaller, faster, flexible, and energy-efficient devices. Two-dimensional materials offer attractive characteristics because their atomic thickness enables strong electrostatic control and potentially reduces short-channel effects in nanoscale devices.

TMDs are particularly promising for transistor applications because several have suitable semiconductor band gaps. Graphene can serve as a conductive layer or electrode, while hexagonal boron nitride can act as an insulating or protective layer. Heterostructures can therefore provide multifunctional electronic architectures.

Flexible electronics represent another major application. Because many 2D materials are thin and mechanically flexible, they can be integrated into flexible substrates. Potential applications include wearable sensors, electronic skins, flexible displays, and portable healthcare devices. Optoelectronics also benefits from 2D materials. Their strong light-matter interactions and thickness-dependent optical properties make them attractive for photodetectors and light-sensitive devices.

However, practical electronic applications require uniform large-area films, reliable contacts, low defect densities, stable operation, and compatibility with established manufacturing processes. These requirements remain major barriers to widespread commercial adoption.

9. Energy Storage and Conversion

Two-dimensional materials have considerable potential for energy-storage systems because of their high surface areas and short ion-diffusion distances. They have been investigated as electrodes, conductive additives, catalysts, and components of composite architectures.

In lithium-ion batteries, layered materials can provide pathways for ion insertion and transport. Their nanoscale thickness can reduce diffusion distances and improve reaction kinetics. However, high surface area may also increase undesirable side reactions, emphasizing the need for careful interface engineering.

Supercapacitors are another important application. Conductive 2D materials can provide rapid charge transport and high accessible surface areas. MXenes have been particularly investigated because of their combination of conductivity, layered structure, and surface chemistry.

Fuel cells and electrochemical hydrogen production also benefit from 2D catalysts. Defects and edge sites can be engineered to increase catalytic activity. Combining 2D materials with other nanostructures can further improve electron transport and active-site availability.

Nevertheless, long-term stability and scalable electrode fabrication remain significant issues. Future research must therefore move beyond laboratory performance metrics and consider complete device-level performance.

10. Environmental and Biomedical Applications

The large surface area and tunable surface chemistry of 2D materials create opportunities for environmental applications. Membranes based on graphene derivatives and other layered materials have been studied for water purification, ion separation, and desalination.

Adsorption-based environmental remediation is another area of interest. Functionalized 2D materials can interact with heavy metals, organic pollutants, and other contaminants. Their performance can be improved by controlling pore structures and surface functional groups.

Biomedical applications include biosensors, drug-delivery systems, imaging, antimicrobial surfaces, and tissue-engineering platforms. Graphene derivatives and other 2D materials can provide high surface areas for biomolecule attachment and signal generation.

However, biomedical and environmental applications require careful assessment of toxicity, persistence, biodegradation, and biological interactions. The behavior of a material in laboratory conditions may differ from its behavior in complex biological or environmental systems. Therefore, safety evaluation must accompany technological development.

11. Challenges and Limitations

The most important challenge facing 2D materials is scalability. Many research demonstrations rely on small flakes or specialized laboratory equipment. Industrial applications require large-area production with consistent thickness, composition, defect density, and surface chemistry. Another challenge is reproducibility. Two samples nominally described as the same 2D material may display significantly different properties because of variations in synthesis and processing.

Environmental stability is also important. Some 2D materials are sensitive to oxygen, moisture, temperature, or light. Protective coatings and encapsulation may be required, increasing device complexity.

Cost is an additional consideration. Even when the raw material is inexpensive, specialized synthesis, purification, transfer, and characterization can make the final product costly.

Health and environmental risks require further investigation. Nanomaterials can interact with biological systems in complex ways, and their effects may depend on size, shape, surface chemistry, dose, and exposure conditions.

Finally, integration with existing technologies remains challenging. New materials must be compatible with established semiconductor, battery, manufacturing, and packaging processes before they can achieve large-scale commercial adoption.

12. Future Research Directions

Future 2D materials research is likely to focus on controlled synthesis, sustainable manufacturing, heterostructure design, artificial intelligence, and multifunctional devices. AI-assisted materials discovery could help identify new compositions and predict properties before experimental synthesis.

Large-scale manufacturing will remain a central priority. Researchers will increasingly seek low-cost, low-energy, and environmentally responsible production methods. Roll-to-roll processing, solution-based deposition, scalable CVD, and other continuous manufacturing approaches could contribute to industrialization.

Another important direction is sustainable design. Researchers must consider not only material performance but also precursor availability, chemical hazards, energy consumption, recyclability, and end-of-life behavior.

Integration with other advanced technologies will also increase. Two-dimensional materials may be combined with three-dimensional nanostructures, polymers, biomaterials, quantum technologies, and additive manufacturing.

The development of standardized testing protocols will be equally important. Consistent definitions, measurement methods, and reporting standards can improve comparison among studies and accelerate technological translation.

13. Conclusion

Two-dimensional materials have become a central research area within contemporary materials science because their atomic-scale structures enable remarkable and tunable properties. Graphene, transition-metal dichalcogenides, MXenes, black phosphorus, hexagonal boron nitride, and other materials offer opportunities across electronics, optoelectronics, energy, catalysis, sensing, healthcare, and environmental technologies.

The field is now moving beyond the discovery of individual materials toward controlled heterostructure engineering and multifunctional systems. Such approaches could generate properties that are not available in conventional bulk materials. At the same time, significant challenges remain in scalable production, reproducibility, environmental stability, safety, cost, and integration with existing industrial processes.

The future success of 2D materials will therefore depend on a balanced approach. Exceptional laboratory performance must be combined with manufacturability, reliability, sustainability, and safety. Advances in artificial intelligence, computational modeling, automated experimentation, and sustainable synthesis could accelerate this transition. If these challenges are successfully addressed, two-dimensional materials may become important building blocks for next-generation electronics, energy systems, medical technologies, and environmentally sustainable industrial applications.

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