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Review Article

2D Materials Beyond Graphene for Energy Storage and Conversion: Recent Advances and Future Perspectives

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Abstract: Two-dimensional (2D) materials have emerged as a major class of advanced materials for energy storage and conversion technologies. Although graphene initiated this research field, its zero bandgap, limited chemical tunability, and restacking tendency restrict its performance in many practical energy systems. These limitations have driven the development of a broad range of 2D materials beyond graphene, including MXenes, transition metal dichalcogenides, black phosphorus, metal oxides and hydroxides, layered double hydroxides, and other emerging atomically thin systems. These materials offer diverse crystal structures, tunable electronic properties, rich surface chemistry, and high surface-to-volume ratios, making them attractive for batteries, supercapacitors, electrocatalysis, and photoelectrochemical applications. This review provides a comprehensive overview of recent progress in 2D materials beyond graphene for energy storage and conversion. Key aspects discussed include synthesis strategies, defect and interface engineering, heterostructure design, and structure–property relationships. The performance of these materials in lithium-ion and beyond-lithium batteries, supercapacitors, electrocatalytic reactions, and solar-driven energy systems is critically examined. Recent advances in characterization techniques, computational modelling, and machine learning-assisted discovery are also highlighted for their role in accelerating material development. Despite significant laboratory-level success, several challenges remain, particularly in scalable synthesis, long-term stability, standardised benchmarking, and system-level integration. Addressing these issues is essential for translating promising material properties into reliable and commercially viable energy technologies. Overall, this review outlines current achievements, identifies critical knowledge gaps, and presents future perspectives for advancing 2D materials beyond graphene toward sustainable and practical energy solution.

Keywords: 2D Materials, Mxenes, Batteries, Energy Storage, Graphene Sustainability.

1. Introduction

1.1 The Post-Graphene Era in 2D Materials

The discovery of graphene in 2004 marked an important change in materials science. Graphene showed that a single atomic layer could provide high electrical conductivity, strong mechanical strength, and a large surface area. These features attracted strong interest for energy-related uses. However, later studies showed that graphene also has clear limitations. The absence of a band gap limits its use as a semiconductor electrode. Its flat carbon network shows weak redox activity. The number of active sites for faradaic reactions remains lower than that of many transition-metal compounds. These drawbacks reduce its direct use in many energy storage and conversion systems. Due to these limits, research moved beyond graphene and entered what is now called the post-graphene era. This phase focuses on a wide range of layered and quasi-two-dimensional materials designed for energy applications. This shift occurred due to three main reasons. First, atomically thin materials show unique electronic, electrochemical, and mechanical behaviour. Second, new classes of 2D materials became available, such as transition-metal dichalcogenides, MXenes, phosphorene, layered metal oxides and hydroxides, and monoelemental sheets known as Xenes. These materials allow control over composition, surface chemistry, and interlayer spacing. Third, these materials are now actively used in devices for batteries, supercapacitors, electrocatalysis, and photo-electrochemical systems. In this post-graphene phase, the combined effect of atomic thickness, tunable electronic structure, and ion-accessible layers has been applied more effectively to sustainable energy technologies [1, 2]

A major benefit of 2D materials for energy use is their high surface-to-volume ratio. This feature increases the number of active sites and reduces ion transport distance. In layered structures, ions can move or insert between van der Waals gaps or modified interlayers. This behaviour supports fast charge storage and high pseudocapacitive response compared to bulk materials. The thin layers can also absorb strain during repeated charge and discharge cycles, which improves mechanical stability. The flexible nature of 2D sheets supports free-standing films, binder-free electrodes, and flexible devices. Such designs are important for modern energy systems. These advantages are now used to tune surface terminations, phase structure, stacking order, and interlayer distance in materials beyond graphene. For example, MXenes allow control over interlayer spacing and surface groups such as –O, –OH, and –F, which improves ion access and conductivity [3]. Transition-metal dichalcogenides can switch between metallic and semiconducting phases, which helps both catalysis and charge storage [4] this review presents a detailed overview of 2D materials beyond graphene with emphasis on energy storage and conversion. The aims include explaining the shift from graphene to other 2D materials, describing the advantages of layered thin structures for energy systems, and classifying major 2D material families such as MXenes, TMDs, phosphorene, layered oxides and hydroxides, and Xenes. The discussion sets the base for later sections on batteries, supercapacitors, electrocatalysis, photo-electrochemistry, and hybrid devices. Figure 1 shows the key milestones of 2D materials used in perovskite solar cells over the last decade. Overall, the post-graphene era represents a major expansion from carbon-based materials to a broad library of 2D systems with controlled structure and chemistry. This transition supports new solutions for current challenges in energy storage and conversion.

1.2 Energy Storage and Conversion Challenges

The global move toward low-carbon energy has increased the need for efficient energy storage and conversion systems. Renewable sources such as solar and wind show irregular output. This mismatch between energy generation and demand creates strong pressure on energy storage systems to balance supply, support grid stability, and allow energy trading. Despite progress, current storage technologies still face limits in energy density, power density, lifespan, safety, cost, and large-scale use [6–8]. In energy conversion systems such as water splitting and carbon dioxide reduction, slow reaction rates, low selectivity, material degradation, and high energy losses restrict practical deployment. A key challenge lies in achieving high energy density together with high power density while maintaining long cycle life and safety. Lithium-ion batteries dominate the market but approach their practical energy limits. Safety risks and high cost also restrict their large-scale grid use. Supercapacitors provide fast charging and long cycle life but store much less energy and often work at lower voltages [9, 10]. Lithium-ion batteries typically deliver energy density between 100 and 300 Wh kg^{-1} with moderate to high power density and a cycle life of 500 to 2000 cycles. This balance makes them suitable for electronics and electric vehicles [11]. However, cost, safety concerns, limited lifespan, and dependence on scarce materials limit broader use. Supercapacitors, in contrast, offer very high-power density and can exceed 100,000 cycles, but their energy density remains low at about 5 to 30 Wh kg^{-1}[12].

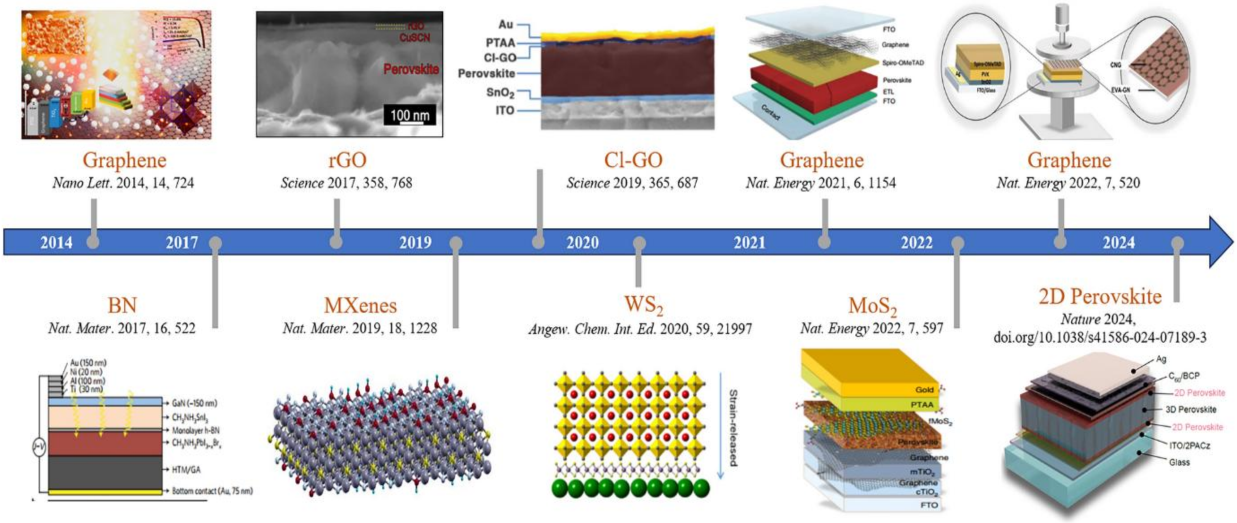

Figure 1. The key milestones of 2D materials-incorporated PSCs over the past decade (Adapted from Shen *et al.,* 2024, Springer Nature, CC BY 4.0) [5].

Hybrid and next-generation systems that use advanced 2D materials aim to improve both energy and power, with targets above 300 Wh kg^{-1} and 10,000 W kg^{-1} [13]. These systems still face challenges related to stability, cost, and scale-up.

Energy conversion processes also show major barriers. In water splitting, the oxygen evolution reaction remains slow and needs high overpotential, which causes catalyst degradation over time [14]. Battery systems based on sodium, magnesium, or aluminium face problems due to larger ion size, slow diffusion, unstable interfaces, and dendrite growth [15]. At the system level, many studies do not fully consider technology readiness, life-cycle emissions, or social and economic factors. A recent analysis highlighted the lack of such criteria in many comparisons of energy storage options [16]. Other common challenges also affect performance. Large-scale manufacturing remains difficult because many materials show poor reproducibility, high synthesis cost, and uneven quality. Stability under real operating conditions, such as temperature changes and mechanical stress, often reduces performance. Interface design between electrode and electrolyte plays a key role and often limits device efficiency more than the active material itself. In addition, the absence of standard testing protocols makes comparison between studies unreliable. Therefore, high material capacity alone is not enough. The material must fit into a scalable, stable, safe, and cost-effective system. Balancing energy, power, cost, and durability remains essential. At this point, 2D materials beyond graphene offer strong potential, but the gap between material discovery and device application remains a major challenge. In summary, energy storage and conversion face four main challenges: balancing energy density, power density, and cycle life; improving speed and stability of conversion reactions; ensuring large-scale manufacturing and durability; and developing standard benchmarks with system-level readiness. This review discusses how 2D materials may help address these issues and support sustainable energy solutions.

1.3 Classification of 2D Materials beyond Graphene

After the success of graphene, many new two-dimensional materials have emerged. Each group shows unique structure, electronic behaviour, and interlayer chemistry that overcome graphene's limitations in energy systems. Clear classification helps in understanding their roles in energy storage and conversion. One important class includes MXenes, which are 2D transition-metal carbides and nitrides with general formula $M_{n+1}X_nT_x$. Here, M represents an early transition metal, X is carbon or nitrogen, and T_x refers to surface groups. MXenes show high electrical conductivity, high capacitance, and adjustable surface chemistry. Reviews describe MXenes as promising materials for advanced energy storage and electrochemical applications [17, 18]. Their layered structure, hydrophilic surface, and tunable spacing support ion insertion and fast charge storage.

Another major group is transition-metal dichalcogenides with formula MX_2, such as MoS_2 and WS_2. These materials consist of layers held by weak van der Waals forces, which allows easy exfoliation. They show semiconducting or metallic behaviour depending on structure and phase. Their tunable band gaps and redox-active metal centres support energy storage and catalytic reactions. MoS_2 has been widely studied for such applications [19]. These materials form a large part of the 2D materials library for energy use [20]. Monoelemental 2D materials, known as Xenes, form another important group. Black phosphorus, or phosphorene in thin layers, shows a natural band gap, anisotropic charge transport, and thickness-dependent electronic properties. Studies highlight its advantages over graphene in band-gap control and redox activity [21]. Its layered structure and high theoretical capacity make it suitable for energy storage. Layered metal oxides and hydroxides, such as layered double hydroxides and cobalt or nickel hydroxides, also play an important role. Though sometimes overlooked in 2D discussions, their thin nanosheet form, rich redox chemistry, and high ion accessibility make them effective for energy devices. Recent reviews discuss their preparation and application [22].

Insulating 2D materials like hexagonal boron nitride serve as protective or supporting layers. They offer chemical stability and structural support in heterostructures, even if they do not directly store charge. New and emerging 2D materials such as tellurene, antimonene, and bismuth oxyselenide are also gaining attention. These materials remain at an early stage but show promise due to tunable electronic structure and high surface area [23] overall, classification of 2D materials beyond graphene is based on function rather than names alone. Each group offers specific structural and chemical advantages for energy devices. Understanding these features helps guide material design, stacking strategies, and device integration for improved energy storage and conversion.

2. Synthesis and Structural Engineering

2.1 Top-Down Synthesis Approaches

Top-down synthesis remains an important route to produce two-dimensional materials with atomic or few-layer thickness. This approach starts from bulk layered solids and separates them into thin sheets. Common top-down methods include chemical and electrochemical etching, liquid-phase exfoliation, and mechanical exfoliation. Each method differs in how it breaks interlayer bonding, controls sheet size, and affects defect density. These features strongly influence performance in energy storage and conversion devices. Chemical and electrochemical etching methods have played a major role in the synthesis of MXenes. In a typical process, aluminium or another A-layer is selectively removed from the MAX phase, which results in layered MXene sheets. These sheets are then delaminated into thin flakes. Studies report that etching remains the main route for MXene synthesis, and the choice of etchant, intercalation ions, and delamination agents directly affects flake size, conductivity, and surface chemistry [24]. The etching process introduces surface groups such as –O, –OH, and –F. These groups influence hydrophilicity, layer spacing, and ion access, which are important for battery and supercapacitor electrodes.

Liquid-phase exfoliation is a scalable method suitable for many layered materials, including transition-metal dichalcogenides, metal oxides, hydroxides, and new Xenes. In this process, bulk materials are dispersed in suitable solvents and exposed to sonication or shear force to separate layers. Surfactants or intercalants often assist this separation. Key factors include solvent choice, sonication energy, and centrifugation speed. These parameters control yield, flake thickness, and defect formation [25] Recent advances such as vortex-fluidic and continuous-flow systems have improved yield. For example, about 73% conversion of MoS_2 into few-layer sheets was achieved using a vortex-fluidic device [26].

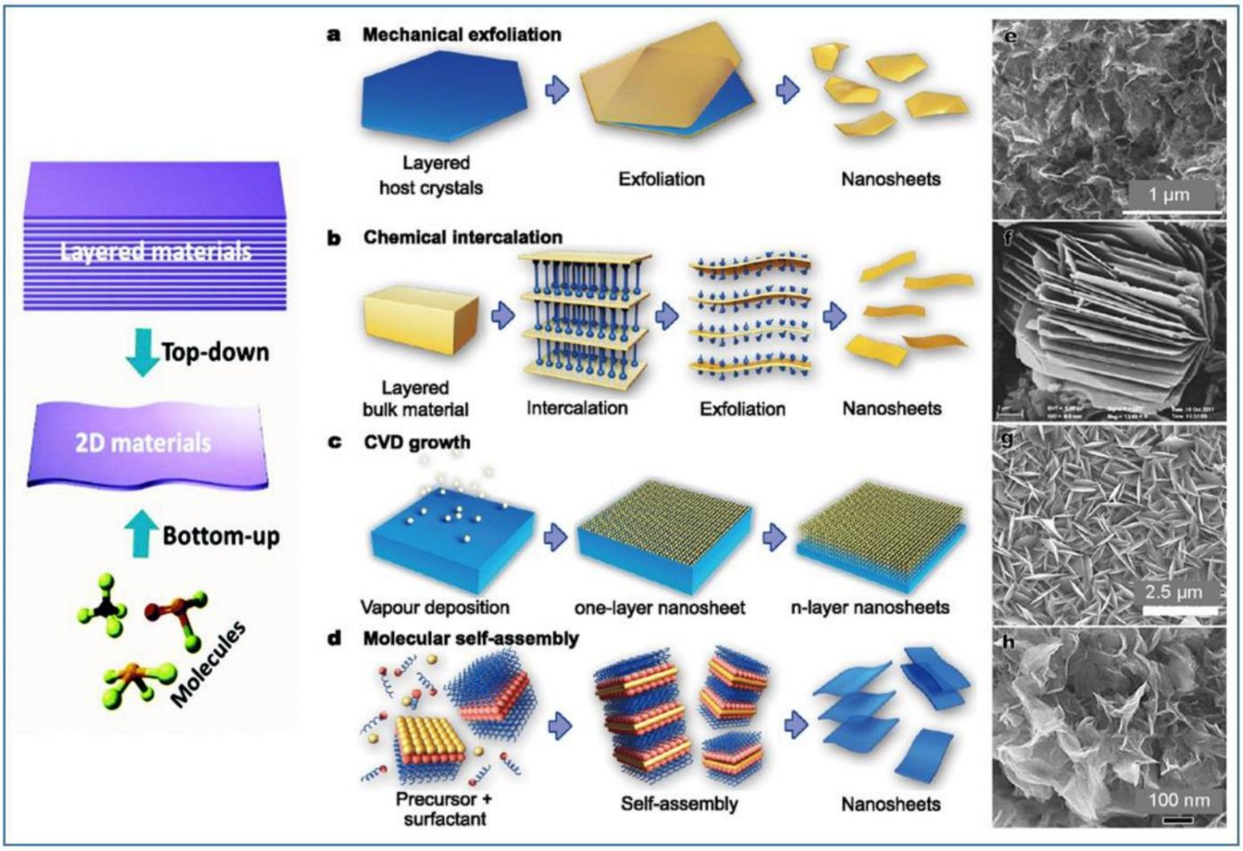

Figure 2. Examples of top-down and bottom-up strategies for the synthesis of 2D layered nanostructures: **(a)** mechanical exfoliation of layered host materials, **(b)** chemical intercalation induced exfoliation, **(c)** chemical vapor deposition (CVD) growth, and **(d)** wet-chemical self-assembly. Scanning electron microscopy (SEM) images of 2D nanomaterials obtained with the corresponding techniques: **(e-h)** TiO2 and (f) VO2 nanosheets. (Adapted from Anwar *et al.,* 2024, Springer Nature, CC BY 4.0) [27].

Despite these gains, liquid-phase exfoliation can introduce defects, uneven thickness, and sheet re-aggregation, which reduce reproducibility and stability in energy devices. Mechanical exfoliation produces high-quality and highly crystalline 2D sheets by physically cleaving bulk crystals. However, this method suffers from very low yield, poor thickness control, and limited scalability. Even with improved sonication or shear-assisted techniques, control over defect density and lateral size remains difficult. Therefore, mechanical exfoliation is mainly used for fundamental studies rather than practical energy-device fabrication.

Each top-down approach shows specific strengths and limitations. Etched MXenes provide high conductivity and fast ion transport due to tailored surface terminations. Liquid-phase exfoliation offers scalable production but often lacks uniformity. Mechanical exfoliation yields high crystal quality but is unsuitable for large-scale use. Several challenges remain across all top-down methods. Uniform thickness and consistent lateral size are difficult to achieve. Defect control requires careful balance, as excessive defects reduce conductivity and cycle life. Removal of etchants and surfactants increases cost and environmental burden. In addition, converting nanosheets into practical electrodes requires careful control of film formation, binder interaction, and electrical contact. Overall, top-down synthesis remains essential for expanding the use of 2D materials in energy systems. Etching methods for MXenes, scalable exfoliation routes, and high-quality mechanical methods together form a strong materials platform. Future progress depends on improving uniformity, reducing defects, increasing yield, and ensuring compatibility with device-scale fabrication. Figure 2 illustrates common top-down and bottom-up synthesis strategies for 2D layered nanostructures.

2.2 Bottom-Up Synthesis Methods

Bottom-up synthesis offers a controlled route to fabricate atomically thin 2D materials with defined thickness, crystal quality, and substrate compatibility. Major bottom-up techniques include chemical vapour deposition, molecular beam epitaxy, and hydrothermal or solvothermal synthesis. These methods are important for energy storage and conversion because they allow control over composition and interface quality. Chemical vapour deposition is widely used to grow large-area 2D films such as MoS_2, WS_2, and hexagonal boron nitride. Recent studies focus on reducing growth temperature, improving film uniformity, and enabling growth on flexible substrates. Low-temperature CVD below 500 °C has shown promise for producing controlled 2D layers on non-traditional substrates by careful precursor and seed selection [28]. Such advances support flexible and binder-free energy devices. However, high cost, substrate transfer steps, and contamination remain barriers for large-scale battery and supercapacitor electrodes. Industrial-scale CVD with consistent thickness and reproducibility remains a key requirement [29]. Molecular beam epitaxy provides precise atomic-level control and enables layer-by-layer growth with clean interfaces. This method supports the formation of high-quality van der Waals heterostructures [30]. Such precision benefits energy devices where interface quality affects charge transport and ion storage. However, high equipment cost, slow growth rate, and limited substrate size restrict its use in large-scale energy applications.

Hydrothermal and solvothermal methods use solution-phase reactions to form 2D nanosheets under moderate conditions. These routes are suitable for layered oxides, hydroxides, LDHs, and some TMDs. They offer low cost, high yield, and scalability. Growth parameters such as solvent type, temperature, and reaction time control sheet thickness and morphology [31]. These nanosheets are easy to process into electrodes and often show high redox activity. However, they may suffer from size variation, residual surfactants, lower conductivity, and limited large-area uniformity. Each bottom-up method involves trade-offs. CVD provides high quality but at higher cost. MBE offers the best control but lacks scalability. Solution-based methods allow large-scale production but need post-treatment to improve conductivity and uniformity. For energy devices, synthesis choice affects electrode thickness, ion transport, mechanical stability, and overall cost. From a device perspective, bottom-up materials must integrate well with current collectors, binders, and large-scale manufacturing. CVD films require careful transfer or direct growth on collectors. Solution-grown sheets must retain layered structure during coating and compaction. Defect tuning, doping, and surface modification often start at this synthesis stage and influence final device performance. In summary, bottom-up methods form the foundation for producing 2D materials for energy applications. Their success depends on balancing quality, scalability, and cost. Future work should focus on low-temperature CVD, scalable alternatives to MBE, and high-yield solution routes with minimal post-processing to close the gap between material synthesis and device production.

2.3 Defect Engineering and Functionalization

Defect engineering and functionalization play a key role in improving the performance of 2D materials beyond graphene. These strategies involve controlled creation of vacancies, heteroatom substitution, edge modification, and surface termination. Such changes alter electronic structure, ion transport, catalytic activity, and interlayer chemistry. Functionalization further adjusts surface interaction with electrolytes and reactants, which supports better device operation. Vacancy engineering has shown strong impact on electrochemical behaviour. Studies report that defects expose active sites, modify band structure, and improve ion access, which enhances redox kinetics [32]. In TMDs such as MoS_2, chalcogen vacancies reduce ion diffusion barriers and improve pseudocapacitive response. Similar effects appear in oxide and hydroxide nanosheets. Heteroatom doping and edge modification further tune electronic states, which is beneficial for reactions such as hydrogen and oxygen evolution.

Surface termination control is especially important for MXenes. Termination groups such as –O, –OH, and –F influence conductivity, wettability, and interlayer spacing. Adjusting these groups can improve reversible ion intercalation and cycling stability. For example, reducing –F content and increasing –O termination in $Ti_3C_2T_x$ has shown improved capacity and durability. Edge functionalization and atom anchoring increase active site density and improve structural stability. Single-atom decoration at vacancy sites in TMDs enhances catalytic activity and durability due to improved charge distribution [33]. Functionalization of phosphorene improves alkali-ion storage and reduces surface oxidation. Controlled covalent functionalization of graphitic materials also supports interface tuning for electronic and energy applications [34]. Figure 3 illustrates controlled covalent functionalization under microfluidic conditions. Despite these benefits, defect engineering requires careful control. High defect density can weaken structure, reduce conductivity, and shorten cycle life, as observed in defect-rich carbon electrodes [35]. Doping and functionalization must preserve layered structure and avoid unwanted phase changes. Performance depends on defect type, concentration, and spatial distribution.

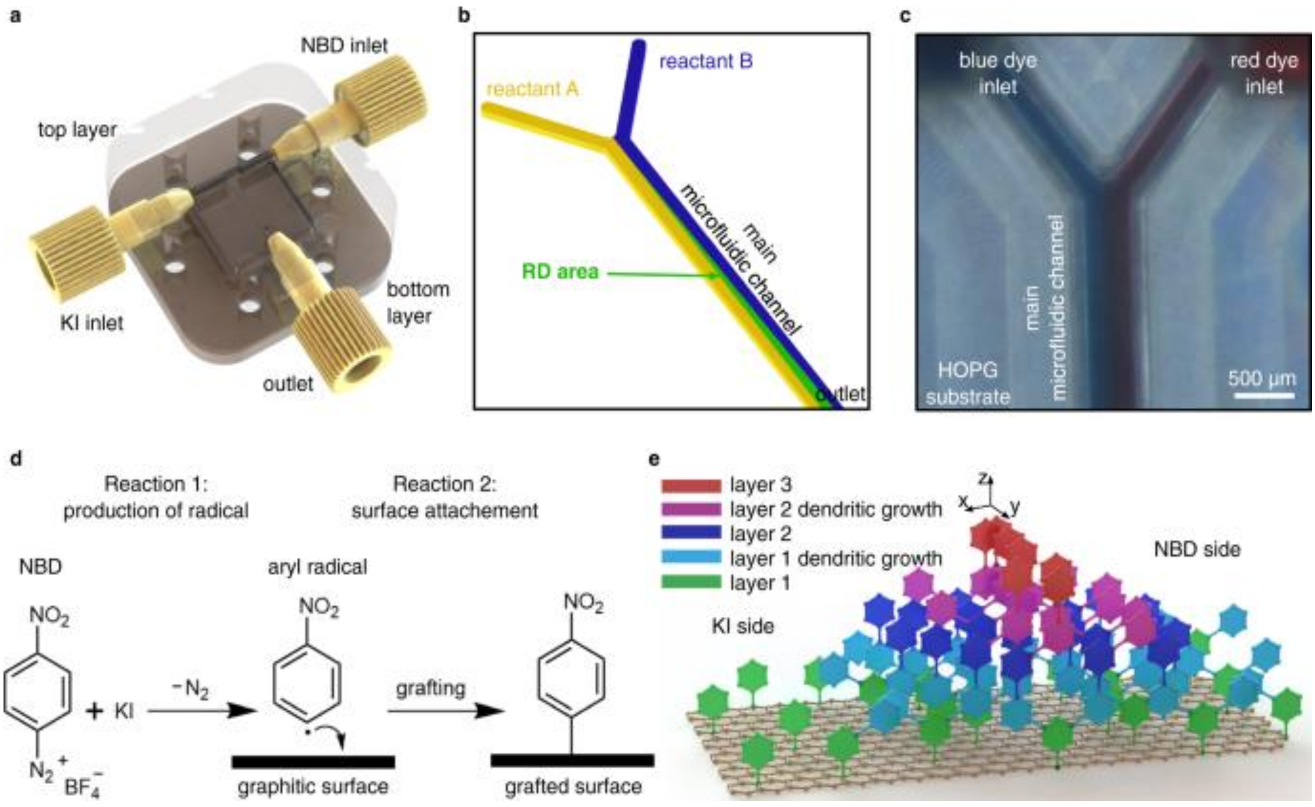

Figure 3. **a** Schematic drawing of the assembled microfluidic device. **b** Illustration of the main microfluidic channel. **c** Micrograph of the assembled microfluidic device. **d** Schematic reactions of NBD with KI on a graphitic surface. **e** Illustration showing the dendric growth of reactions presented in d (Xia *et al.,* 2022, Springer Nature, CC BY 4.0) [33].

For practical devices, engineered defects must remain stable during long-term cycling and under varying temperature and chemical conditions. Advanced in-situ and operando techniques help track defect evolution during operation. Overall, defect engineering and functionalization offer powerful tools to improve ion transport, conductivity, catalytic activity, and stability. Future research must focus on scalable defect control and direct integration into device architectures.

2.4 Heterostructure Construction

Heterostructure construction combines different 2D materials into a single system to achieve functions not possible with individual layers. In energy storage and conversion, heterostructures improve charge transport, ion access, electronic alignment, and mechanical stability. The layered nature of 2D materials supports van der Waals assembly without strict lattice matching. Vertical heterostructures involve stacking different 2D layers. These structures enable band alignment control and charge separation. In energy conversion devices, Type-II heterojunctions improve electron–hole separation, which benefits photoelectrochemical reactions [36]. In batteries and supercapacitors, stacking conductive MXenes with redox-active layers combines high conductivity with high capacity. Reviews show that MXene-based heterostructures improve ion diffusion and cycling stability [37].

Lateral heterostructures connect different 2D materials within the same plane. These structures offer sharp interfaces, fast in-plane charge transport, and high edge-site density. Such features are useful for flexible devices and microsupercapacitors. Lateral coupling has shown reduced overpotential and improved durability in electrocatalysis [38] Van der Waals assembly methods allow stacking of metals, semiconductors, and insulators without lattice constraints. These assemblies preserve layer integrity and introduce minimal strain. Built-in electric fields at interfaces improve charge separation and ion transport. Reviews highlight improved light absorption and catalytic activity in such heterostructures [39]. Each heterostructure type has trade-offs. Vertical stacks offer uniform thickness but may face interlayer resistance. Lateral structures provide better edge access but involve complex synthesis. Solution-assembled heterostructures support scalability but may need post-treatment. Overall, heterostructure construction enables improved transport, stability, and multifunctionality in energy devices. Future work must focus on scalable synthesis, interface control, and clear links between heterostructure design and device performance. Figure 4 shows an example of interface investigation using advanced microscopy. Table 1 list the important 2D materials and their energy relevant characteristics.

Table 1. Key Families of 2D Materials and Their Energy-Relevant Characteristics

No.	2D Material Class	Typical Synthesis Method(s)	Surface Chemistry	Representative Applications	Strengths	Challenges	References
1	Ti3C2Tx MXene	HF etching of Ti3AlC2 MAX phase	Surface terminations (-OH, -F, -O)	Supercapacitors, Li-ion batteries	Metallic conductivity, high volumetric capacitance (417.4 F/g)	Oxidation instability, moisture sensitivity	[40]
2	Ti3C2Tx MXene	LiF/HCl etching (MILD method)	Layered structure with tunable interlayer spacing	Symmetric supercapacitors	High specific capacitance (402 F/g), conductivity (210 S/cm)	Low yield in traditional methods	[41]
3	Ti3C2Tx MXene	Hydrothermal synthesis	Ti3C2Tx with oxygen-containing groups	Energy storage devices	Stability enhancement, easier processability	Quality control challenges	[42]
4	Ti3C2Tx/SnO composite	One-step hydrothermal	SnO nanoparticles on MXene	Asymmetric supercapacitors	Prevents aggregation, 29.3 mAh/g at 5 mV/s	Moderate energy density (26.7 Wh/kg)	[43]
5	Ti3C2Tx MXene	Ionic liquid etching (TMATFB)	Oxygen-rich functional	Sodium-ion batteries	Safer synthesis, 267.5 mAh/g	Lower capacity vs conventional	[44]

			groups		after 100 cycles	methods	
6	Ti3C2Tx MXene	Chemical etching	Layered 2D structure	Li-ion and Na-ion batteries	High electrical conductivity, large surface area	Environmental instability	[45]
7	Ti3C2Tx MXene	Top-down synthesis	MXene nanosheets	Batteries and supercapacitors	Tunable surface chemistry, hydrophilicity	Oxidation under ambient conditions	[46]
8	Ti3C2Tx MXene	Selective etching	2D carbide/nitride layers	Sodium-ion batteries	Operando XAS insights, reversible Na+ intercalation	Complex reaction mechanisms	[47]
9	MoS2	Liquid-phase exfoliation	Layered hexagonal structure	Li-ion batteries, supercapacitors	High theoretical capacity (~670 mAh/g), tunable bandgap	Low intrinsic conductivity, volume expansion	[48]
10	MoS2	CVD, hydrothermal	2H and 1T phases	Energy storage devices	Phase-dependent properties, large interlayer spacing	Stability issues during cycling	[49]
11	MoS2 composites	Hydrothermal, solvothermal	MoS2 with metal oxides/carbon	Li-ion and Na-ion batteries	Enhanced conductivity, improved stability	Complex synthesis procedures	[50]
12	MoS2/ternary nanocomposites	Sol-gel, hydrothermal	MoS2 with conducting polymers/carbon	Supercapacitors, batteries	Synergistic effects, enhanced capacitance	Material compatibility issues	[51]
13	1T-MoS2	Phase engineering	Metallic 1T phase	HER catalysis	High catalytic activity, enhanced conductivity	Phase stability challenges	[52]
14	Al,P-doped MoS2	One-step hydrothermal	Doped nanosheets on carbon cloth	Asymmetric supercapacitors	449.2 F/g, 30.07 Wh/kg energy density	Doping optimization needed	[53]
15	3R-MoS2	DFT-based design	Rhombohedral phase	Aluminum-ion batteries	High theoretical capacity for Al3+ storage	Experimental validation needed	[54]
16	MoS2 (various morphologies)	Microwave, electrochemical	Nanostructured forms	Post-lithium batteries (Na, K)	Versatile for multiple battery chemistries	Rate capability limitations	[55]
17	WS2	CVD, liquid exfoliation	Layered dichalcogenide	Li-ion and Na-ion batteries	Similar to MoS2, good stability	Lower capacity than MoS2	[56]
18	WSe2	Mechanical/chemical exfoliation	Transition metal diselenide	Photovoltaic, batteries	1.3 eV bandgap, high absorption coefficient	Limited research vs MoS2	[57]
19	Black Phosphorus (BP)	Mechanical exfoliation	Puckered layered structure	Li-ion batteries	Ultra-high theoretical capacity (2596 mAh/g)	Air/moisture instability, degradation	[58]
20	Phosphorene (few-layer BP)	Liquid exfoliation, CVD	Monolayer/few-layer BP	Supercapacitors, batteries	High carrier mobility (~1000 cm^2/V·s), anisotropic properties	Environmental sensitivity, scalability	[59]

21	FL-BP/c-CN composite	Freeze drying, sonication	0D/2D heterostructure	Flexible supercapacitors	203.25 mF/cm^2, prevents restacking	Complex fabrication	[60]
22	Phosphorene	Chemical synthesis (80°C)	2D nanosheets	Supercapacitors with polyaniline	335.54 F/g at 1.6 A/g	Low-temperature synthesis advantages	[61]
23	BP/CNT hybrid	Microfluidic-spinning	Chemically bridged heterostructure	Flexible supercapacitors	96.5 mWh/cm^3, 308.7 F/cm^3 volumetric capacitance	Manufacturing complexity	[62]
24	Black Phosphorus	Various top-down methods	Few-layer structure	Batteries, electrocatalysis	Tunable bandgap (0.3-2.0 eV)	Storage and handling difficulties	[63]
25	Phosphorene	Sonication exfoliation	2D monolayer	Energy storage	High surface area, flexibility	Poor air stability	[64]
26	2D BP	Mechanical cleavage, electrochemical	Layered phosphorene	Li-ion battery anodes	Exceptional theoretical capacity	Synthesis scalability issues	[65]
27	BP composites	Top-down/bottom-up	BP with protective coatings	Various batteries	Improved cycle life with passivation	Cost and complexity	[66]
28	NiFe-LDH	Coprecipitation	Layered double hydroxide structure	Li-ion and Na-ion batteries	477 mAh/g theoretical capacity, low-cost synthesis	Initial capacity loss issues	[67]
29	NiFe-NO3 LDH	One-pot coprecipitation	Nitrate intercalated LDH	Sodium-ion batteries	Simple, scalable process, 256.9 mAh/g	Moderate cycle stability	[67]
30	NiFe LDH/Fe-NC-CNT	Precipitation, carbonization	LDH on carbon framework	Zinc-air batteries	818 mAh/g capacity, bifunctional catalyst	Complex multi-step synthesis	[68]
31	NiFe-LDH with Ag	In-situ growth	P-n heterostructure	Water splitting, OER	Enhanced electron transfer, OER activity	Precious metal usage	[69]
32	LaCoO3/NiFe-LDH	In-situ growth	P-n heterostructure	OER for water splitting	Photogenerated carrier assistance, oxygen vacancy formation	Complex synthesis	[70]
33	Co9S8@NiFe-LDH	Multi-step synthesis	Core-shell structure	Zinc-air batteries	Bifunctional ORR/OER, 1.62 V OER potential	Multi-component complexity	[71]
34	NiFe-LDH/RGO/CNFs	One-step hydrothermal	Composite structure	Asymmetric supercapacitors	1330.2 F/g, 97.1% retention after 2500 cycles	Optimization required	[72]
35	NiFe-LDH	Solvent-free method	Nanospherical architectures	HER and OER catalysis	Green synthesis, enhanced active sites	Scalability assessment needed	[73]
36	La-doped NiFe-LDH	Electrodeposition	Doped layered structure	Overall water splitting	399 mV@50 mA/cm^2 (OER), 223 mV (HER)	Requires conducting substrate	[74]
37	NiFe-LDH based composites	Various methods	2D sheet-like structures	Flexible supercapacitors	Easy production, low cost, versatile composition	Conductivity limitations	[75]

38	h-BN	CVD, mechanical exfoliation	Hexagonal boron-nitrogen lattice	Thermal management, dielectric applications	Wide bandgap (~5.5 eV), high thermal conductivity, electrical insulation	Limited electrochemical activity	[76]
39	h-BN nanosheets (BNNS)	Liquid-phase sonication	Exfoliated monolayers	Thermal interface materials	400 W/m·K in-plane thermal conductivity	Cross-plane conductivity reduction	[77]
40	Doped h-BN	Heteroatom doping	Functionalized BN	HER, OER, NRR catalysis	Enhanced catalytic activity via doping	Inert nature requires modification	[78]
41	h-BN quantum dots (BNQDs)	Chemical synthesis	0D quantum structures	Energy conversion, sensing	Quantum confinement effects, tunable properties	Scalability challenges	[79]
42	h-BN/CuS composite	Ultrasonic exfoliation	Hybrid heterostructure	Supercapacitors	Enhanced conductivity through compositing	Optimization needed	[80]
43	Bilayer h-BN	Theoretical (DFT)	Interlayer cavity structure	Hydrogen storage	4 wt% H2 storage capacity	Theoretical study, needs validation	[81]
44	h-BN derivatives	Various functionalization	Surface-modified h-BN	Electrocatalysis	Chemical stability, thermal endurance	Requires surface activation	[82]
45	h-BN nanosheets	Top-down methods	2D insulating layers	Electronic devices, sensors	Atomically flat, no dangling bonds	Limited direct energy storage	[83]
46	A-HNT-h-BN composite	Ultrasonication	Nanoclay composite	Hydrogen storage	2.88 wt% H2 capacity at 50°C	Below DOE targets	[84]
47	VS2	Hydrothermal synthesis	Metallic 1T phase	Supercapacitors, Li-ion batteries	Metallic conductivity (~3×10^3 S/cm), high theoretical capacity (1397 mAh/g)	Structural instability during cycling	[85]
48	VS2-BP hybrid	One-pot hydrothermal	Vanadium disulfide-black phosphorus	All-solid-state supercapacitors	203.25 mF/cm^2, 28.22 µWh/cm^2 energy density	Optimization of BP concentration critical	[86]
49	VS2 nanosheets	Single-step hydrothermal (220°C)	Hexagonal phase-pure structure	Symmetric supercapacitors	106 F/g, 94% retention after 9000 cycles	Moderate specific capacitance	[87]
50	VS2@PDA	Dopamine coating	Core-shell structure	"Fast-charging" Li-ion batteries	682.03 mAh/g, 99.78% efficiency after 400 cycles	Complex surface modification	[88]
51	VS2-NC composite	Freeze drying, calcination	VS2 in N-doped carbon matrix	Li-ion batteries, supercapacitors	Enhanced stability, hierarchical structure	Multi-step synthesis	[89]
52	VS2	Various methods	Layered metallic structure	Multiple battery types (Li, Na, Zn)	Multielectron storage capability	Peierls distortion issues	[90]
53	TiS2-coated VS2	CVD with conformal coating	~2.5 nm TiS2 protective layer	Li-ion battery cathodes	180 mAh/g @ 200 mA/g, improved	Complex coating process	[91]

					stability		
54	NiS2/V2O3 heterostructure	Hydrothermal + sulfurization	Spherical composite	Asymmetric supercapacitors	1295 F/g, 35.1 Wh/kg, 85.8% retention after 3000 cycles	Multi-component complexity	[92]
55	BiCo-MOF@VS2	MOF intercalation on VS2	MOF on nanosheet support	Supercapacitors	472 F/g specific capacitance	Novel material, needs further study	[93]
56	VS2 nanomaterial	Facile hydrothermal	1T metallic phase	Supercapacitors	Low cost, large scale, highly crystalline	Performance optimization needed	[94]
57	VS2 nanosheets	Layer-by-layer stacking	Intercalation structure	Na-ion storage	High-rate pseudocapacitance	Requires further development	[95]
58	SnSe-MnSe@rGO	Multi-component synthesis	Heterostructured composite	Li-ion batteries, supercapacitors	High energy density asymmetric design	Complex multi-metal system	[96]

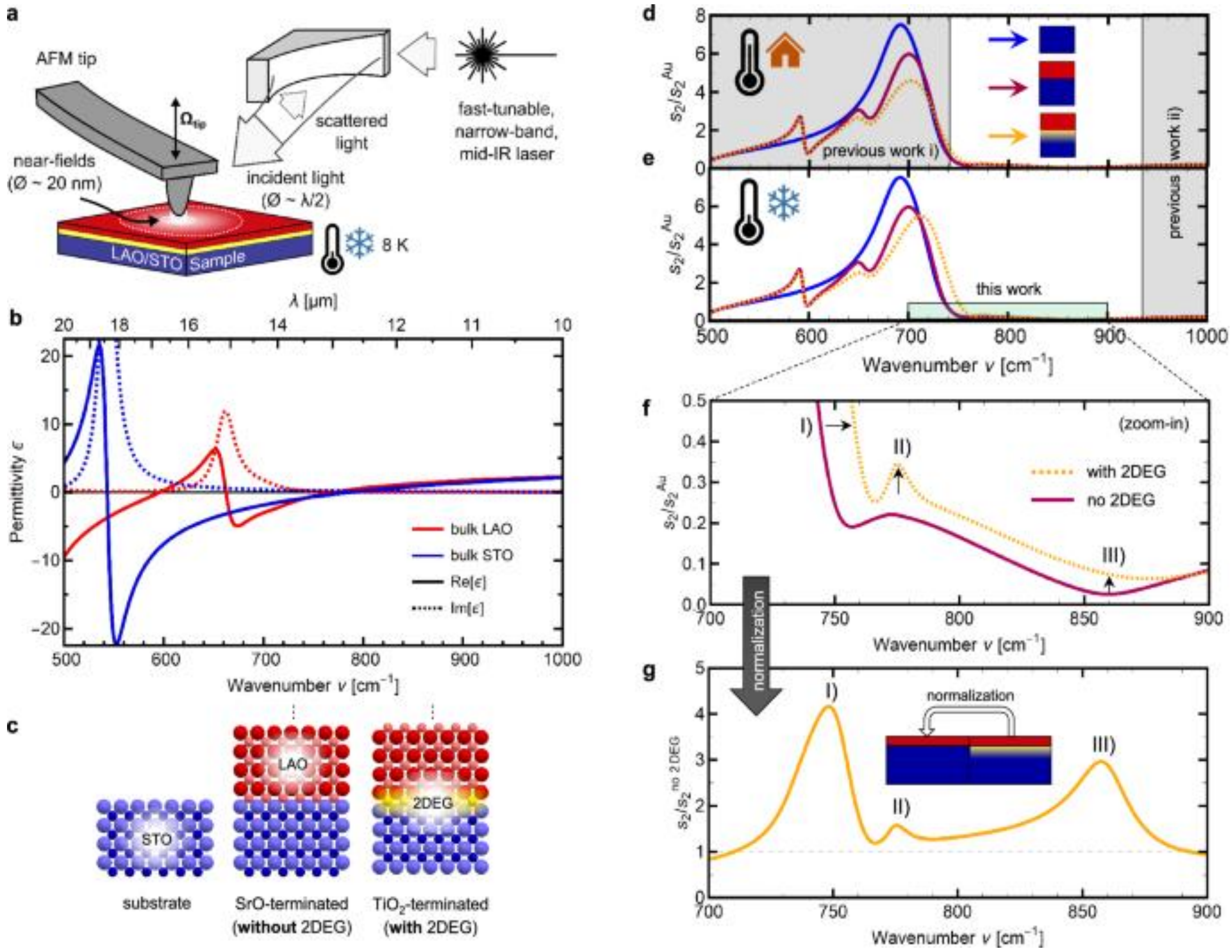

Figure 4. **a** Experimental setup showing the LAO/STO sample and the metal-coated AFM tip. **b** Real (solid lines) and imaginary part (dashed lines) of the dielectric functions of STO (blue) and LAO (red). **c** STO single crystals were epitaxially covered with LAO. **d** Simulation of the Au-normalized near-field amplitude spectra. **e** Simulation of s2/s2Au at cryogenic temperatures. **f** Zoom-in of Figure 4d. **g** Characteristic response with three separate maxima (Barnett *et al.,* 2025, Springer Nature, CC BY 4.0) [97].

3. Lithium-Ion and Beyond-Lithium Batteries

3.1 MXenes as Battery Electrodes

MXenes are a family of two-dimensional materials with the general formula $M_{n+1}X_nT_x$, where M is a transition metal, X is carbon or nitrogen, and T_x represents surface groups. These materials have gained strong interest for battery electrodes because they show high electrical conductivity, layered structures, and adjustable surface chemistry. In lithium-ion and beyond-lithium batteries, MXenes offer both fast electron transport and easy ion movement. This combination is difficult to achieve in many traditional materials such as graphite, metal oxides, or transition metal dichalcogenides. A recent review reports that MXenes and MXene-based composites are among the most promising candidates for next-generation rechargeable batteries and discusses their synthesis, electrode design, and current challenges [98].

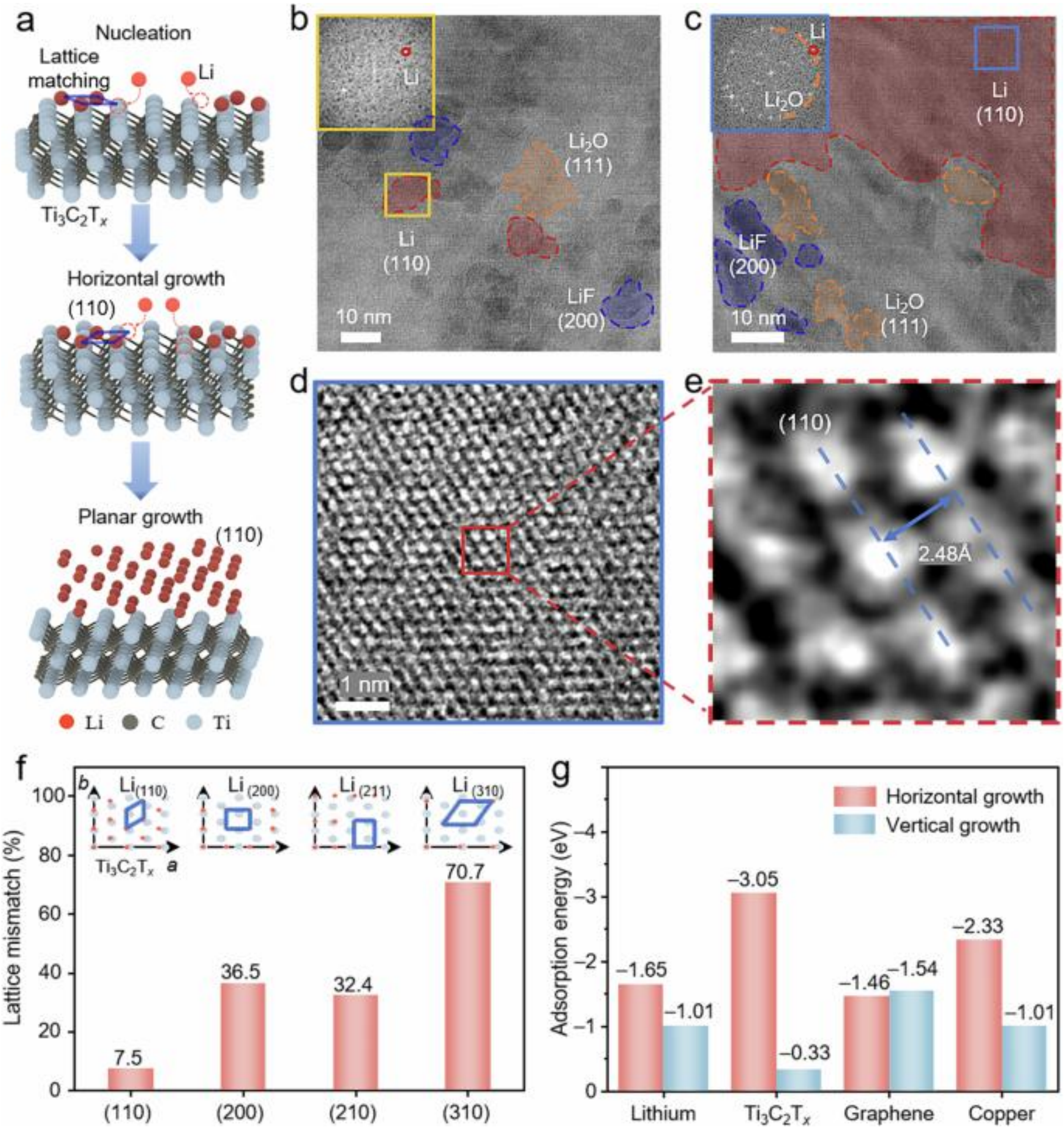

Figure 5. **a** Schematic diagram of lithium nucleation on MXene $Ti_3C_2T_x$ interface. (**b**) and (**c**) Red, blue and yellow regions represent crystalline Li metal, LiF and Li_2O nanocrystals, respectively. **d** Magnified image of boxed regions in blue from (**c**). **e** Atomic-resolution TEM image of the boxed regions from (**d**), **f** Lattice mismatch of lithium and the hexagonal crystal plane of MXene $Ti_3C_2T_x$ interface. **g** Adsorption energies of Li atoms (Chen *et al.,* 2025, Springer Nature, CC BY 4.0) [103]

The electrochemical performance of MXene electrodes mainly depends on their intercalation behaviour. Unlike graphite, where lithium ions enter fixed graphitic layers, MXenes allow control of the interlayer distance through surface groups such as –O, –OH, and –F, as well as through inserted species. This feature enables smooth insertion of Li^+ and other ions while maintaining good electrical pathways. For example, Ti_3C_2@TiO_2 hybrid electrodes with expanded interlayers delivered a reversible capacity of about 302 mAh g^{-1} at 200 mA g^{-1} after 500 cycles. This performance arises from a mix of intercalation and surface-driven charge storage [99]. Such results show that MXenes operate through combined mechanisms, including intercalation, surface redox reactions, and pseudocapacitance, which support high power output with moderate energy density. MXenes also show strong compatibility with composite electrode designs. MXene sheets act as conductive frameworks, host layers, and buffer components for high-capacity materials such as silicon, tin, and conversion-type oxides. These roles help reduce volume expansion during cycling. Studies reviewed in recent literature show that MXene-based composites prevent sheet restacking, increase interlayer spacing, and absorb mechanical strain [100]. In practical electrodes, these effects improve rate performance, cycle life, and structural stability.

However, several challenges still limit the direct use of MXenes in batteries. When used alone, MXenes usually show lower gravimetric capacity than silicon or conversion oxides. As a result, composite approaches become necessary. MXenes also oxidise easily, especially in air or water, which raises concerns about long-term stability. This issue has been highlighted as a key barrier for large-scale use [101]. In addition, layer restacking and limited ion access can reduce performance, making structural tuning such as porosity control and interlayer expansion essential. From a performance point of view, MXene electrodes often show excellent rate capability and stable cycling, though their specific capacity remains moderate. For instance, holey Ti_3C_2-based composites retained about 80% capacity after 2,000 cycles and delivered an energy density of nearly 110 Wh kg^{-1} in a lithium-ion capacitor setup [102]. Although this value is lower than that of high-energy batteries, it highlights the advantage of MXenes in fast-charging and high-power applications.

MXenes are also under study for sodium, potassium, and multivalent ion batteries. Their adjustable interlayer spacing and conductive nature allow them to host larger ions and multivalent species. Both theoretical and experimental studies suggest that suitable surface terminations help accommodate these ions [104]. This adaptability positions MXenes as versatile electrode platforms for multiple battery chemistries. Figure 5 presents experimental and theoretical insights into lithium plating behaviour at MXene interfaces in MXene-modified graphite electrodes. In summary, MXenes are among the most promising two-dimensional materials for battery electrodes. They offer high conductivity, adjustable interlayers, and flexible chemistry. Their main strength lies in high-power and fast-charging systems and in composite electrode designs. For real-world use, future work must improve capacity, enhance air stability, refine composite structures, and evaluate performance under practical conditions.

3.2 Transition Metal Dichalcogenides in Batteries

Transition metal dichalcogenides, such as MoS_2 and WS_2, are two-dimensional materials with layered structures and high theoretical capacities. These materials consist of metal layers placed between chalcogen layers, forming van der Waals gaps that allow ion insertion and tolerate volume changes during cycling. Recent reviews highlight their potential in batteries and energy devices due to their tunable layers and active redox behaviour [105]. An important feature of TMDs is their phase-dependent electrochemical behaviour. The 2H phase is semiconducting, while the 1T phase shows metallic conductivity. The 1T phase provides higher electrical conductivity, more active sites, and wider interlayer spacing, which improves lithium insertion and removal. For example, stabilised 1T-MoS_2 in all-solid-state lithium-ion batteries showed better rate and cycle performance than the 2H phase [106]. Studies also stress that phase conversion or combination with conductive additives is essential to overcome the low conductivity of pristine 2H-MoS_2 [107].

TMD electrodes often undergo more complex reactions than simple intercalation. In MoS_2, lithium first inserts into the layers and later forms Li_2S and metallic Mo through conversion reactions. This process gives high capacity but also causes large volume change, which leads to particle damage and capacity loss. Research on few-layer MoS_2 nanosheets showed improved capacity but also reported restacking and agglomeration as major issues [108]. To manage these problems, researchers use nanoscale designs, carbon supports, heterostructures, and binder-free electrodes to control structure and maintain contact. Beyond lithium-ion batteries, TMDs are also studied for sodium, potassium, and multivalent ion systems. Their larger interlayer spacing allows storage of bigger ions. A recent study on MoS_2, WS_2, and $MoWS_2$ flakes reported reversible behaviour in sodium- and potassium-ion batteries, with MoS_2 reaching over 1,000 mAh g^{-1} in sodium-ion cells [109]. These results confirm the flexibility of TMDs, though long-term stability remains a concern. Overall, TMDs are versatile electrode materials with tunable phases, high capacity, and structural flexibility. To achieve practical battery performance, further work must focus on phase control, morphology design, conductive integration, and long-term cycling under realistic conditions.

3.3 Black Phosphorus for High-Capacity Anodes

Black phosphorus has attracted renewed attention as a high-capacity anode due to its very high theoretical capacity of about 2,596 mAh g^{-1} in lithium-ion batteries. Its layered and anisotropic structure offers advantages beyond conventional graphite [110]. Black phosphorus stores lithium through both intercalation and alloying reactions, which leads to high gravimetric and volumetric capacity. The crystal structure of black phosphorus consists of puckered layers with zig-zag and armchair directions. This structure allows fast ion movement along specific directions and provides space to reduce mechanical stress during cycling. Recent studies on black phosphorus–graphite–carbon nanotube composites reported initial capacities near 1,375 mAh g^{-1} and stable cycling over 450 cycles [111]. These results show that composite design and conductive networks greatly improve performance. Despite these advantages, black phosphorus faces serious stability issues. During full lithiation, it undergoes volume expansion of about 300%, which causes cracking, loss of contact, and fast capacity decay. Advanced studies using electrochemical atomic force microscopy revealed surface wrinkling and layer separation during cycling. Molecular-level studies further identified degradation pathways under electrochemical and ambient conditions [112].

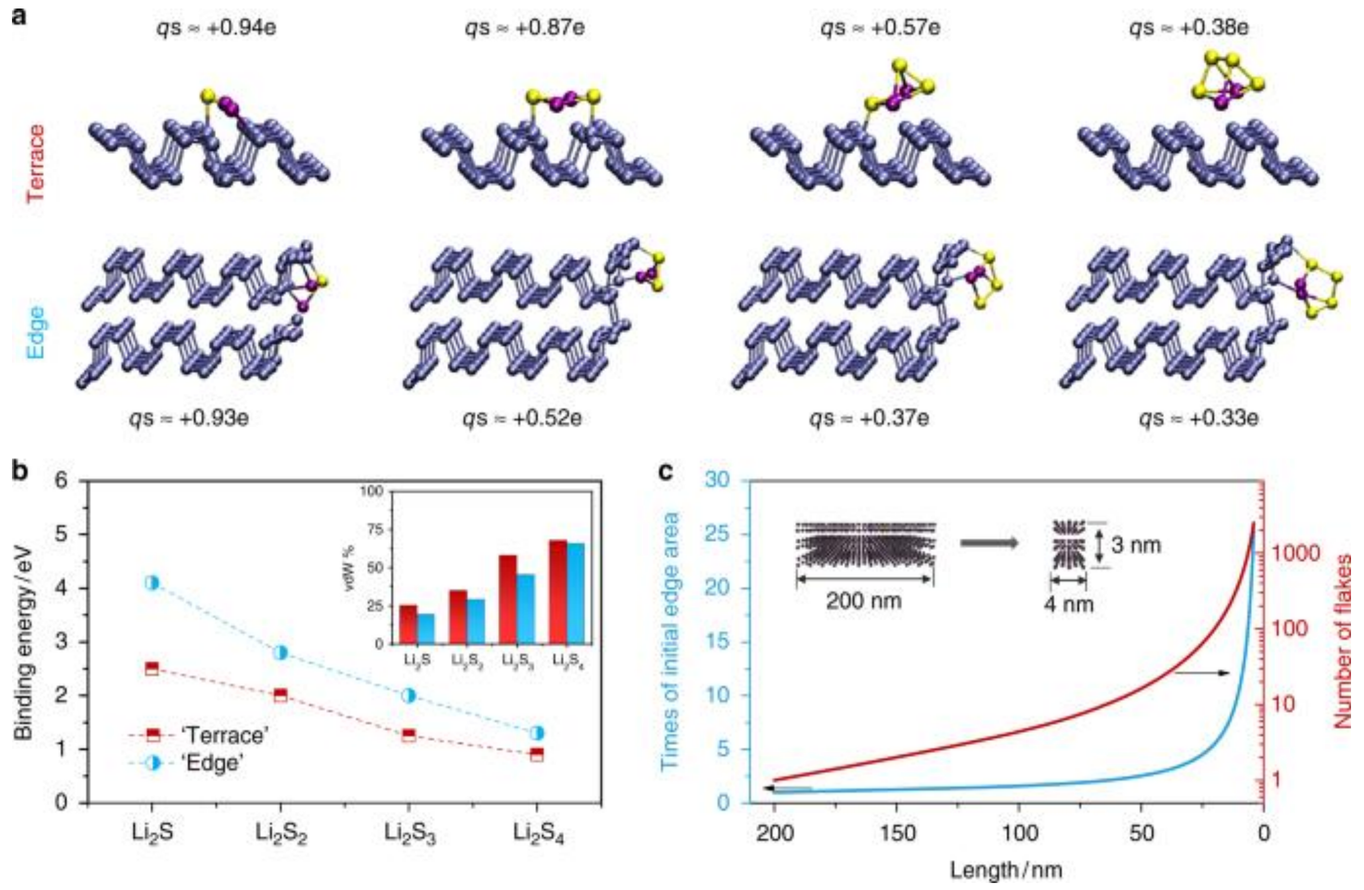

Figure 6. **a** Lithium polysulfides (LiPSs) adsorbed on black phosphorus (BP). **b** Binding energies of LiPSs. **c** the increase of exposed edge area and the number of flakes by downsizing flake to quantum dots (Xu *et al.,* 2018, Springer Nature, CC BY 4.0) [113].

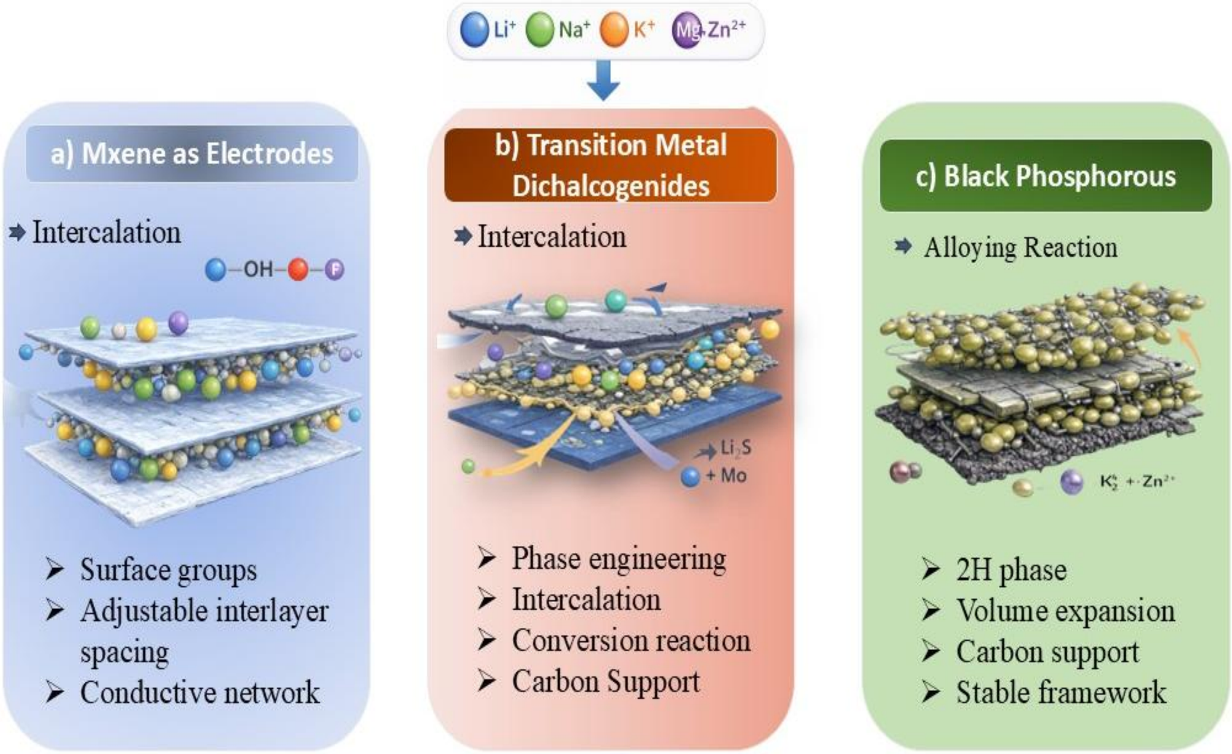

Figure 7. schematic illustration of charge storage mechanisms and structural roles of two-dimensional materials in rechargeable batteries.

In order to overcome these problems, researchers focus on protective matrices and interface engineering. For example, black phosphorus confined in metal–organic framework glass matrices showed stable capacity retention of about 98% after 1,000 cycles [114]. Similarly, lithium fluoride-rich interphases on black phosphorus–carbon composites improved cycling stability at high current densities [115]. Figure 6 illustrates lithium polysulfide adsorption on black phosphorus surfaces and the effect of size reduction on exposed edge area [116]. In conclusion, black phosphorus offers very high capacity and favourable ion transport, but severe volume change and interface instability limit its direct use. Successful application depends on composite design, stable interphases, nanoscale control, and scalable synthesis. With these advances, black phosphorus may become a strong candidate for future high-energy batteries. Figure 7 is a schematic illustration of charge storage mechanisms and structural roles of two-dimensional materials in rechargeable batteries.

3.4 Sodium-Ion, Potassium-Ion, and Multivalent Batteries

Beyond-lithium battery systems such as sodium-, potassium-, and multivalent-ion batteries are gaining attention due to lower cost, resource availability, and safety benefits. Two-dimensional materials are well suited for these systems because of their layered structures, large surface areas, and adjustable interlayer spacing. These features help accommodate larger ions and complex charge storage processes. In sodium- and potassium-ion batteries, the larger size of Na^+ and K^+ ions slows diffusion and increases mechanical stress. Reviews highlight that 2D materials help address these issues through easy ion pathways and flexible structures [117]. MXenes with expanded interlayers and hydrophilic surfaces improve sodium-ion transport and cycling stability [118]. Porous Ti_3C_2 MXene anodes showed stable performance at high current densities in sodium-ion batteries [119].

For potassium-ion batteries, even larger ion size creates greater strain. Few-layer materials such as bismuthene and antimonene show good potassium storage and long cycle life, sometimes exceeding 2,500 cycles [120]. These results stress the importance of strong mechanical frameworks and conductive networks. From a commercial view, sodium-ion batteries are closer to large-scale use due to low cost. Two-dimensional electrodes can further improve rate performance and durability. However, challenges remain in producing high-quality materials at scale and maintaining high electrode density. Potassium and multivalent systems still require major improvements in cycle life and full-cell stability. Overall, two-dimensional materials offer a strong path toward sodium-, potassium-, and multivalent-ion batteries. Through interlayer tuning, conductive design, and strain management, these materials can address the limits of larger ions. Future progress depends on realistic testing, scalable fabrication, and complete cell demonstrations.

Evaluation of advanced battery electrodes must focus on capacity, rate capability, and cycle life, along with clear links between structure and performance. High capacity alone is not sufficient without stable cycling and good rate behaviour. For example, coated $LiCoO_2$-based full cells have shown high energy density and strong rate performance under demanding conditions [121]. In contrast, several studies caution that many two-dimensional electrodes show weaker rate performance due to ion transport limits in dense electrodes. Structure–performance analysis shows that metallic phases, surface chemistry, and morphology strongly affect outcomes. Metallic 1T-MoS_2 improves rate capability but still suffers from volume change. MXenes benefit from conductivity, but surface terminations and restacking limit accessible capacity. Black phosphorus shows very high capacity but struggles with cycle stability. Porosity, ion pathways, and electronic connectivity must remain balanced. High surface area alone does not ensure fast performance if ions or electrons face transport barriers. Long-term cycle life, especially under high loading and realistic conditions, is essential for practical use. In summary, two-dimensional battery electrodes must achieve balanced improvement in capacity, rate capability, and durability. Progress depends on managing volume change, improving transport pathways, and realistic benchmarking. Continuous comparison with standard materials is essential for advancing energy storage technologies.

4. Supercapacitors and Hybrid Energy Storage

4.1 Pseudocapacitive 2D Materials

In modern supercapacitors, pseudocapacitive two-dimensional materials have gained strong attention because they store charge through fast surface or near-surface redox reactions. These reactions occur along with high electrical conductivity and open layered structures. Unlike electrical double-layer capacitors, which store charge only by ion adsorption, pseudocapacitive electrodes store charge through reversible electron transfer linked with surface reactions or ion insertion. This process increases energy density while keeping high power output. The introduction of two-dimensional materials, especially MXenes with the formula $M_{n+1}X_nT_x$, has further advanced this field. These materials offer metallic or near-metallic conductivity, adjustable surface groups, and stacked layers that support both ion movement and electron flow [122].

Among these materials, $Ti_3C_2T_x$ MXenes show very high volumetric capacitance, often above 1,000 F cm^{-3} in film form when used with aqueous electrolytes. This performance mainly comes from proton insertion and surface redox reactions linked with the carbide layers and oxygen-based surface groups [123]. These values are much higher than those of conventional carbon electrodes, which typically show only 100–200 F cm^{-3}. Recent studies also report $Ti_3C_2T_x$ combined with polyaniline films reaching a volumetric capacitance of 2,368 F cm^{-3} with stable performance over 10,000 cycles, showing both high energy storage and long-term durability when electrode structure is well controlled [124]

Charge storage in pseudocapacitive two-dimensional systems occurs through a combination of fast ion insertion into interlayers or edge sites, surface redox reactions linked with surface groups, and smooth electron transport across the layered network. This combined behaviour allows these materials to match the fast response of double-layer capacitors while offering higher charge storage. However, this performance strongly depends on interlayer spacing, surface chemistry, electrode thickness, and packing density. When the sheets restack tightly, ion movement becomes difficult, and the charge storage shifts towards slower processes. Therefore, studies highlight the need for structural design methods such as spacers, vertical alignment, and surface control to keep redox sites accessible and maintain fast charge–discharge behaviour [125]

Apart from MXenes, two-dimensional metal oxides and hydroxides, such as layered double hydroxides and cobalt or nickel-based oxides, also show pseudocapacitive behaviour. Their thin structure and active redox sites improve performance compared to bulk forms. However, their lower electrical conductivity often limits rate capability when compared with metallic two-dimensional materials. Device-level performance also depends strongly on electrode design. In practical systems, volumetric and areal capacitance values are often more meaningful than gravimetric values. Thick electrodes with high mass loading may show good per-gram capacitance but perform poorly in real devices. Reviews report that MXene-based microsupercapacitors can reach volumetric energy densities of about 30–40 Wh L^{-1}, which is higher than activated carbon devices but still lower than battery systems [126]. In summary, pseudocapacitive two-dimensional materials, especially conductive layered systems such as MXenes, form an important link between high-power supercapacitors and higher-energy batteries. Their fast and reversible redox behaviour, along with good conductivity and layered structure, makes them suitable for next-generation energy storage. To move toward real applications, future work must address electrode structure, volumetric performance, large-scale fabrication, and long-term stability together with material design.

4.2 Interlayer Engineering for Enhanced Capacitance

Interlayer engineering has become a key approach to improve the capacitive performance of two-dimensional materials used in supercapacitors. This strategy focuses on adjusting the spacing between layers, adding conductive spacers, and improving ion access and electron transport. In pseudocapacitive materials such as $Ti_3C_2T_x$ MXenes and layered metal oxides, the interlayer structure controls both the number of active redox sites and the speed of ion and electron movement. A detailed review explains that widening the interlayer spacing in MXenes directly improves capacitance by reducing restacking and creating easier paths for ion transport [127]. One important study demonstrated this effect by inserting alkyl-ammonium ions into $Ti_3C_2T_x$ MXene layers, which expanded the spacing to about 2.2 nm. When tested in an ionic liquid electrolyte, the material showed a specific capacitance of around 257 F g^{-1}, corresponding to nearly 492 F cm^{-3}, along with better cycling stability than the unmodified MXene [127]. This result confirmed that controlled interlayer expansion supports ion movement even for large ions, while maintaining good power and durability.

Figure 8 shows a schematic of interlayer structure engineering in MXene hybrid films. It highlights the difficulty of inserting large multivalent ions such as Zn^{2+} and demonstrates how one-dimensional spacers widen the gap between MXene sheets. This design allows fast and reversible ion insertion and removal [128]. The benefits of interlayer engineering arise from three main effects. Expanded spacing shortens ion diffusion paths and reduces resistance. Spacer molecules prevent layer collapse and keep internal surfaces open. When conductive spacers are used, the electronic network remains continuous even with larger spacing. For example, MXene films with polyvinyl alcohol nanofibers as spacers showed increased interlayer distance while keeping good electrical contact. This design improved both rate performance and volumetric capacitance [129]

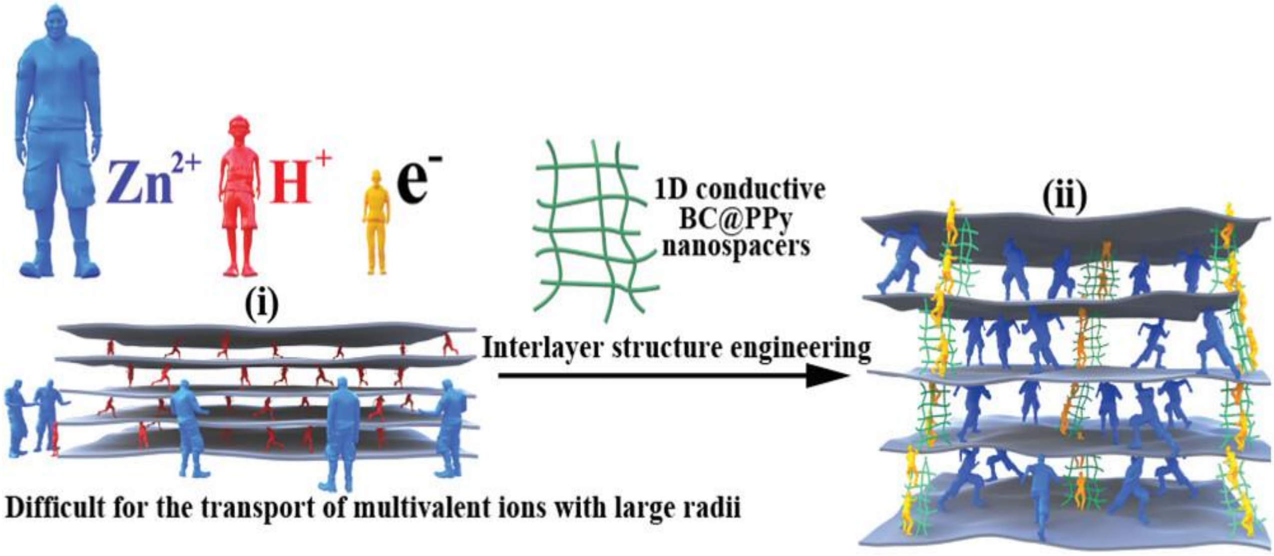

Figure 8. Illustration of the proposed interlayer structure engineering of MXene hybrid film: **i)** an intercalation of multivalent ions with large ionic radius. **ii)** Insertion of 1D nanospacers to widen the space between MXene nanosheets (Cheng *et al.,* 2021, Wiley Advanced, CC BY 4.0) [128]

However, interlayer expansion must be carefully controlled. Too much spacing reduces packing density and may lower volumetric capacitance. Insulating spacers can also increase electrical resistance. Therefore, a balance between ion access, conductivity, and compact structure is necessary. Recent reviews highlight that the best performance occurs when interlayer spacing, surface chemistry, and electrode composition are optimised together [130]. In practice, interlayer engineering uses several methods. These include chemical pre-insertion of ions or molecules to fix spacing, addition of pillar structures to maintain separation during cycling, and formation of hybrid composites with conductive materials such as graphene or carbon nanotubes. These approaches often lead to strong improvements in volumetric capacitance. For example, a pillared MXene composite reached more than 1,200 F cm^{-3} in microsupercapacitor devices, which is much higher than unmodified MXene films [131]. In conclusion, interlayer engineering is a powerful structural tool for improving two-dimensional pseudocapacitive materials. Careful control of layer spacing, prevention of restacking, and preservation of electrical pathways allow higher volumetric energy storage without losing power or stability. Future studies should focus on scalable methods for uniform interlayer expansion in thick electrodes, clear evaluation of packing density effects, and direct measurement of volumetric energy density in full-cell devices under practical conditions.

4.3 Asymmetric and Hybrid Supercapacitors

In recent years, asymmetric and hybrid supercapacitors have gained strong importance because they connect the performance gap between conventional electric double-layer capacitors and batteries. Unlike symmetric devices that use the same material on both electrodes, asymmetric supercapacitors use different electrode chemistries. Usually, a high-capacity pseudocapacitive or battery-type material acts as the positive electrode, while a fast capacitive material serves as the negative electrode. This design allows a wider operating voltage, higher energy density, and good power delivery. Two-dimensional materials beyond graphene, such as MXenes, transition metal dichalcogenides, and functional metal-oxide nanosheets, suit this architecture well due to their large surface area, adjustable layer structure, and fast ion transport.

A clear example is an asymmetric supercapacitor that used sulfur-doped VSe_2 combined with carbon nanotubes as the positive electrode and two-dimensional borocarbonitride as the negative electrode. This device delivered an areal energy density of about 36.3 μWh cm^{-2} and retained nearly 87.2 % of its capacitance after 5,000 cycles [132]. In this system, the strong pseudocapacitive response of the sulfur-doped VSe_2 worked well with the double-layer behaviour of the borocarbonitride electrode. This pairing extended the voltage range and improved energy storage while maintaining good reversibility. Another reported system used a binder-free $Ti_3C_2T_x$ MXene and cellulose nanofiber anode with a polyaniline-coated carbon cloth cathode. This all-solid-state asymmetric device showed good flexibility and stable cycling performance [133].

The performance of asymmetric and hybrid supercapacitors depends on careful control of electrode material choice, operating voltage, and charge balance between electrodes. Two-dimensional materials support fast ion access and smooth electron flow, which enables high rate capability. However, the electrolyte and device design must safely support the wider voltage window without causing side reactions or electrode damage. Since hybrid systems often combine a redox-active electrode with a capacitive one, both electrodes must operate in matching potential ranges to ensure long-term stability. Well-designed two-dimensional hybrid devices usually show near-rectangular cyclic voltammetry curves, low internal resistance, high coulombic efficiency, and stable capacitance over thousands of cycles.

Performance comparisons clearly show the advantage of hybrid designs. A recent review reported that supercapacitors based on layered two-dimensional materials achieved energy densities above 40 Wh kg^{-1} at power densities greater than 1 kW kg^{-1}, while maintaining more than 80 % capacity after over 10,000 cycles [134]. This balance of high power and high energy comes from the synergy between two-dimensional materials and complementary electrode chemistries. Key design aspects include proper control of electrode thickness and mass loading to avoid imbalance, use of materials that resist layer restacking, and selection of electrolytes that remain stable across extended voltage ranges. In summary, asymmetric and hybrid supercapacitors provide an effective route to exploit the advantages of two-dimensional materials beyond graphene. Their large surface area, adjustable layer spacing, and fast charge transport help overcome the limits of symmetric capacitors. Future studies should focus on better electrode matching, higher areal and volumetric energy density, scalable fabrication methods, and long-term testing under realistic device conditions. The combination of advanced two-dimensional materials with hybrid device designs holds strong potential for next-generation energy storage systems that demand both high energy and high power.

4.4 Flexible and Wearable Energy Storage

The rapid growth of wearable electronics, such as health monitors, smart fabrics, flexible displays, and skin-mounted sensors, has created a strong need for energy storage devices that combine high performance with flexibility and durability. In this area, two-dimensional materials beyond graphene play a key role because of their thin structure, large surface area, adjustable layer spacing, and good electrical conductivity. These properties allow the design of electrodes that bend, stretch, and conform to soft surfaces without losing performance. Recent studies show that MXenes, transition metal dichalcogenides, two-dimensional metal oxides, hydroxides, and conductive polymer composites can form freestanding films, fibres, textiles, or surface coatings suitable for wearable devices. One notable example is a textile-based supercapacitor formed by coating fabric with a high loading of $Ti_3C_2T_x$ MXene. This device delivered an areal energy density of 0.401 mWh cm^{-2} at a power density of 0.248 mW cm^{-2} using a 6 V stack. It successfully powered a wireless temperature sensor for 96 minutes while undergoing bending and folding, which confirmed its suitability for wearable use [135]. Another recent Perspective highlighted MXene-based wearable supercapacitors for healthcare applications. It emphasized how metallic conductivity, hydrophilic nature, mechanical flexibility, and high volumetric capacitance together make these materials suitable for smart wearable systems [136].

Device design and material assembly play a major role in transferring two-dimensional materials into wearable energy storage. Freestanding films remove the need for heavy current collectors and help reduce device thickness. Fibre- and textile-based electrodes formed from two-dimensional materials combined with polymers or carbon networks support twisting, stretching, and close contact with the body. A recent review described conductive polymer and two-dimensional material nanocomposites as strong candidates for flexible supercapacitors. In these systems, the polymer provides mechanical strength, while the layered material supports fast charge transport and ion access [137]. Despite these advances, maintaining high areal and volumetric energy density during repeated mechanical deformation remains difficult. Challenges include controlling the interface between layers and the textile or polymer support, preventing sheet restacking under strain, and keeping electrolyte access stable during movement.

Mechanical durability in wearable supercapacitors is usually assessed by monitoring capacitance retention during repeated bending, twisting, or stretching cycles. A recent review highlighted that, apart from the active material, the substrate, electrolyte, packaging, and electrical connections all influence the balance between performance and durability [138]. The flexible nature of two-dimensional materials helps reduce stress mismatch between the electrode and substrate. This property improves stability by lowering the risk of cracking or delamination during repeated deformation. From a performance viewpoint, flexible supercapacitors based on two-dimensional materials now report areal capacitances from several hundred millifarads per square centimetre to values exceeding one farad per square centimetre. These values are suitable for low-power wearable electronics. Many devices also show stable operation over more than 10,000 bending cycles. Still, further improvement is needed in increasing areal loading without losing flexibility, scaling fabrication to large textile areas, developing safe and washable gel or solid electrolytes, and reporting volumetric metrics rather than only mass-based values. Integration of energy storage with sensing, energy harvesting, and wireless communication also remains at an early stage.

Figure 9 shows an all-flexible ECG sensing system powered by a flexible energy harvesting and storage system. The device records clear ECG signals and demonstrates on-skin charging of a smartphone under outdoor light conditions. The system also shows comparable charging rates for smart devices when compared with commercial USB sources [140]. In conclusion, flexible and wearable energy storage represents a field where two-dimensional materials beyond graphene show strong advantages. Their layered structure, high conductivity, and processability allow the fabrication of electrodes that adapt to movement while delivering reliable energy storage. Future work should focus on scalable production of two-dimensional material-coated textiles, integrated devices that combine storage and sensing, electrolytes suitable for daily wear, and deeper understanding of how mechanical deformation affects long-term performance.

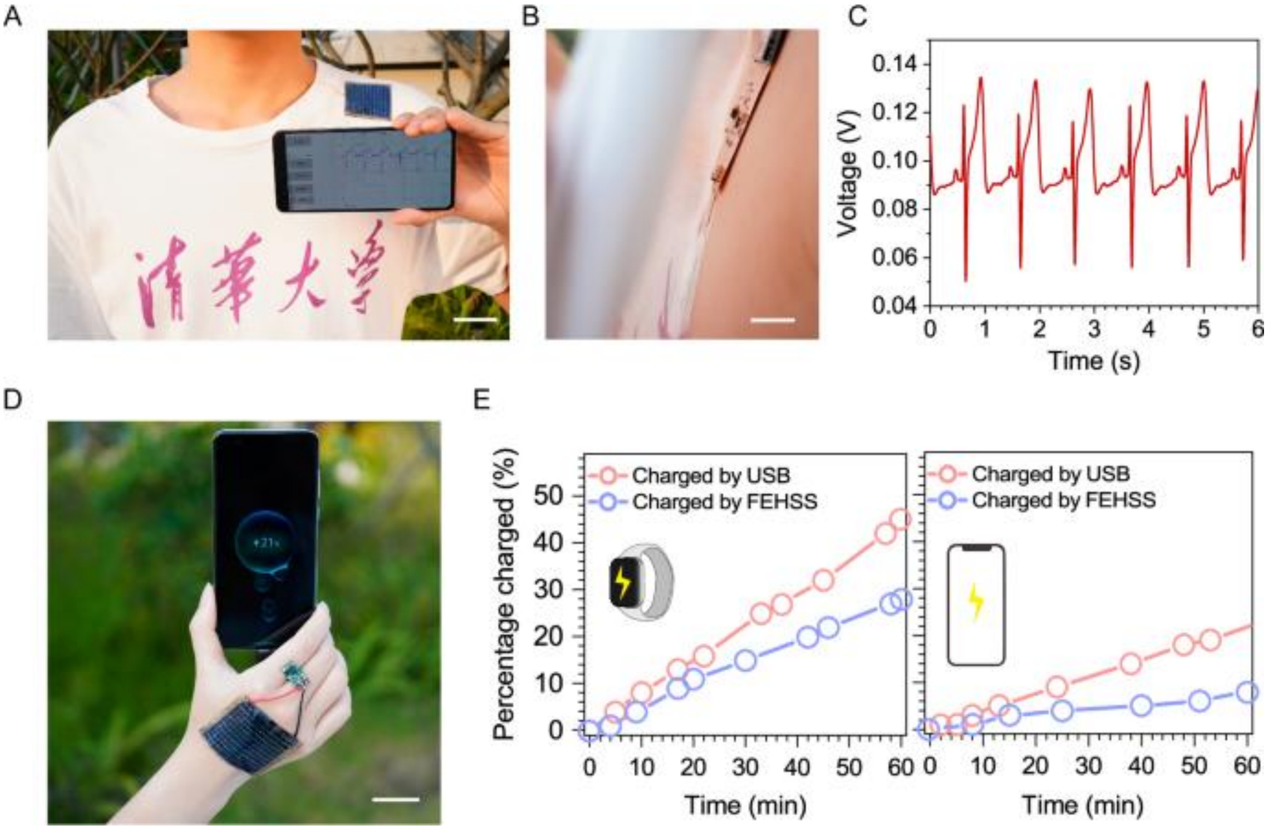

Figure 9. A, B Photographs of an all-flexible ECG sensing system powered by our FEHSS. C ECG signal obtained from the flexible ECG electrodes. D Photograph demonstrating an on-skin FEHSS charging a smartphone. E Smartwatch (left) and smartphone (right) charging rate using commercial USB (pink) and FEHSS (purple) (Saifi *et al.*, 2024, Springer Nature, CC BY 4.0) [139].

With continued progress, two-dimensional materials can support lightweight, flexible, and autonomous power sources for next-generation wearable electronics.

5. Electrocatalysis: HER, OER and ORR

5.1 Hydrogen Evolution Reaction (HER)

The hydrogen evolution reaction is a key process in water splitting for clean hydrogen production. It remains an important focus because low-cost and stable catalysts are required for large-scale use. Two-dimensional materials beyond graphene have shown strong potential in this field. Their atomic-scale thickness, large surface area, exposed edge sites, and adjustable electronic structure support efficient catalytic activity. These materials act not only as active catalysts but also as conductive supports and interfacial layers that improve charge transfer. A recent review explained the multiple roles of two-dimensional materials in HER systems and highlighted their contribution as catalytic layers and electron transport media [141]. Effective HER catalysis using two-dimensional materials depends on three closely linked factors. These include the creation of active sites, smooth transport of electrons and ions, and structural stability during operation. For HER pathways such as Volmer–Heyrovsky and Volmer–Tafel, the hydrogen adsorption free energy should be close to zero to achieve fast reaction rates. Two-dimensional materials allow this tuning through heteroatom doping, phase control, surface termination, and defect or edge formation. For example, MXenes such as $Ti_3C_2T_x$ show strong HER activity when doped or surface-modified. These materials deliver overpotentials close to platinum catalysts and show Tafel slopes of about 30–40 mV dec^{-1} in both acidic and alkaline media [142].

Apart from active site control, the layered nature of two-dimensional materials supports efficient electron movement and fast ion diffusion. This feature is important because poor charge transport can limit HER performance even when many active sites are present. As a result, two-dimensional materials often serve as conductive backbones, charge-transfer layers, or growth platforms for nanoscale catalysts. In one study, a MXene sheet reduced interfacial resistance and improved electron transfer and hydrogen bubble release compared to conventional carbon supports [143].

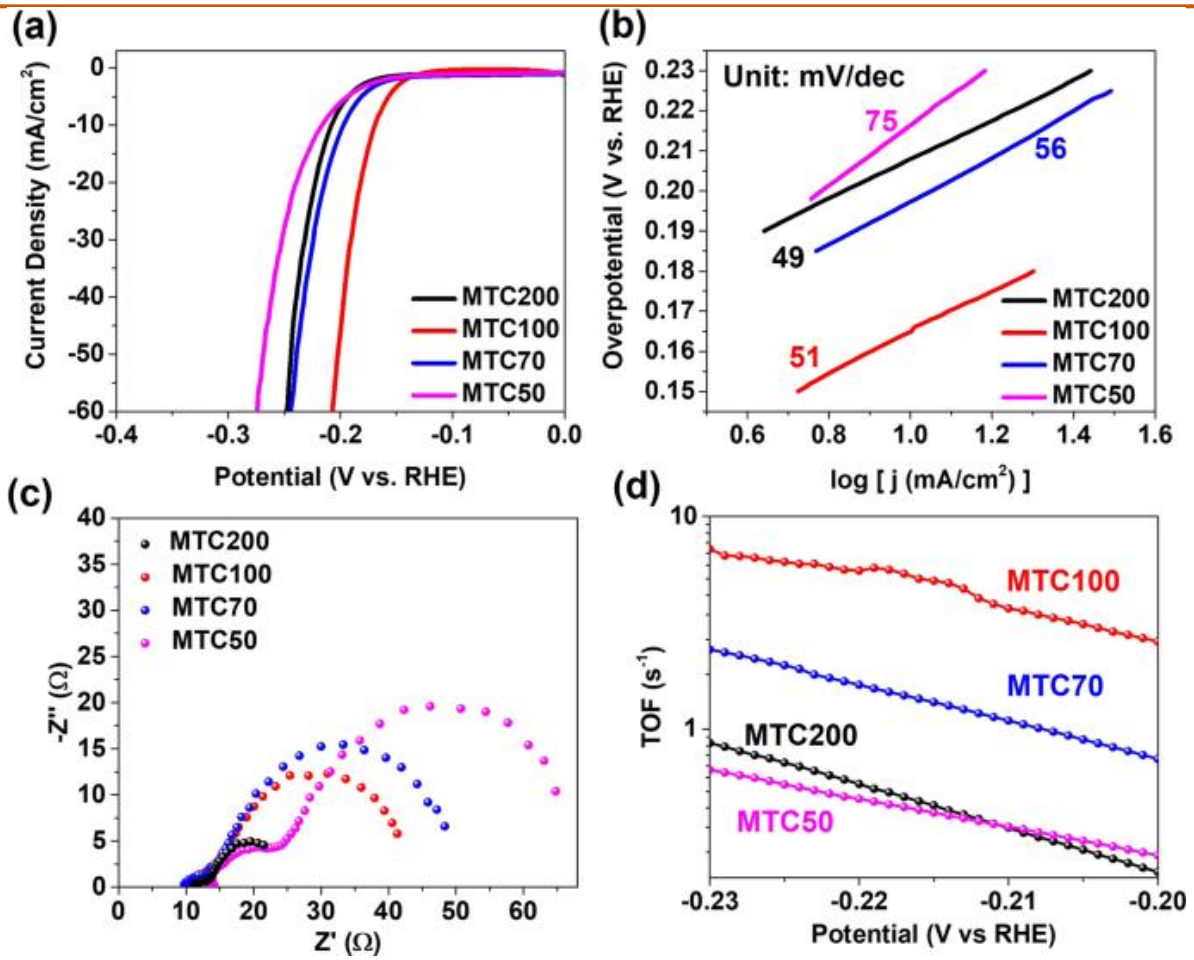

Figure 10. The electrochemical results of MTC hybrids with different CNT ratios (Wei *et al.,* 2022, Springer Nature, CC BY 4.0) [145]

Long-term structural stability also plays a major role in HER performance, especially under harsh acidic or alkaline conditions and high current operation. Two-dimensional materials show advantages due to their thin structure, which lowers stress buildup, and their stacked layers, which support easy gas release. Defect and edge engineering also helps prevent structural damage. A recent study reported that controlled wrinkle formation in two-dimensional transition metal dichalcogenide heterostructures improved HER activity. The induced strain adjusted hydrogen adsorption energy and reduced the overpotential to about −0.18 V while improving durability [144].

Figure 10 shows electrochemical results of MTC hybrid catalysts with different carbon nanotube ratios. Polarization curves, Tafel plots, Nyquist plots, and turnover frequency trends clearly indicate the influence of conductive additives on HER performance [145]. In summary, two-dimensional materials have advanced from early laboratory demonstrations to functional components of advanced HER systems. Their thin structure, flexible chemistry, and strong interfacial properties make them suitable for hydrogen production using earth-abundant elements. However, further progress is required to scale synthesis, integrate these materials into high-current electrolyzers, ensure long-term durability, and establish common performance benchmarks. Addressing these issues will support the transition of two-dimensional HER catalysts from research studies to commercial hydrogen technologies.

5.2 Oxygen Evolution Reaction (OER)

The oxygen evolution reaction is one of the most challenging steps in electrochemical energy conversion systems such as water electrolysis and metal–air batteries. This reaction involves slow kinetics and multiple electron transfer steps, which lead to high energy losses. Two-dimensional materials beyond graphene offer effective solutions due to their thin structure, large surface area, tunable electronic properties, and efficient mass transport. Materials such as layered double hydroxides, transition metal oxide or hydroxide nanosheets, and MXenes have gained strong attention. A recent review showed that reducing bulk oxides into ultrathin two-dimensional sheets increases active site exposure and improves adsorption of OER intermediates, which lowers overpotential [146]. The design of two-dimensional OER catalysts focuses on controlling surface chemistry, defect density, and interface structure. These factors directly influence the difficult step of oxygen–oxygen bond formation. For instance, NiFe layered double hydroxide nanosheets show much higher OER activity than bulk forms. This improvement comes from better hydroxide ion access and lower charge-transfer resistance [147]. MXenes such as $Ti_3C_2T_x$ also play an important role as conductive supports or functional platforms for oxide and hydroxide catalysts. Their metallic conductivity and surface terminations help reduce charge-transfer losses and support stable operation under oxidative conditions [148].

Studies on reaction mechanisms reveal that strong interaction between two-dimensional supports and catalytic species helps adjust the energy of key intermediates such as O* and OOH*. This adjustment lowers both overpotential and Tafel slope. An example is the $NiFe_2O_4/Ti_3C_2$ composite, which showed excellent bifunctional activity. It achieved an overpotential of 181 mV for OER and 157 mV for HER at 10 $mA\ cm^{-2}$ in both alkaline and acidic environments [149]. Such performance results from expanded catalyst–support interfaces, fast ion transport through thin nanosheets, and improved structural stability at high current density. Performance comparison across systems highlights the strength of two-dimensional designs. For example, $Cu_2S–Ti_3C_2T_x$ MXene heterostructures delivered an overpotential of 250 mV at 25 $mA\ cm^{-2}$, a Tafel slope of 61 $mV\ dec^{-1}$, and stable operation after 2,000 cycles [150]. These results match or exceed many bulk oxide catalysts under alkaline conditions, showing the benefit of two-dimensional architectures.

Figure 11 illustrates OER performance in proton exchange membrane water electrolysis devices. The data compare polarization behaviour, overpotential components, and long-term stability for different anode catalysts. The results confirm reduced resistance and improved durability for two-dimensional material-based electrodes [152]. Despite clear progress, challenges remain for two-dimensional OER catalysts. High active material loading often leads to layer restacking, which restricts ion transport and increases resistance. The strong oxidative environment also demands high corrosion resistance, which requires surface protection or stable heterostructure design. In addition, translating excellent laboratory results into large-area electrolyzers with high current density and long service life remains difficult.

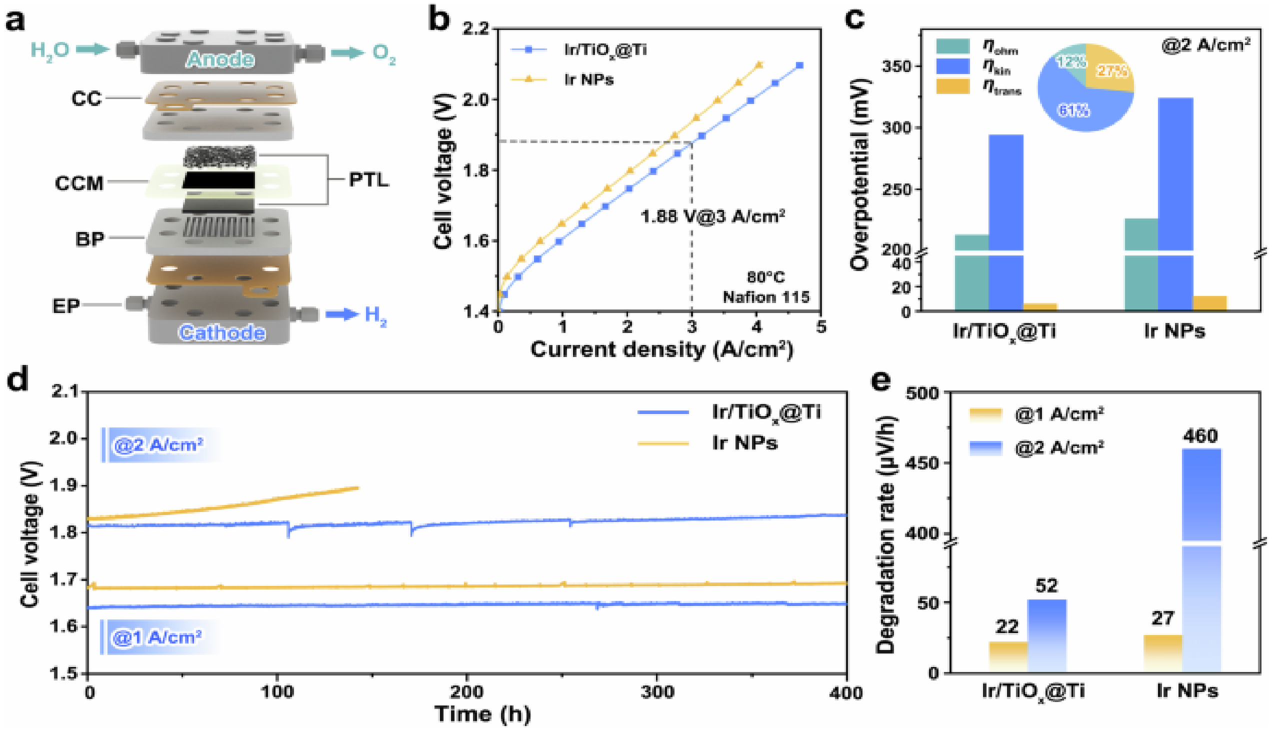

Figure 11. **a** Schematic diagram of PEMWE. **b** Steady-state polarization curves of PEMWE using Ir/TiOx@Ti and Ir NPs as anode catalysts. **c** Comparison of ohmic overpotential, kinetic overpotential, and transport overpotential of PEMWE. **d** Chronopotentiometry curves of PEMWEs. **e** Voltage degradation rates of PEMWEs (Zhang *et al.,* 2025, Springer Nature, CC BY 4.0) [151].

Uniform testing standards and detailed reporting of mass activity, stability, and full-cell performance are still needed. In conclusion, two-dimensional materials have introduced new possibilities in OER electrocatalysis by combining catalytic activity, electrical conductivity, and mechanical stability. Their layered structure and tunable surfaces support low overpotential and fast reaction kinetics. Future progress depends on scalable fabrication, deeper understanding of active site changes during operation, and successful integration into practical electrolyzer systems. These efforts are essential for developing efficient and sustainable energy conversion technologies based on hydrogen and oxygen reactions.

5.3 Oxygen Reduction Reaction (ORR)

The oxygen reduction reaction is one of the slowest and most complex reactions in electrochemical energy systems. It plays a key role in fuel cells, metal–air batteries, and related clean energy technologies. Two-dimensional materials beyond graphene are now widely studied as ORR electrocatalysts. Their atomic-level thickness exposes a large number of active sites and allows control over electronic structure. These features support their use in well-designed electrode structures. Recent studies report that materials such as transition-metal-doped carbons, two-dimensional metal–organic frameworks, layered transition metal dichalcogenides, and MXene-based derivatives show strong ORR activity. Several systems approach or even exceed the performance of conventional Pt/C catalysts. A theoretical study on conductive two-dimensional MOFs reported a low ORR overpotential of about 0.20 V for a four-electron pathway in RhN_2O_2-HTC, highlighting the promise of two-dimensional catalysts for selective ORR [153].

Effective ORR catalysis requires both high intrinsic activity and stable mass transport. Catalytic activity depends strongly on the adsorption strength of ORR intermediates such as OOH*, O*, and OH*. Proper tuning of these adsorption energies supports the preferred four-electron pathway and suppresses the undesired hydrogen peroxide route. Two-dimensional materials allow such tuning through heteroatom doping, defect introduction, phase control, and heterostructure formation. These approaches adjust the local electronic environment and improve reaction kinetics. A detailed review on two-dimensional transition metal dichalcogenides reported that defect control and phase engineering reduce ORR overpotential and improve durability in alkaline media [154]. From a transport viewpoint, ultrathin sheets shorten electron and ion diffusion paths. When combined with conductive frameworks such as graphene, carbon nanotubes, or metallic MXenes, these systems show higher current density and stable operation at high rates.

Several two-dimensional ORR catalysts have shown strong performance in practical testing. Many systems display half-wave potentials close to or higher than commercial Pt/C catalysts in alkaline electrolyte. For example, a layered two-dimensional MOF achieved a half-wave potential of 0.83 V with an electron transfer number close to four in a zinc–air battery cathode. This performance exceeded that of 20 wt% Pt/C tested under the same conditions, which showed a half-wave potential of 0.78 V [155]. These results confirm that controlled structure and chemistry in two-dimensional materials directly improve ORR efficiency.

Despite clear progress, important limitations remain. Most two-dimensional ORR catalysts are tested using rotating disk electrode methods at low current density. Their behaviour in full fuel cells or metal–air batteries remains limited. Stability under acidic conditions is also weaker for many non-noble two-dimensional materials when compared with platinum-based catalysts, especially in proton exchange membrane systems. In addition, comparison across studies is difficult due to differences in testing methods, electrode loading, and mass transport conditions. Large-scale synthesis and long-term durability of defect-rich or heterostructured two-dimensional catalysts also require further improvement before commercial use. In conclusion, two-dimensional materials offer a flexible and powerful platform for ORR catalysis. Their adjustable surface chemistry, thin transport pathways, and strong catalytic metrics challenge the dominance of precious metals. Future studies should focus on device-level testing, long-term operation under realistic conditions, and unified reporting standards. Progress will depend on combining material design, in situ characterisation, theoretical insight, and scalable fabrication to enable practical ORR systems based on two-dimensional catalysts.

5.4 Bifunctional and Trifunctional Catalysts

Modern energy systems require electrocatalysts that can support more than one reaction. Bifunctional catalysts support both hydrogen evolution and oxygen evolution, while trifunctional catalysts also enable oxygen reduction. Two-dimensional materials beyond graphene have emerged as strong candidates for such multifunctional catalysis. Their large surface area, high defect density, adjustable electronic structure, and easy hybrid formation allow activity across different reactions. These features support their use in overall water splitting and rechargeable metal–air batteries. A recent review highlighted that two-dimensional materials provide an ideal platform for multifunctional electrocatalysis due to their structural and chemical flexibility [156].

Multifunctional performance depends on careful control of active sites and interfaces. Each reaction has different requirements. Oxygen evolution needs strong binding of oxygen intermediates under high potential, while hydrogen evolution prefers near-zero hydrogen adsorption energy. A single catalyst must balance these demands. Two-dimensional materials such as transition metal dichalcogenides, layered double hydroxides, MXene derivatives, and two-dimensional MOFs offer wide chemical diversity to tune surface properties. One example is a hybrid catalyst composed of WS_2 nanosheets embedded in a UiO-66 MOF framework. This system achieved low overpotentials of about 121 mV for hydrogen evolution and 220 mV for oxygen evolution at 10 mA cm^{-2}, showing effective bifunctional activity [157].

Trifunctional catalysis places even higher demands on material design. A single electrode must support hydrogen evolution, oxygen evolution, and oxygen reduction. This requirement demands balanced surface chemistry, strong conductivity, and stable morphology. MXene-derived heterostructures offer a useful solution. Conductive carbide layers enable fast electron flow, while surface-attached metal oxides or hydroxides provide oxygen evolution sites. Nearby heteroatom-doped carbon regions support oxygen reduction. Such integrated systems allow one electrode to operate under both anodic and cathodic conditions. A recent study discussed future directions for two-dimensional bifunctional materials and outlined design principles for full water-splitting systems [158].

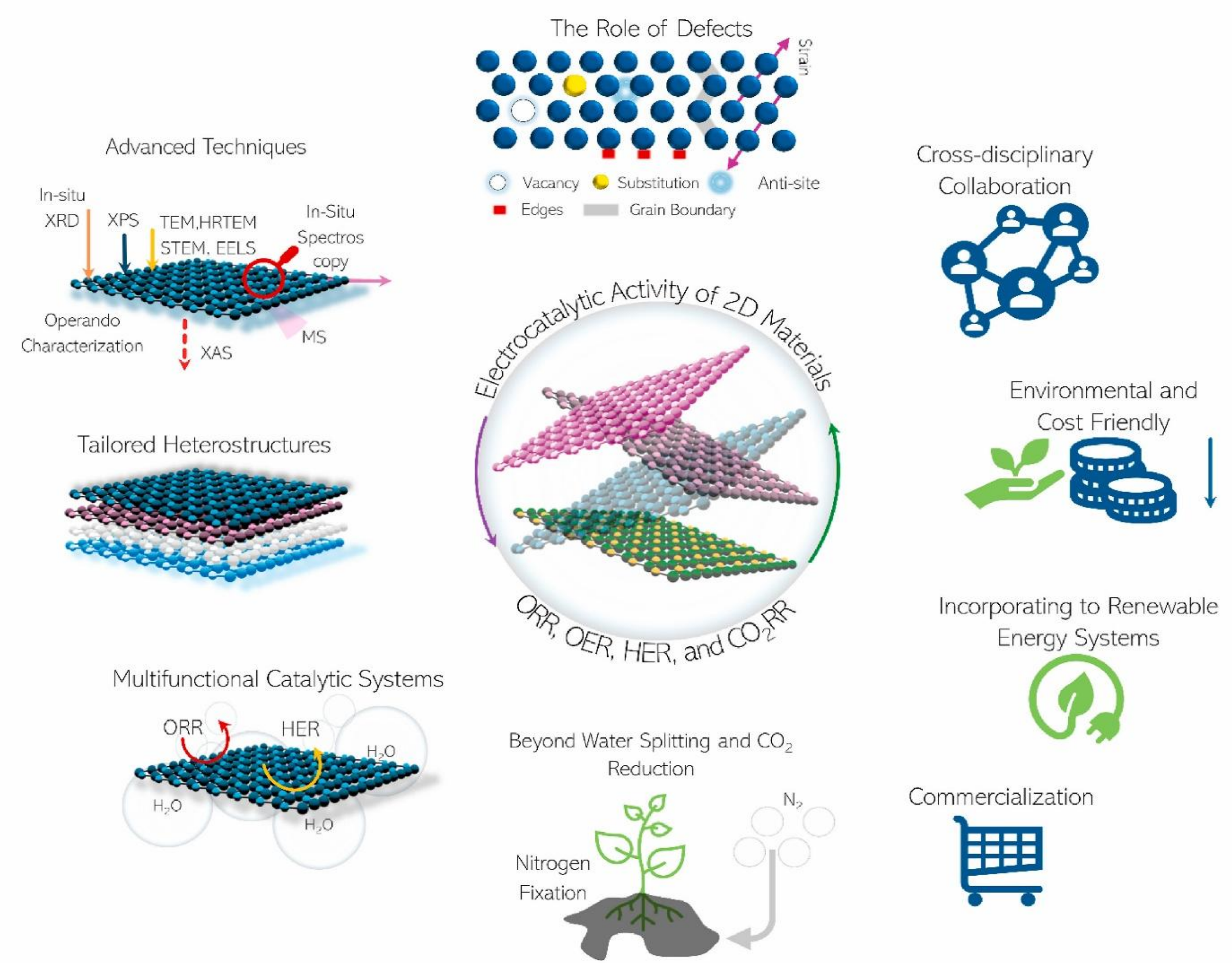

Figure 12. The schematic model of 2D materials with adapted properties for actual electrocatalytic applications (Raza *et al.,* 2024, Elsevier, CC BY-NC-ND 4.0) [159].

Figure 12 illustrates how tailored two-dimensional materials support real electrocatalytic applications through adapted surface and structural properties [159]. Despite strong progress, challenges remain. Most multifunctional two-dimensional catalysts are tested in half-cell setups. Real devices require high current density, large electrode area, and long operating time. Achieving high activity for multiple reactions in one material often leads to trade-offs in binding strength and stability. As a result, composite and heterostructure designs dominate, but these increase system complexity and may affect scalability. Long-term stability under cycling, extreme pH, and mechanical stress also remains a major concern. Thin two-dimensional sheets may collapse or detach without proper structural support. In conclusion, bifunctional and trifunctional catalysts based on two-dimensional materials represent a key direction for integrated energy conversion. Their adjustable chemistry, high conductivity, and flexible structure support multiple reactions in a single platform. Future success depends on scalable synthesis, deeper mechanistic understanding during multi-reaction operation, and integration into real devices. Strong coordination between material science, diagnostics, and engineering will be essential to realise multifunctional two-dimensional catalysts for practical energy systems.

5.5 Electrocatalyst Stability and Degradation

The long-term use of two-dimensional electrocatalysts depends strongly on their stability during operation. In real devices, catalysts face harsh conditions such as high current density, changing potential, corrosive electrolyte, gas evolution, and repeated cycling. These conditions accelerate degradation through dissolution, surface passivation, structural change, and loss of electrical contact. Two-dimensional materials are especially sensitive because of their thin layers, large exposed surface, and high defect density. While these features enhance activity, they also increase susceptibility to chemical attack and mechanical damage. A recent review on oxygen evolution catalysts reported that performance loss often arises from surface and structural degradation rather than thermodynamic limits alone [160]. One major degradation pathway involves dissolution or leaching of active metal sites. Under operating conditions, metals in layered double hydroxides, transition metal dichalcogenides, or MXene-derived oxides may oxidise and dissolve into the electrolyte. In NiFe layered double hydroxides, active hydroxide phases may convert into less active oxides, which increases overpotential during cycling. Operando techniques such as X-ray absorption spectroscopy and synchrotron X-ray diffraction reveal changes such as amorphisation, phase separation, and nanosheet delamination during operation [161]. For two-dimensional materials, the high exposure of edges and basal planes further increases vulnerability, making surface stabilisation essential.

Loss of electronic connectivity is another important degradation mechanism. Many two-dimensional catalysts rely on thin films or aligned nanosheet networks. Mechanical stress from gas bubble release, volume change during redox cycling, or repeated loading can cause cracking, delamination, or sheet restacking. These effects increase charge-transfer resistance and reduce active surface area. A study on platinum-based fuel cell electrodes showed that loss of electrochemical surface area due to support corrosion caused major activity decline. Similar effects are now observed in two-dimensional catalyst systems when conductive networks collapse [162]. The use of spacers, flexible binders, or encapsulation layers can improve stability but may reduce access to active sites. Gas bubbles and electrolyte corrosion also affect durability. Gas bubbles can stick to thin nanosheets and apply local stress, which promotes layer detachment and surface damage. Thin two-dimensional layers lack the mechanical support of bulk materials and therefore suffer faster fatigue. In proton exchange membrane fuel cells, prolonged high-current operation caused micro-crack formation and pinholes in catalyst layers, showing that mechanical stability is as important as chemical stability [163]. For two-dimensional catalysts, strong adhesion to the support, controlled bubble release, and hierarchical structures help reduce damage.

Improving stability requires a combined strategy. Stable compositions and surface terminations must resist corrosion. Conductive networks must remain intact through mechanical support and binder design. Gas-induced stress must reduce through surface engineering and porosity control. Operando diagnostic tools are essential to track structural and chemical changes during operation. A recent stability-focused review recommended accelerated durability tests that reflect real operating stress and standard reporting of performance decay over long time scales [164]. In summary, two-dimensional materials offer high activity and flexible design for electrocatalysis, but long-term durability remains a key challenge. Industrial use demands strong control over degradation pathways through combined chemical, mechanical, and interfacial engineering. Future research should focus on scalable stabilisation methods, standard durability testing under realistic conditions, and deeper understanding of how structure and surface chemistry affect long-term performance. Addressing these factors is essential for deploying two-dimensional electrocatalysts in practical and sustainable energy technologies.

6. Photocatalysis and Photo electrochemistry

6.1 2D Semiconductors for Solar Energy Conversion

Two-dimensional semiconductors provide a strong platform for solar energy conversion. Their atomic thickness allows efficient light absorption and fast charge movement. These materials support exciton separation and effective interface control. Their bandgap can be tuned by changing thickness or stacking order. They also show strong interaction with light and offer a large surface area. These features make them suitable for advanced solar devices. In recent years, materials such as transition metal dichalcogenides, black phosphorus, graphitic carbon nitride, MXenes, and two-dimensional perovskites have gained attention. They are used in photovoltaic cells, photoelectrochemical systems, and tandem devices. A recent review discussed how ultrathin materials improve solar conversion by linking structure, properties, and function in perovskites, TMDs, and MXenes [165].

In photovoltaic applications, two-dimensional semiconductors serve multiple roles. They act as light absorbers, charge transport layers, and interface modifiers. Monolayer TMDs such as MoS_2, WS_2, and WSe_2 show direct bandgaps in the visible to near-infrared range. These properties support flexible and ultrathin solar cells. High exciton binding energy remains a challenge, as it affects charge separation. Even so, device models using TMD absorbers and spacer-based superlattices predict efficiencies above 10% under ideal conditions [166]. In perovskite solar cells, two-dimensional materials reduce surface defects and improve energy alignment. They also increase resistance to moisture and oxygen. A recent study reported that large-area perovskite modules retained stable performance during long-term outdoor operation when two-dimensional layers were added [167].

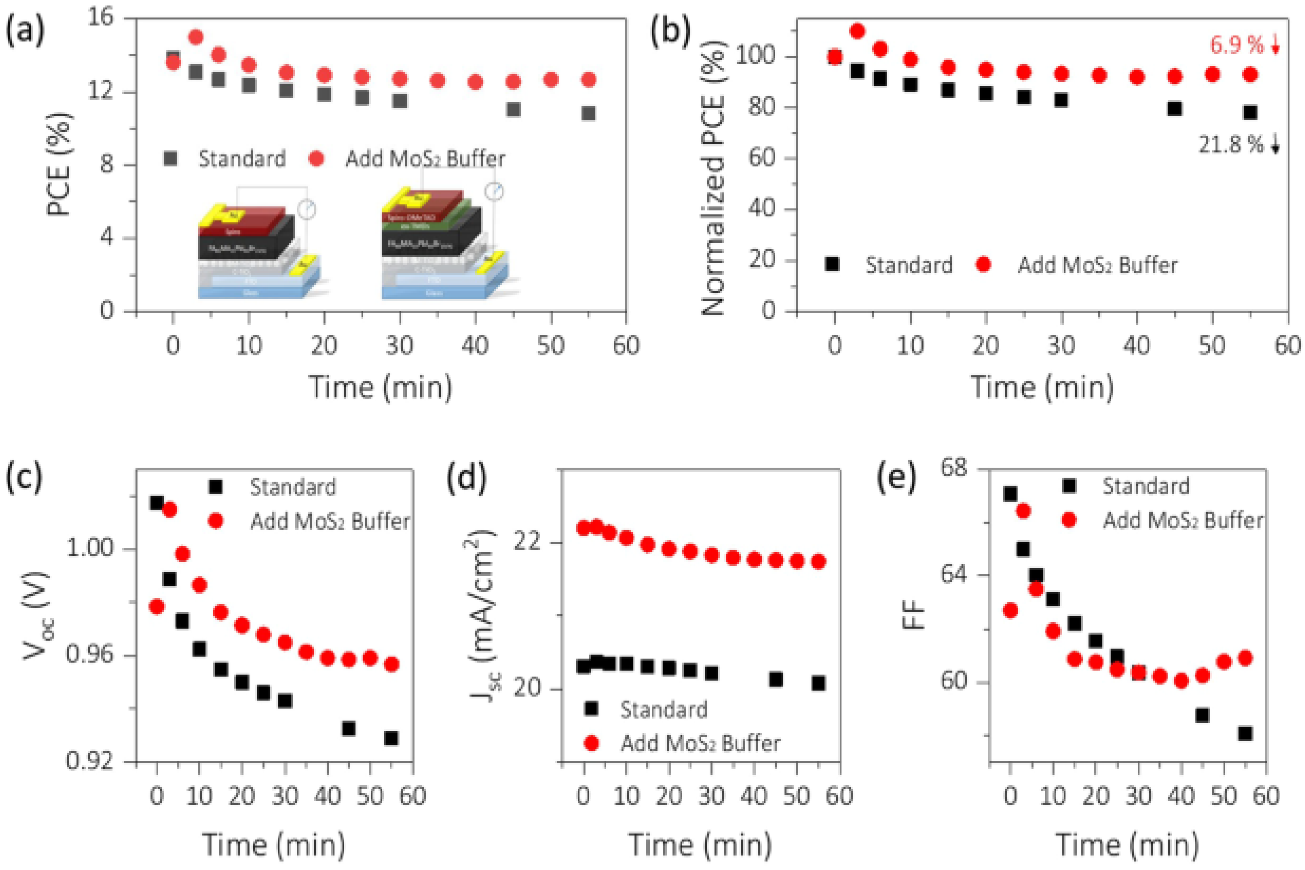

Figure 13. Stability of the PCSs with and without a MoS2 buffer layer. **a** PCE, **b** normalized PCE, **c** Voc, **d** Jsc, and **e** FF of PSCs with and without a MoS2 buffer layer (Liang *et al.,* 2020, Springer Nature, CC BY 4.0) [168].

Figure 13 shows the effect of a MoS_2 buffer layer on perovskite solar cell stability. The results compare power conversion efficiency, open-circuit voltage, short-circuit current, and fill factor for devices with and without the buffer layer [169] Two-dimensional semiconductors also play an important role in photoelectrochemical applications. Their thin structure supports quick charge separation and short transport paths. Strong light absorption leads to high carrier generation. A detailed review on PEC water splitting explained that two-dimensional sheets act not only as absorbers but also as protective layers and charge transfer bridges. They also form efficient heterojunctions that improve both activity and durability [170] these roles show that two-dimensional semiconductors go beyond traditional bulk materials by combining light capture, charge transport, and catalytic support in a single thin layer.

Despite progress, several design challenges remain. The thin nature of two-dimensional semiconductors limits total light absorption. This issue requires light-trapping designs, plasmonic support, or stacked heterostructures. For example, TMDC-based superlattice structures with spacers improved internal light scattering and achieved simulated efficiencies of about 12.9% [171] High exciton binding energy also restricts free carrier generation. This problem demands careful heterojunction design, doping, and built-in electric fields. Device integration remains another concern. Large-area fabrication, interface stability, and process compatibility need further work. Studies on two-dimensional perovskite hybrid devices showed that inserting thin layers reduced ion migration and improved moisture resistance, leading to longer device lifetime [172]. In summary, two-dimensional semiconductors show rapid progress in solar energy conversion. Precise control over thickness, composition, and interfaces supports high device performance. These materials offer strong potential for next-generation solar cells and solar fuel systems. Future work should focus on scalable synthesis, stable device integration, better light absorption methods, and long-term testing under real conditions. These efforts will help expand their use in flexible, wearable, and large-area renewable energy technologies.

6.2 Z-Scheme and Heterostructure Photo catalysts

Two-dimensional materials have become important in Z-scheme and heterostructure photocatalysis. These systems help overcome the limits of single-component photocatalysts. They improve light absorption, charge separation, and redox strength at the same time. The thin structure, large surface area, and tunable band structure of two-dimensional materials support strong interface formation. A recent review highlighted that 2D/2D heterojunctions are widely used because van der Waals contact improves electric field formation and reduces resistance at the interface [173]. The Z-scheme mechanism allows electrons to remain in one material and holes in another. This design preserves strong reduction and oxidation ability. In two-dimensional systems, this approach is highly effective. A narrow bandgap material absorbs visible light, while a wide bandgap partner supports oxidation. Their layered contact enables direct charge transfer without mediators. A theoretical study on a GeC/BSe heterostructure confirmed stable Z-scheme alignment suitable for water splitting [174] such studies show how two-dimensional heterostructures combine strong light absorption with suitable redox potential.

In experiments, 2D Z-scheme systems show improved hydrogen evolution, oxygen evolution, pollutant removal, and carbon dioxide reduction. A review covering more than 3000 studies reported better charge separation and higher visible-light use compared to bulk systems [175]. The improvement comes from better interface contact and shorter carrier paths. A WO_3/g-C_3N_4 Z-scheme heterostructure showed enhanced degradation and nitrogen fixation due to efficient charge separation and extended interface area [176]. Successful Z-scheme design depends on several factors. Proper band alignment is required to guide electron flow. A strong internal electric field helps reduce recombination. Adequate light absorption must be maintained while limiting carrier loss. Stability under light and water exposure remains critical. Many two-dimensional assemblies face structural degradation during long-term operation.

Figure 14 illustrates photoluminescence and absorption behaviour in WSe_2/MoS_2 heterostructures, along with charge transfer and exciton behaviour under light excitation [177] despite progress, challenges remain. Many systems perform well only under laboratory conditions. Long-term unassisted water splitting is still rare. Structural restacking and corrosion reduce durability in water. Large-scale synthesis with uniform interfaces remains difficult. Inconsistent testing methods also limit comparison across studies. In conclusion, Z-scheme photocatalysts based on two-dimensional materials offer strong potential for solar energy conversion.

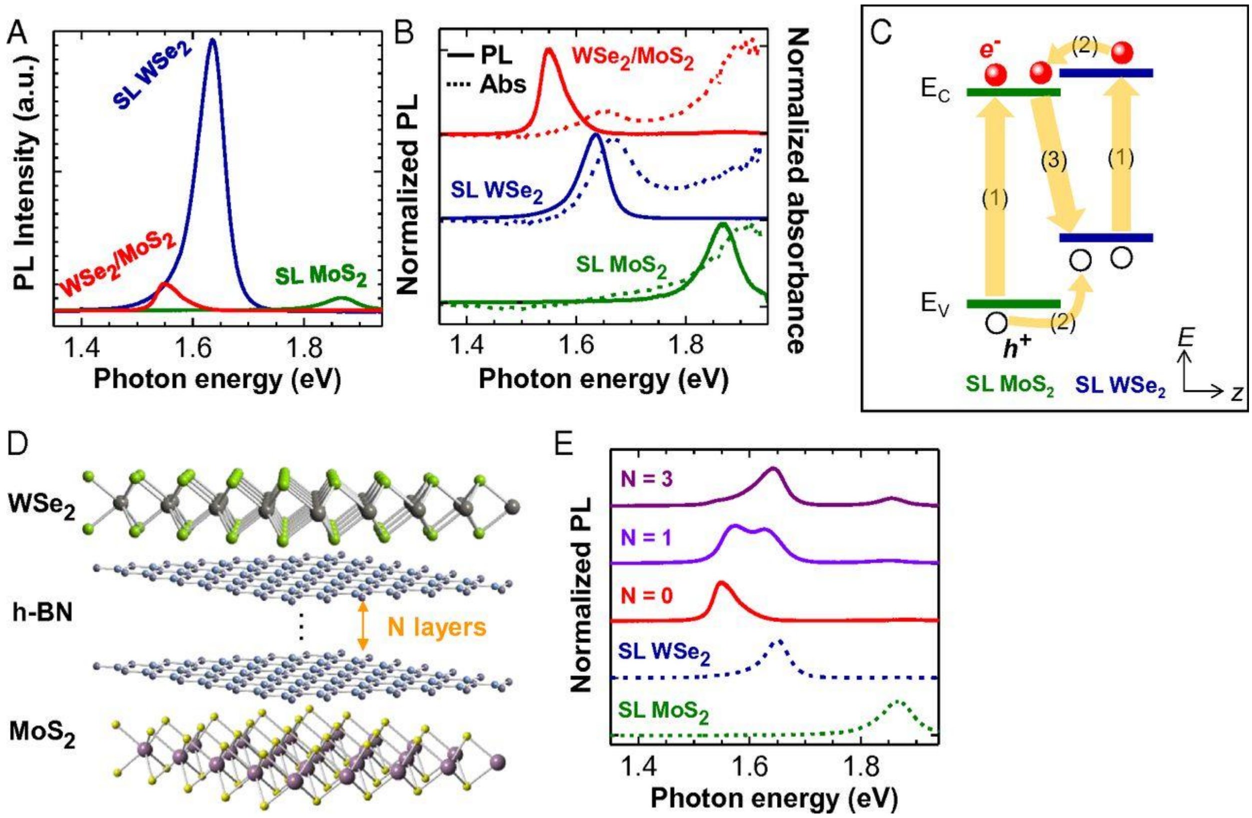

Figure 14. Photoluminescence and absorption from WSe2/MoS2 hetero-bilayers. **(A)** PL spectra. **(B)** Normalized PL (solid lines) and absorbance (dashed lines) spectra. **(C)** Band diagram of WSe_2/MoS_2 hetero-bilayer under photo excitation. **(D)** An atomistic illustration of the heterostructure of single-layer WSe_2/single-layer MoS_2. **(E)** Normalized PL spectra (Fang *et al.,* 2014, PNAS, CC BY 4.0) [177]

Their thin structure and tailored interfaces support efficient charge flow and redox reactions. Future research must focus on stable device operation, scalable fabrication, and standard performance evaluation. These efforts will support their role in advanced solar fuel technologies

6.3 Photo electrochemical Cells

Two-dimensional materials are reshaping photoelectrochemical cell design. In these systems, sunlight drives chemical reactions such as water splitting. Effective PEC operation needs strong light absorption, charge separation, and surface catalysis. Two-dimensional materials support all these processes together. A recent review highlighted their roles as absorbers, transport layers, catalysts, and protective coatings in PEC water splitting [178]. Photo electrodes based on two-dimensional materials benefit from thin geometry and tunable band structure. Few-layer TMDs and black phosphorus absorb visible light efficiently and allow fast carrier extraction. Conductive materials such as MXenes and graphene improve electron transport. A study showed that combining graphene or carbon nanotubes with g-C_3N_4 increased photocurrent and carrier lifetime [179]. Two-dimensional materials also improve interface quality. They reduce surface recombination and support catalytic reactions. They act as protective layers against corrosion. In one study, an MXene-derived Ti-rich layer on α-Fe_2O_3 nanorods reduced charge recombination and improved electron transport. The modified electrode showed seven times higher PEC performance than the pristine sample. Transient absorption studies confirmed longer hole lifetime and improved charge separation [180] These results show how two-dimensional materials solve key PEC limitations.

However, challenges remain for commercial use. Large-area fabrication with uniform quality is difficult. Many devices still rely on sacrificial agents and half-cell setups. A review on tandem PEC cells reported that stable solar-to-hydrogen efficiency above 10% for long durations is still uncommon [180]. Stability under sunlight and corrosive environments also needs more study. Delamination and oxidation of thin layers reduce lifetime. Reporting standards also vary, which limits comparison. In conclusion, PEC cells provide a strong platform for two-dimensional materials in solar fuel production. Their unique properties improve light capture, charge transport, and surface reactions. Future work must focus on device-level development, large-scale fabrication, stable interfaces, and long-term testing. With these advances, two-dimensional material-based PEC systems can become efficient and reliable solutions for solar energy conversion.

7. Emerging Applications and Cross-Cutting Themes

7.1 CO_2 Reduction and Artificial Photosynthesis

Reducing carbon dioxide into useful fuels through photocatalytic and photoelectrochemical routes is central to sustainable energy cycles. This approach, often called artificial photosynthesis, aims to close the carbon loop using sunlight. Two-dimensional materials beyond graphene have gained strong attention in this field. Their large surface area, adjustable band structure, quantum confinement effects, and efficient charge transport support improved CO_2 conversion. These properties help overcome common limits of bulk catalysts, such as weak light use, slow surface reactions, and poor selectivity toward multi-electron products. A recent review reported that two-dimensional transition metal dichalcogenides, layered perovskites, and MXene-based materials help link light absorption, charge separation, and product selectivity in CO_2 photoreduction systems [181].

Effective CO_2 reduction depends on three connected steps. These include strong light absorption, fast movement of photocharges to active sites, and surface reactions that favour CO_2 conversion over unwanted reactions like hydrogen evolution. Two-dimensional materials support all three steps. Monolayer TMDs such as MoS_2 and WS_2 show direct bandgaps, which improve light absorption and carrier lifetime. Their thin layers shorten the distance that charges must travel to reach reactive sites. Two-dimensional perovskites and layered MOF systems also act as light absorbers and stable platforms for CO_2 binding. These materials help anchor co-catalysts, stabilise reaction intermediates, and guide selective product formation. Recent studies show progress through advanced catalyst design. One example reported a surfactant-free palladium nanosheet placed on graphitic carbon nitride. This 2D/2D structure showed higher selectivity for CO and methane under visible light compared to surfactant-covered systems. The clean interface improved charge transfer and maximised contact area between layers [182]. Such planar interfaces are now common in artificial photosynthesis research. They allow fast charge injection and better control over surface chemistry. These features are important for managing multi-electron and multi-proton reactions that form fuels such as CO, CH_4, methanol, or ethylene.

Despite progress, major challenges remain. CO_2 reduction competes strongly with hydrogen evolution in water-based systems. Both reactions occur at similar potentials, which reduces product selectivity. A review highlighted low selectivity as a key limitation in CO_2 conversion [182]. Even with improved light capture and charge transport, surface chemistry must still control CO_2 adsorption, weaken C=O bonds, suppress hydrogen formation, and stabilise multi-carbon products. Many studies also rely on small-scale tests using sacrificial agents rather than full water–CO_2 systems under sunlight. Stability is another concern, as thin materials can degrade, peel, or corrode during long operation.

Figure 15 presents photocatalytic and electrochemical results for gersiloxene-based systems, including hydrogen and carbon monoxide evolution, photostability, impedance behaviour, and transient photocurrent response [183]. In summary, two-dimensional materials offer strong potential for CO_2 reduction and artificial photosynthesis. Their ability to combine light absorption, fast charge movement, and tuned surface chemistry supports efficient solar fuel generation. Future work should focus on scalable material growth, full-device operation without bias, realistic solar testing, and long-term durability. Strong links between material design, reaction mechanism, and system performance will be essential to move this technology toward practical use.

7.2 Nitrogen Reduction Reaction (NRR)

Electrochemical nitrogen reduction provides a promising route for ammonia production under ambient conditions. This method offers an energy-saving alternative to the Haber–Bosch process. Two-dimensional materials beyond graphene, such as TMDs, MXenes, metal–organic frameworks, and carbon nitride nanosheets, have shown strong potential for this reaction. Their thin structure shortens charge transport paths and exposes more active sites. Adjustable surface chemistry also supports nitrogen adsorption and activation. A detailed review reported that control of active sites, suppression of hydrogen evolution, and stronger nitrogen binding are key challenges in two-dimensional NRR systems [184].

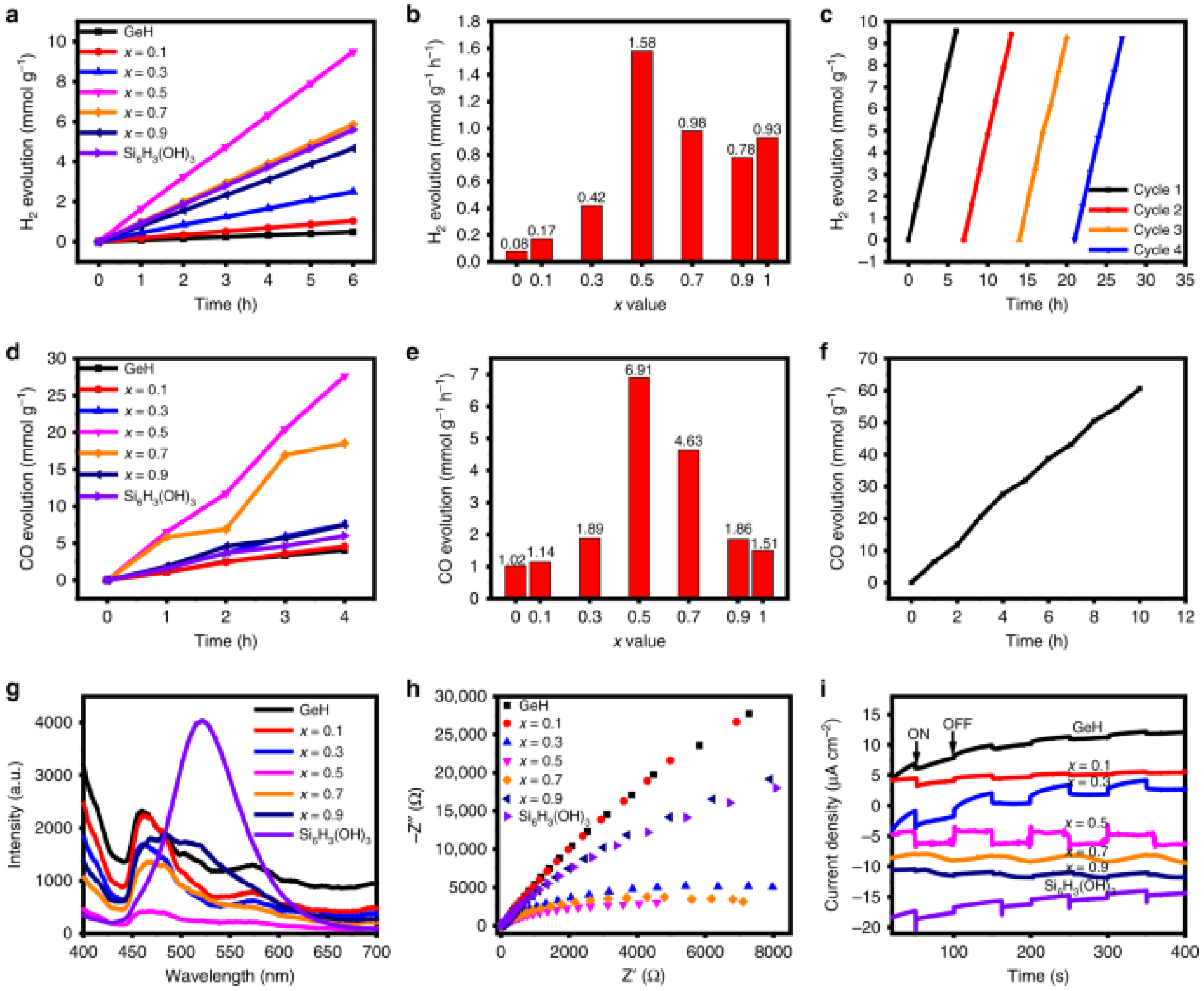

Figure 15. Photocatalytic performance and electrochemical characterization. a, b Time-dependent photocatalytic hydrogen evolution **(a)** and HERs **(b)** of gersiloxenes, GeH and Si6H3(OH)3. **c** Photostability for H2 production. **d, e** Time-dependent photocatalytic CO evolution **(d)** and COERs **(e)** of gersiloxenes, GeH and Si6H3(OH)3. f Time-dependent photocatalytic CO evolution. **g–i** PL spectra **(g),** EIS Nyquist plots **(h)** and transient photocurrent responses (i) of gersiloxenes, GeH and Si6H3(OH)3 (Zhao *et al.,* 2020, Springer Nature, CC BY 4.0) [183].

In these systems, nitrogen adsorption, intermediate stabilisation, and hydrogen suppression must occur together. Two-dimensional carbon nitride sheets are effective supports for single-atom catalysts. Their planar structure allows precise control over electronic properties and isolated metal centres. A recent machine-learning study developed a descriptor that links metal properties and carbon-to-nitrogen ratio. This approach guided the design of catalysts with very low energy barriers for nitrogen reduction [185]. TMD nanosheets such as MoS_2 also show improved ammonia selectivity when combined with $g\text{-}C_3N_4$. The engineered interface improves charge flow and favours nitrogen-related intermediates over hydrogen adsorption [186].

Heterostructure design further improves performance. A $MoS_2/g\text{-}C_3N_4$ face-to-face heterojunction showed higher ammonia yield and Faradaic efficiency. The interface promoted fast electron transfer and reduced hydrogen evolution by stabilising nitrogen intermediates on Mo edge sites [187]. MXene-based materials also show promise. Studies revealed that hydroxyl-terminated MXenes enhance nitrogen reduction more effectively than fluorine-terminated ones. This finding highlights the importance of surface termination in two-dimensional catalysts [188]. Comparative analysis across studies shows clear trends. Catalyst performance depends strongly on defect density, atom dispersion, and interface structure. Adjusting these parameters directly affects ammonia yield and efficiency.

However, practical challenges remain. Hydrogen evolution still dominates in aqueous systems, often limiting ammonia efficiency to below 30%.

Proton control and selective nitrogen adsorption remain difficult. Many catalysts show good performance only in half-cell tests or with additives. Long-term stability under continuous operation is rarely demonstrated. Atomically thin materials may degrade under harsh electrolytes. Standard testing methods and accurate ammonia detection are also lacking. Large-scale synthesis with controlled defects remains difficult. In conclusion, two-dimensional materials provide a strong platform for nitrogen reduction. They allow precise control over active sites and charge transport. Future progress requires scalable synthesis, stable device operation, and reliable benchmarking. With these advances, two-dimensional catalysts can support sustainable ammonia production.

7.3 Thermal Energy Harvesting and Thermoelectrics

Thermal energy harvesting through thermoelectric conversion has gained renewed interest with the rise of two-dimensional materials. These materials help address the long-standing trade-off between electrical conductivity, thermal conductivity, and Seebeck coefficient. Two-dimensional chalcogenides, conductive MOFs, and van der Waals heterostructures show clear advantages. Their thin geometry reduces heat transport, while lateral size supports charge flow. Band structure tuning also improves carrier movement. A recent review highlighted the importance of morphology control, doping, and hybrid structures for improving thermoelectric performance [189]. In two-dimensional systems, low thermal conductivity arises from strong phonon scattering at boundaries and interfaces. At the same time, charge transport remains effective along the plane. For example, two-dimensional SnSe alloys prepared through electric-current-assisted sintering showed improved room-temperature performance [190]. Other studies reported that anisotropic phonon transport in layered materials helps reduce heat flow, which improves thermoelectric efficiency [191]. Heterostructure design plays a key role in further improvement. Stacking different two-dimensional layers enhances phonon scattering while preserving electrical pathways. A study showed that MXene-modified Bi_2Te_3 modules achieved higher efficiency for waste heat recovery [192]. Conductive MOFs also show promise due to their low thermal conductivity and adjustable electrical properties [193].

Figure 16 illustrates the design and fabrication of flexible thermoelectric generators using Bi_2Te_3-based legs and soft interfaces, including large-area devices compatible with human skin [194]. Despite progress, challenges remain. Most two-dimensional thermoelectric materials are still produced at laboratory scale. Scaling to large-area, uniform films is difficult. Introducing defects reduces heat flow but can harm charge transport. Stability under repeated heating and bending also needs attention. Standard device-level testing methods are still evolving. In summary, two-dimensional materials are reshaping thermoelectric energy harvesting. Their tunable electronic and thermal properties support next-generation devices. Future work should focus on scalable manufacturing, stable module design, and real-world testing to support waste heat recovery applications.

7.4 Integration with Device Architectures

The practical use of two-dimensional materials depends on successful device integration. While many studies focus on material properties, real applications require integration with substrates, interfaces, packaging, and system components. Recent reviews emphasise that although two-dimensional materials offer large surface area and flexibility, challenges such as adhesion, strain, and reliability remain [195]. In micro-energy devices, two-dimensional materials support compact design. Thin electrodes shorten ion paths and increase capacitance. Printing methods such as inkjet and laser writing allow direct fabrication on silicon or flexible substrates. MXenes and TMDs have been used to build micro-supercapacitors with high areal capacitance. Interface quality between electrode and current collector remains critical. A review on flexible electronics highlighted that while thin materials support bending, processing steps often reduce durability [196].

Wearable systems also benefit from two-dimensional materials. MXene films laminated onto textiles maintain performance under bending and stretching. Reviews report that energy storage, sensing, and communication can be combined on a single flexible platform using two-dimensional materials [197]. Device integration involves careful design of electrodes, electrolytes, packaging, and electronic connections. Additive manufacturing offers new opportunities. Printable inks containing two-dimensional sheets allow fabrication of complex three-dimensional structures. These include interdigitated energy devices and hybrid modules. However, challenges include nanosheet alignment, dispersion control, and stress management.

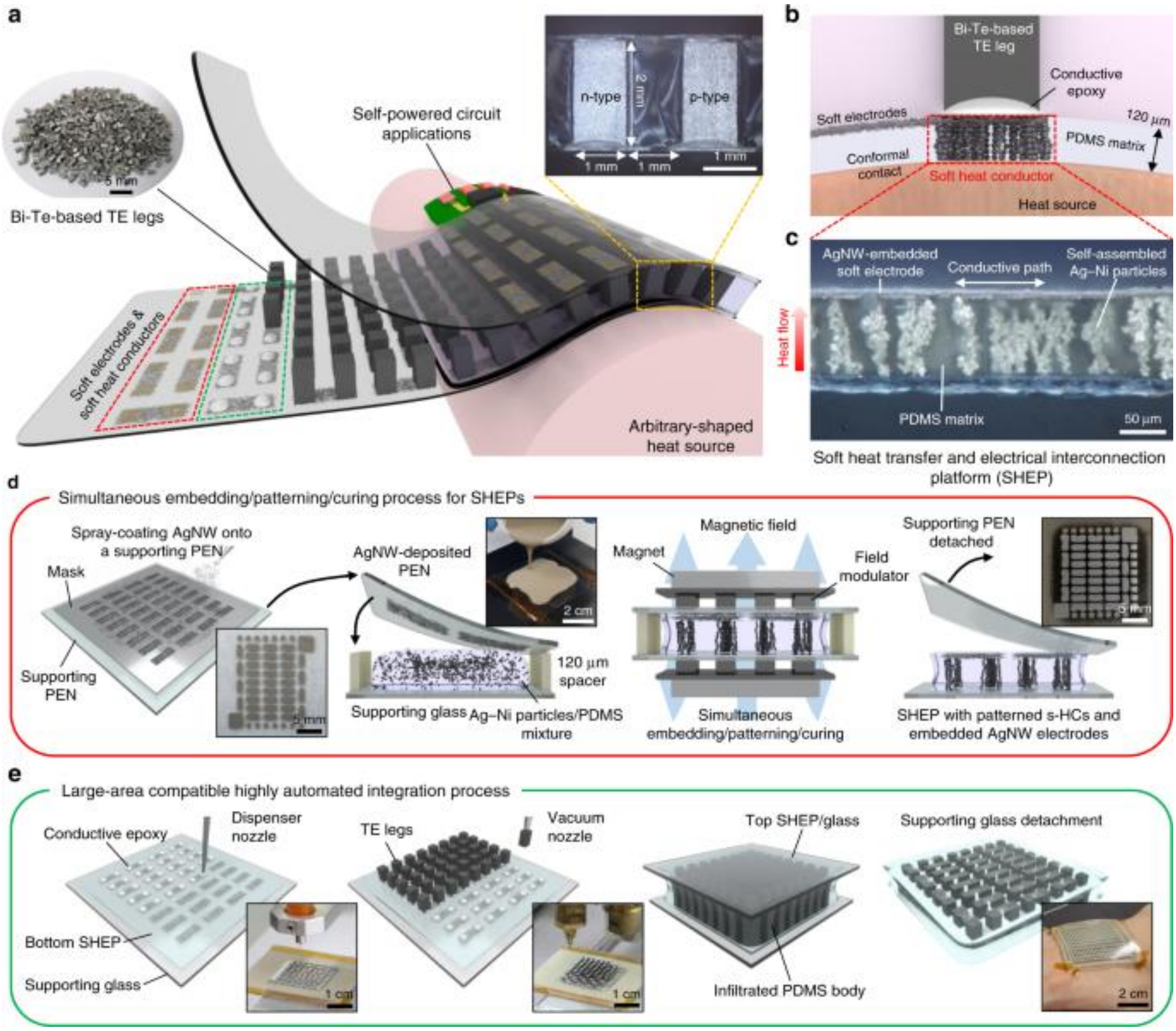

Figure 16. **a** Conceptual illustration of a compliant TEG. **b** Schematic illustration showing the structure of the compliant TEG. **c** Microscopic image of the soft heat transfer and electrical interconnection platform (SHEP). **d** Schematic illustration and photographs of simultaneous embedding/patterning/curing process for the SHEPs. **e** Schematic illustration and photographs of a large-area compatible fully automated integration process (Lee *et al.,* 2020, Springer Nature, CC BY 4.0) [194].

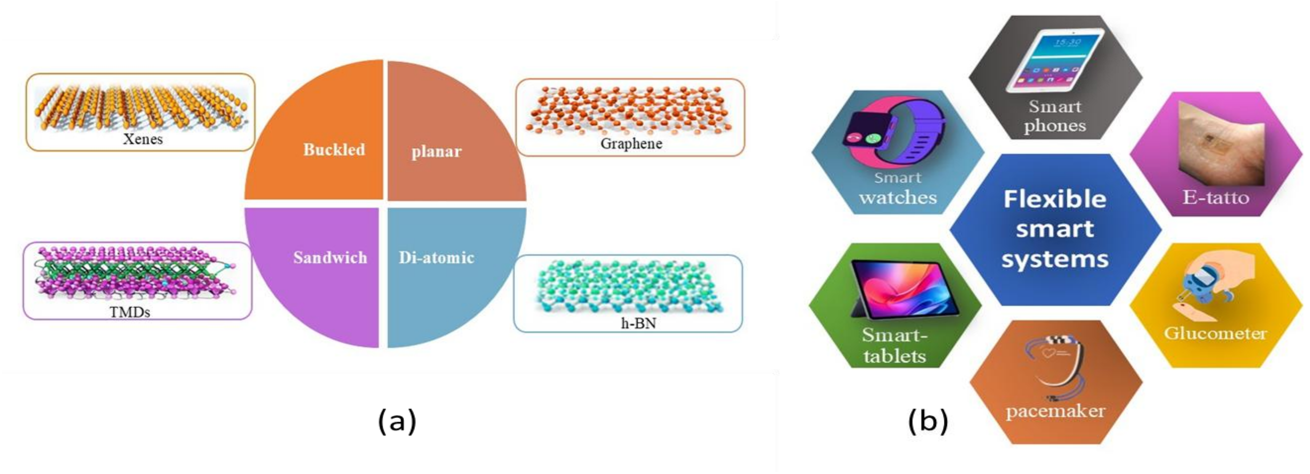

Figure 17. Three-dimensional illustrations of contemporary **(a)** 2D monolayers and their role in **(b)** flexible smart systems.

Despite advances, integration challenges remain. Large-area film transfer often leads to wrinkles or contamination. Contact resistance limits charge flow. Mechanical fatigue under repeated bending is rarely tested. Thermal mismatch and environmental stability also need attention. Scaling from prototypes to roll-to-roll production remains difficult. Figure 17 shows examples of two-dimensional monolayers and their role in flexible smart systems, including wireless communication applications [198]. In conclusion, device integration is key for translating two-dimensional materials into real technologies. Progress requires improved interface control, mechanical reliability, and scalable manufacturing. Addressing these issues will help bring two-dimensional materials from laboratory research to practical energy systems.

8. Characterization Techniques and Computational Insights

8.1 Advanced Structural Characterization

The rapid growth of two-dimensional materials beyond graphene has increased the need for advanced characterization methods. These techniques help to study atomic structure, defects, interfaces, and changes during operation. Modern tools such as aberration-corrected transmission electron microscopy (AC-TEM), aberration-corrected scanning transmission electron microscopy (AC-STEM), synchrotron-based X-ray methods, and scanning probe techniques now provide very high spatial resolution. Many of these methods also operate under in-situ or operando conditions. A focused review on two-dimensional materials reported that AC-STEM allows direct observation of atomic vacancies, dopants, edge structures, stacking faults, and heterointerfaces in monolayer and few-layer systems. The same study noted challenges related to sample preparation, beam damage, and interpretation of strain and defect contrast [199].

Atomic-scale characterization plays a central role in linking structure with material performance. AC-STEM imaging can resolve features below one ångström and map lattice distortion, stacking angle, atomic occupancy, and interface disorder. These parameters strongly influence electronic, optical, and catalytic properties. In transition metal dichalcogenides and MXenes, defects such as metal or chalcogen vacancies, antisite defects, and intercalated species affect electron transport, active site density, and mechanical stability. AC-STEM combined with electron energy loss spectroscopy enables simultaneous spatial and chemical mapping of these defects. A wide-ranging review explained how microscopy, spectroscopy, and machine learning now work together to improve atomic-level understanding of two-dimensional materials [200].

Synchrotron-based X-ray techniques provide information that local imaging alone cannot capture. Operando and in-situ X-ray absorption spectroscopy and X-ray diffraction help track oxidation states, coordination changes, and lattice variation during real operation. These tools are especially important for energy materials under electrochemical cycling or thermal stress. A recent review highlighted that improved operando cell designs now allow direct observation of structural evolution and interface changes in photoelectrochemical and battery systems [201]. For layered two-dimensional materials such as MXenes and transition metal dichalcogenides, these techniques help monitor interlayer spacing, surface termination chemistry, and defect formation during operation. Scanning probe techniques further complement electron and X-ray methods. Advanced atomic force microscopy modes now measure not only surface morphology but also mechanical, electrical, optical, and magnetic properties at the nanoscale. A review described how these methods reveal local variations in stiffness, charge transport, work function, and response to strain across two-dimensional sheets [202]. Such insights are critical for flexible and wearable energy devices, where mechanical deformation can strongly affect material integrity and performance.

Despite major progress, several challenges remain. Preparing clean and damage-free samples for AC-STEM is difficult, especially for beam-sensitive and ultrathin materials. Oxidation and delamination further complicate analysis. Data interpretation must also consider surface effects, strain, twist angles, and quantum confinement, which differ from bulk materials. Operando studies face trade-offs between spatial resolution, time resolution, and realistic operating conditions. Large data sets from techniques such as 4D-STEM, hyperspectral EELS, and time-resolved XAS require machine learning for analysis, yet standard processing and reporting methods are still developing. In summary, advanced structural characterization is essential for understanding two-dimensional materials beyond graphene. The combination of atomic-scale imaging, operando spectroscopy, and nanoscale probing provides a detailed picture of how defects, interfaces, and dynamic changes control material behaviour. Future progress depends on better sample preparation, improved operando platforms for realistic conditions, and standard data analysis methods that allow comparison across studies.

8.2 Operando and In-Situ Techniques

Two-dimensional materials show strong structural sensitivity during operation in energy storage and conversion devices. Their behaviour changes under electrical bias, heat, and chemical environments. Operando and in-situ techniques help capture these changes in real time. These methods track structural, chemical, and morphological evolution while the device operates. They are now essential for studying two-dimensional materials in batteries, supercapacitors, electrocatalysts, and photoelectrochemical systems. A review on in-situ techniques for electrocatalysis showed how these methods reveal reaction pathways, phase changes, and active-site evolution during operation [203]. The need for operando studies arises from the thin nature of two-dimensional materials. Their high surface area and defect density lead to frequent changes in structure and chemistry during use. In transition metal dichalcogenide electrocatalysts, chalcogen vacancies can form, migrate, or disappear under applied current. These changes affect performance and can only be linked to activity through real-time observation. In-situ scanning transmission electron microscopy and synchrotron X-ray absorption under bias provide this information. A comprehensive review of battery electrodes described how optical stress sensors, X-ray tomography, Raman mapping, and infrared spectroscopy track chemical and mechanical changes during cycling [204].

Operando techniques capture transient states that ex-situ methods often miss. In MXenes, ion intercalation causes rapid changes in interlayer spacing and surface termination chemistry. Expansion or delamination can occur within seconds. In-situ X-ray diffraction and X-ray absorption spectroscopy under bias directly reveal lattice changes and oxidation state shifts. A review of operando cell designs described these methods as powerful tools for advanced battery development [205]. In two-dimensional heterostructures, operando spectroscopic imaging has shown how charge transfer alters band alignment and interlayer coupling during bias or illumination. For example, operando photoemission imaging revealed energy landscape changes in a two-dimensional transistor during operation [206].

Several challenges still limit operando studies of two-dimensional materials. Many materials are sensitive to electron beams, air, or vacuum, which complicates cell design. Most operando cells suit bulk materials and provide weak signals for ultrathin layers. Achieving both high spatial and temporal resolution remains difficult. Faster processes such as ion motion often reduce image quality or environmental control. Large and complex data sets require advanced analysis tools, including machine learning, which are still developing for two-dimensional systems. Standard protocols for cell design, testing conditions, and data reporting are also lacking. A review on in-situ infrared spectroscopy noted that few studies currently apply these techniques to energy materials [206]. In conclusion, operando and in-situ techniques are essential for understanding two-dimensional materials under real working conditions. These methods move analysis beyond static images to dynamic mechanisms. Future work should focus on cell designs suitable for ultrathin layers, better balance between resolution and realism, strong data analysis frameworks, and standard testing practices. These steps will help unlock the full potential of two-dimensional materials in energy technologies.

8.3 Computational Modeling and Predictions

Computational modeling plays a key role in the development of two-dimensional materials beyond graphene. Density functional theory has become a standard tool to study electronic structure, defects, interfaces, and catalytic reactions. Recent advances include high-throughput calculations and machine-learning-assisted screening. These approaches expand the range of materials that can be studied efficiently. One study used machine learning with density functional theory to screen about 4,500 MXene systems and identify promising hydrogen evolution catalysts at much lower computational cost [207].

Computational methods support research in several ways. First, they explain mechanisms by identifying reaction pathways, adsorption energies, and electronic changes caused by strain or doping. A large computational study screened over 226,000 bilayer heterostructures and classified their band alignment types and lattice mismatch. This database supports device design using two-dimensional heterostructures [208]. Second, computational screening speeds up material discovery by combining first-principles calculations with machine learning filters. This approach helps identify suitable compositions, terminations, and phases more quickly [209].

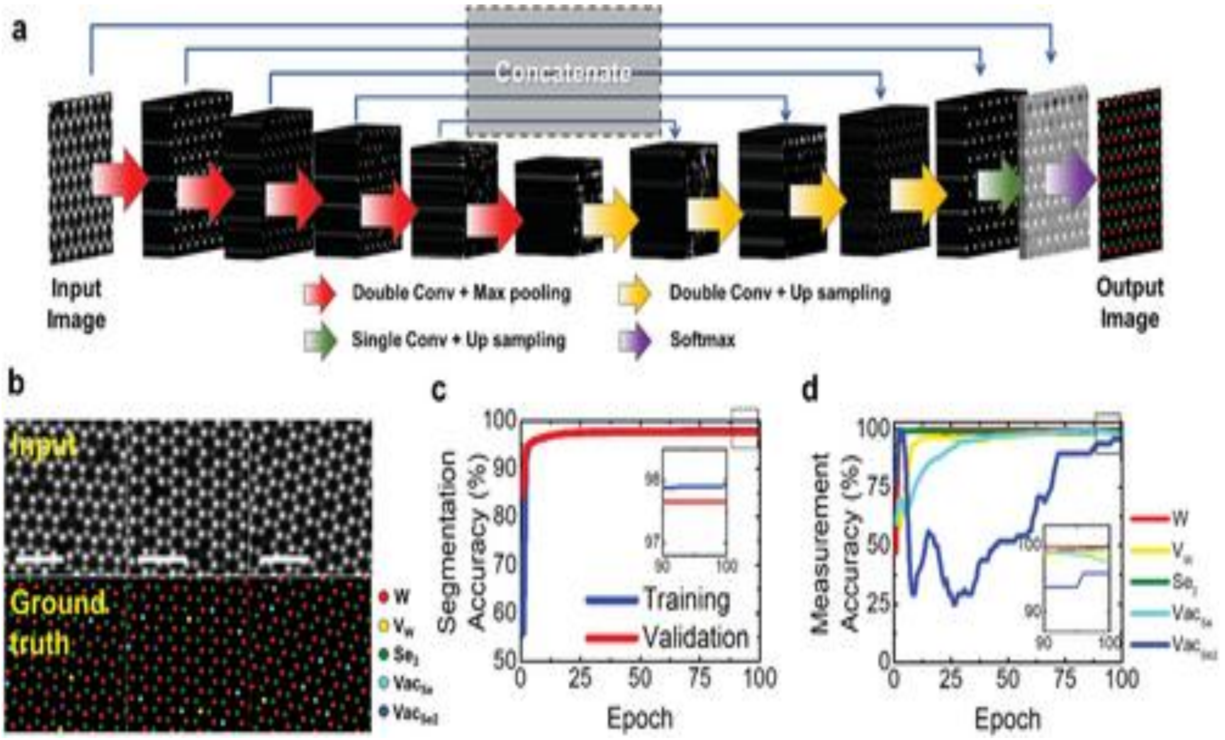

Figure 18. **a)** Deep neural networks model **b)** Examples of training dataset of atom segmentation model. **c)** Pixel-level accuracy graph. **d)** Measurement accuracy graph (Yang *et al.,* 2021, Wiley Advanced, CC BY 4.0) [212].

Third, predictive design allows researchers to estimate how defects, doping, or interfaces will change performance before synthesis.

For energy storage and conversion, modeling helps understand ion intercalation, surface reactions, strain effects, and transport properties. Density functional theory studies have shown how heteroatom doping alters adsorption energy, diffusion barriers, and electronic structure in two-dimensional anode materials [210]. Machine learning methods also play a growing role. A graph neural network model predicted work functions of two-dimensional materials with high accuracy, showing how data-driven tools complement first-principles calculations [211].

Figure 18 shows a deep-learning-based method for atomic site classification using ADF-STEM images of V-WSe_2. The model achieved high accuracy compared to human analysis [212]. Despite strong progress, challenges remain. Standard density functional theory struggles with van der Waals interactions, strong correlations, and excited states in two-dimensional systems. A benchmark study showed that advanced methods improve accuracy only slightly but at high computational cost [213]. Machine learning methods also face issues related to data bias, model transferability, and reproducibility [214]. Another challenge is the gap between ideal models and real devices. Effects such as grain boundaries, contamination, stress, and ageing are difficult to include in simulations. Multiscale modeling that links atomic-level calculations to device-level behaviour is still developing. Standard benchmarks and shared data practices are also limited. In summary, computational modeling is central to advancing two-dimensional materials for energy applications. The combination of first-principles methods, high-throughput screening, and machine learning accelerates discovery and guides experiments. Future work should improve accuracy beyond standard methods, connect models across length scales, and adopt shared standards for data and workflows. With these advances, computational tools will strongly drive the rational design of next-generation two-dimensional energy materials.

9. Challenges and Perspectives

9.1 Synthesis and Scalability

As research on two-dimensional (2D) materials moves from laboratory studies to real applications, large-scale synthesis and manufacturability have become major concerns, as shown in figure 19. Materials such as transition metal dichalcogenides (TMDs), black phosphorus derivatives, metal-oxide nanosheets, and especially MXenes like $Ti_3C_2T_x$ must be produced in large quantity without losing quality. The synthesis process must also remain low cost, safe, repeatable, and suitable for mass production.

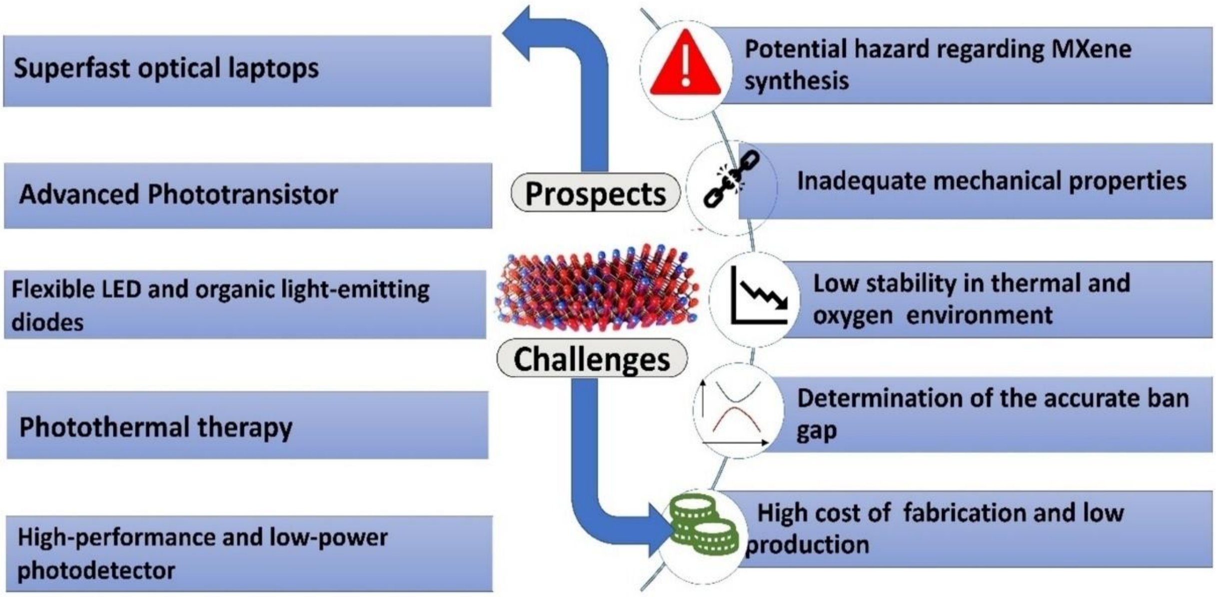

Figure 19. Graphical illustration representing various prospects and challenges of MXene (Hossain *et al.,* 2024, Wiley, CC BY 4.0) [218].

A recent tutorial review reports that although exfoliation and small-scale chemical routes are widely used, industrial production demands new thinking in precursor supply, reactor design, process monitoring, and control of material uniformity [215]. Scalable production of 2D materials requires not only larger batch sizes but also stable control over thickness, lateral size, defect density, purity, surface terminations, and structural quality. This challenge is clearly seen in MXene synthesis. Large-scale etching and delamination of MXenes using fluoride-based or molten-salt routes have enabled production up to hundreds of grams. However, issues related to toxic etchants such as HF, waste handling, oxidation, delamination efficiency, and cost remain unresolved. Bao *et al.* showed that although large-volume MXene synthesis is technically achievable, future progress depends on safer etchants, continuous reactors, and modular production strategies [216]. Bottom-up synthesis methods such as chemical vapour deposition, molecular beam epitaxy, and vapour-phase conversion have also been adapted for 2D materials. These methods aim to achieve wafer-scale uniform films compatible with industrial substrates. Studies on wafer-scale growth of MoS_2, WS_2, and related TMDs on 4–12 inch substrates show that precursor delivery, substrate cleanliness, film transfer, and thickness control remain key limitations [217]. Similar challenges are observed in energy material manufacturing, where uniform coating, electrode size, and production rate are critical factors.

Despite clear progress, several obstacles still limit commercial-scale manufacturing of 2D materials for energy devices. Most synthesis routes remain batch-based with low throughput, while continuous or modular systems are still rare. Large-scale control over defects, surface chemistry, and lateral dimensions is difficult, and such variations strongly affect device performance and lifetime. Environmental and safety concerns linked to hazardous chemicals and waste disposal also require urgent attention, as regulations increasingly favour green synthesis routes. In addition, material production is often disconnected from device fabrication, even though scalability must cover the entire chain from synthesis to module assembly. Finally, the lack of standard metrics for yield, defect density, size distribution, and batch consistency restricts comparison across studies and slows industrial adoption. In summary, scalable synthesis of 2D materials beyond graphene is as important as discovering new materials. For practical energy storage and conversion systems, synthesis methods must deliver large quantities of high-quality material at low cost with minimal environmental impact. At the same time, key properties such as conductivity, surface chemistry, mechanical flexibility, and ion accessibility must be preserved. Achieving this goal will require advances in reactor engineering, materials chemistry, quality control, economic evaluation, and strong collaboration between academia, industry, and policy bodies.

9.2 Stability and Degradation Issues

The real-world use of 2D materials beyond graphene in energy storage and conversion devices depends strongly on their long-term stability. Although many materials show excellent laboratory performance, they often degrade over time through chemical, structural, electrochemical, and mechanical processes. These degradation mechanisms reduce performance, shorten device life, and limit commercial use. Understanding and controlling stability is therefore essential for practical deployment. Chemical instability is one of the most common degradation pathways. Materials such as black phosphorus and several TMDs readily react with oxygen, moisture, or electrolytes, leading to oxidation or surface changes. A large meta-analysis covering 29 different 2D materials reported that degradation rates vary over five orders of magnitude, with composition controlling nearly 85% of this variation [219]. This result highlights the need to evaluate stability alongside performance. Long-term studies on $Ti_3C_2T_x$ MXene films further show that conductivity loss during ambient storage mainly arises from water adsorption and can be partly reversed through vacuum annealing, indicating that some degradation effects are not permanent [220].

In electrochemical systems, structural damage and interface degradation dominate. When 2D materials act as electrodes or catalyst supports, repeated ion insertion and removal cause volume changes, layer separation, phase shifts, and edge corrosion. Defect engineering, while useful for improving activity, may also increase instability, as reactive sites interact more strongly with electrolytes and dissolve or restructure under bias [221]. In TMD electrodes, loss of chalcogen atoms or conversion to oxides during cycling leads to performance decay and higher resistance. Stability therefore depends on a delicate balance between defect density, ion transport, and mechanical strength.

Mechanical stress further contributes to degradation, especially in flexible or wearable devices. Thin 2D layers experience cracking, delamination, and loss of contact when subjected to bending, stretching, or thermal cycling. In batteries, repeated volume expansion during ion storage generates stress that propagates through 2D frameworks and accelerates failure. A recent review reports that without proper interface and stress management, the excellent initial performance of many 2D materials drops quickly under realistic cycling conditions [222]. Environmental factors such as temperature, humidity, electrolyte composition, and reactive species also shape degradation pathways. In photoelectrochemical systems, light, heat, and radicals can trigger surface reconstruction or corrosion. In contrast, controlled use of 2D materials as interlayers in perovskite solar cells has improved moisture resistance, defect passivation, and ion migration control, extending device lifetimes beyond 5000 hours under stress conditions [223]. These examples show that stability challenges can be mitigated through thoughtful material and interface design.

Despite progress, several gaps remain. Long-term stability data under realistic operating conditions are still scarce. Standard testing protocols for stability reporting are lacking, making comparison difficult. The combined effects of chemical, mechanical, and electrochemical degradation in complex 2D systems remain poorly understood. Strategies for repairing or self-healing degraded materials are also at an early stage. In conclusion, while 2D materials beyond graphene offer strong potential for energy technologies, their success depends on stable and durable performance. Addressing degradation requires integrated approaches that combine surface chemistry, mechanical design, interface engineering, and realistic device testing. Only through such efforts can these materials move from laboratory studies to reliable components in sustainable energy systems.

9.3 Interface Engineering

Interface engineering plays a crucial but often underestimated role in the use of 2D materials beyond graphene for energy storage and conversion. The interface between a 2D material and its substrate, electrode, electrolyte, or neighbouring phase controls charge transport, ion movement, chemical stability, mechanical adhesion, and overall device reliability. For materials such as MXenes, TMDs, black phosphorus, and van der Waals heterostructures, precise control of interface chemistry and structure is essential for high performance and long-term stability. A comprehensive review on 2D-material interfaces highlights that interface engineering is central to unlocking the full potential of these materials in electronic and energy devices [224].

From an energy perspective, interfaces serve several interconnected functions. First, they reduce electrical resistance and support efficient charge transfer. Strong and chemically compatible contact between 2D layers and current collectors lowers contact resistance and improves electron and ion flow.

This can be achieved through surface termination control, conductive interlayers, or substrate functionalisation. Second, interfaces influence ion transport and electrochemical stability. Well-designed interfaces must tolerate volume changes during cycling, maintain contact, and suppress unwanted reactions such as electrolyte decomposition. Third, in catalytic and photoelectrochemical systems, interfaces determine energy-level alignment and charge separation efficiency. Introducing 2D materials at catalyst-support junctions can tune band alignment, reduce recombination, and enhance catalytic stability. These effects are clearly discussed in studies on halide-perovskite and 2D-material interfaces [225].

Mechanical aspects of interfaces are equally important, especially for flexible and large-area devices. Repeated bending or thermal cycling can cause delamination, cracking, and increased resistance at poorly designed interfaces. Adhesion layers, gradient structures, or hierarchical anchoring can help absorb stress and maintain contact. Scaling such interface treatments to large substrates while ensuring uniformity and long-term chemical stability remains a manufacturing challenge. Several barriers still limit effective interface engineering. Real interfaces often contain defects, roughness, contamination, and size variations that complicate large-scale control. The relationship between interface chemistry and long-term stability is not well explored, as many studies focus only on initial performance. Designing interfaces that balance ion transport, electrical conduction, mechanical adhesion, and chemical durability involves trade-offs. In addition, standard methods for measuring and reporting interface properties such as adhesion strength, resistance evolution, and delamination are rarely used consistently. In summary, interface engineering is a key factor in advancing 2D materials for energy applications. High material performance alone is insufficient without stable, scalable, and durable interfaces. Future research must focus on precise interface control, systematic measurement under operating stress, and scalable fabrication methods. Strong progress in interface design will be essential for practical deployment of 2D materials beyond graphene.

9.4 Theoretical Understanding Gaps

Although 2D materials beyond graphene have shown strong potential for energy storage and conversion, major gaps remain in theoretical understanding. One key limitation lies in the weak connection between atomic-scale simulations and real device behaviour. Methods such as density functional theory and molecular dynamics provide insights into defects, ion binding, and interlayer interactions. However, linking these results to larger-scale effects such as electrode swelling, fracture, ion networks, and heat flow remains challenging. Recent studies stress that chemical reactions, ion transport, and mechanical deformation are often treated separately instead of as a coupled system [226]. Another limitation arises from simplified modelling assumptions. Many theoretical studies consider ideal, defect-free 2D sheets with fixed terminations and ignore electrolytes, interphases, humidity, and interface dynamics present in real devices. As a result, predicted binding energies or diffusion barriers may not reflect actual performance. Reviews on band-gap engineering in 2D heterostructures report that many models neglect disorder, many-body effects, and environmental factors, which limits their practical relevance [227].

The selection of reliable descriptors for screening 2D materials also remains unclear. Common parameters such as adsorption energy, bandgap, diffusion barrier, and work function do not always correlate across different materials and applications. This reduces the predictive strength of high-throughput and machine-learning models. Although machine-learning tools reduce computational cost, their accuracy strongly depends on training data quality and descriptor choice, and reliability outside trained domains remains uncertain [228]. Dynamic processes such as phase changes, delamination, stress-driven reactions, and interface evolution during cycling are also poorly captured. Many materials undergo significant structural and chemical changes during operation, yet most models remain static and equilibrium-based. Predictive models for heterogeneous 2D–3D interfaces, which are critical for stability, are still limited [229]. Without time-dependent modelling, long-term durability and failure modes are difficult to predict.

Finally, lack of standardisation in computational methods and data sharing further restricts progress. Differences in calculation settings, material models, and reporting formats hinder comparison and reproducibility. Limited access to open datasets also restricts validation and meta-analysis. To address these gaps, future efforts should focus on multi-scale and multi-physics modelling that links chemistry, mechanics, and thermal effects. Models must better represent realistic device environments. Robust and transferable descriptors should be validated across materials and applications. Dynamic simulations that capture long-term evolution are needed. Community-wide standards for data reporting and open databases will also be essential. In conclusion, closing theoretical gaps is critical for transforming 2D materials beyond graphene into practical energy technologies. Improved modelling will strengthen theory–experiment links, enhance predictive accuracy, and support reliable and scalable material design.

9.5 Standardization and Benchmarking

In research on 2D materials beyond graphene, the lack of standardisation and benchmarking remains a major barrier to practical adoption. Although many studies report impressive values for capacity, activity, or conductivity, differences in testing conditions and reporting formats prevent meaningful comparison. A recent review on metrology for 2D materials notes that despite rapid progress, universal measurement standards are still missing, especially for high-volume manufacturing [230]. Standardisation is required at several levels. First, material characterisation must follow consistent definitions for layer number, lateral size, defect density, surface chemistry, and uniformity. Without common metrics, terms such as "few-layer" or "high quality" remain ambiguous. Second, performance benchmarking must adopt standard test conditions. In energy devices, electrolyte composition, mass loading, electrode structure, cycling protocol, and ageing conditions should be clearly defined. Studies have shown that many reports focus on single-device performance without providing statistical variation or yield data, which limits reliability assessment [231]. Third, system-level metrics such as full-cell performance, areal capacity, stability under stress, and environmental impact are often missing, even though they are crucial for real applications.

The absence of standardisation has direct consequences. It slows reproducibility, reduces investor confidence, and delays technology readiness. Industry roadmaps now emphasise the need for standard protocols and metrics, including defect density, uniformity, and production cost per area, as key milestones for the next decade [232]. Implementation remains difficult due to the wide variety of 2D materials, synthesis methods, and applications. Addressing this challenge requires coordinated action. This includes developing certified reference materials, publishing open standard testing protocols, building shared performance databases, and aligning research practices with international standards organisations such as IEEE, ASTM, and SEMI. Commentaries have repeatedly stressed that without unified standards for mobility, defect density, and process repeatability, translation from laboratory research to technology will remain slow [233]. In conclusion, the full potential of 2D materials beyond graphene in sustainable energy systems can only be realised through rigorous standardisation and benchmarking. Novel materials alone are not sufficient. Clear protocols, transparent reporting, and comparable datasets are essential for reproducibility, confidence, and industrial uptake. Future high-impact studies must integrate standard metrics and benchmarking as core elements of their methodology to accelerate translation from research to real-world energy technologies.

10. Future Directions and Outlook

10.1 Emerging 2D Material Families

Research on two-dimensional materials has expanded far beyond graphene as its limitations, such as zero bandgap and restricted chemical control, became clear for many energy applications. Although graphene shows excellent conductivity and strength, it is not ideal for all energy storage and conversion systems. As a result, several new 2D material families have emerged with diverse atomic structures, compositions, and electronic properties. A comprehensive review reports more than 150 graphene-like materials, including layered and non-layered 2D systems, which reflects the rapid growth of this research area [234]. One important group includes mono-elemental 2D materials, often called Xenes, such as phosphorene, antimonene, bismuthene, and tellurene. These materials show thickness-dependent bandgaps, directional charge transport, and strong spin–orbit effects. Such properties make them attractive for energy conversion, sensing, and catalytic applications. Phosphorene, for example, offers a tunable bandgap between 0.3 and 2 eV along with high carrier mobility, which supports its use in photodetection and energy-harvesting devices [235]. However, many Xenes suffer from chemical reactivity and poor environmental stability, which limits their practical use. Another emerging class consists of ternary and quaternary 2D materials, such as MA_2Z_4-type compounds including $MoSi_2N_4$. In these materials, a transition metal layer is sandwiched between functional layers to form a stable but non-natural 2D structure. These systems show high mechanical strength, good thermal conductivity, and semiconducting behaviour with controllable bandgaps. Monolayer $MoSi_2N_4$, for instance, sustains very high tensile stress along both zigzag and armchair directions and also tolerates large strain under biaxial loading

[236]. Such properties make these materials suitable for thermoelectric devices, electrocatalysis, and flexible energy systems.

MXenes form another rapidly growing family of 2D materials. These transition-metal carbides and nitrides build upon the success of $Ti_3C_2T_x$ and related systems. MXenes offer metallic conductivity, flexible mechanical behaviour, and tunable surface terminations such as –O, –OH, and –F. These features support their use as electrodes, conductive frameworks, and charge-storage materials. Future progress depends on expanding MXene compositions beyond titanium-based systems and integrating them into layered and hybrid device structures. In addition, 2D metal oxides, metal halides, layered double hydroxides, and covalent organic frameworks have gained attention. These materials provide high surface area, accessible ion pathways, and abundant active sites. Two-dimensional oxide nanosheets and perovskite-type oxides have been developed for batteries, supercapacitors, and water-splitting reactions. Their tunable interlayer spacing, surface chemistry, and electrochemical stability offer clear advantages. A detailed review highlights the broad chemical flexibility of these 2D systems for energy and catalytic applications [237].

Each emerging material family brings distinct strengths. Xenes provide high mobility and tunable electronic structure. Designer ternary materials offer mechanical strength with controlled bandgaps. MXenes deliver high conductivity and surface control. Oxide and hydroxide nanosheets contribute chemical stability and catalytic activity. However, challenges remain in stability, large-scale synthesis, electrolyte compatibility, and device integration. Systematic efforts are needed to unlock their full potential. In conclusion, the landscape of 2D materials beyond graphene continues to expand rapidly. The focus has shifted from extending graphene properties to designing new 2D chemistries with targeted functions. Real progress in energy technologies will depend on advances in synthesis control, interface design, stability improvement, and scalable manufacturing. Deeper understanding of structure–property relationships and alignment with device requirements will shape future developments.

10.2 AI and Autonomous Discovery

Materials research is undergoing a major shift as artificial intelligence becomes central to the discovery and development of advanced 2D materials. In energy storage and conversion fields such as batteries, supercapacitors, catalysis, and photovoltaics, AI tools help explore large chemical spaces that are difficult to access using traditional methods. A general review highlights how machine-learning techniques support prediction of structural, electronic, mechanical, and chemical properties of 2D materials, thereby speeding up discovery and translation [238]. AI methods such as deep learning, graph neural networks, generative adversarial networks, and reinforcement learning enable several key tasks. These tools allow high-throughput screening of possible structures, identification of hidden design rules, and extraction of meaningful descriptors such as defect energy or surface termination effects. In some systems, AI connects synthesis, characterisation, and feedback into closed-loop discovery pipelines. For example, a study using crystal-graph convolutional neural networks analysed nearly 45,000 structures and identified design rules relevant to mechanical and photovoltaic properties in 2D systems [239]. Other generative frameworks have proposed hundreds of thousands of new 2D material candidates through deep-learning models combined with structural prediction and DFT validation [240].

AI also supports autonomous discovery and optimisation. Integrated workflows that combine formation-energy prediction, interatomic potentials, and genetic algorithms have identified new compounds with more than hundred-fold speed improvement compared to standard DFT screening [241]. These approaches show how combining AI with physical insight can accelerate the materials genome strategy for energy-focused 2D materials. Recent reviews also note that modern AI frameworks now include constraints such as synthesizability, defect tolerance, and scalability, which brings predictions closer to real-world implementation [242]. Despite these advances, challenges remain. AI models depend strongly on data quality, and experimental data for many emerging 2D materials remain limited. Model transferability across different chemistries is uncertain. Bias in datasets and lack of interpretability also restrict confidence in predictions. Autonomous laboratories face practical issues related to synthesis repeatability, quality control, and matching AI outputs with device-level performance. Although generative models can suggest many candidates, successful synthesis and device translation rates remain modest [243]. In summary, AI and autonomous discovery tools are becoming powerful drivers in 2D materials research for energy applications. These methods support large-scale screening, materials design, and optimisation beyond traditional approaches. To fully realise their potential, efforts must focus on building high-quality datasets, improving model transparency, integrating AI with experimental platforms, and linking predictions to device and cost metrics. With these developments, AI-based discovery can become a core pillar of next-generation energy materials research.

10.3 Integration Pathways to Commercialization

Moving 2D materials beyond graphene from laboratory research to commercial energy devices is a complex process. Material innovation alone is not sufficient. Success also depends on manufacturing readiness, supply-chain integration, regulatory approval, and cost competitiveness. Although materials such as MXenes, TMD nanosheets, Xenes, and layered oxides show strong laboratory performance, their commercial impact remains limited due to low production throughput, defect variability, and lack of standard process flows [244]. Technology readiness assessment plays a central role in commercialization. For energy storage applications, this requires a shift from small-scale flakes to large-area films or composites compatible with industrial processes such as roll-to-roll coating and electrode fabrication. MXene electrodes, for instance, show high capacity in laboratory cells, but challenges remain in large-scale synthesis, etchant handling, yield control, and electrode formulation. A review on MXene integration into batteries highlights that these factors must meet industrial reliability standards for commercial success [245]. Control over surface chemistry, defect density, and film uniformity is therefore essential.

Industry partnerships and pilot-scale studies help bridge the gap between research and manufacturing. Collaboration among material suppliers, equipment developers, device manufacturers, and system integrators allows alignment across the value chain. An industrial commentary stresses that translation requires reliable supply, quality assurance, and compatibility with existing energy-device infrastructure [246]. Pilot lines must test not only material performance but also compatibility with binders, coatings, cell assembly, and long-term cycling. Regulatory and environmental factors also influence commercialization. New 2D materials must meet safety, toxicity, recycling, and sustainability standards. Use of hazardous etchants or rare elements can raise regulatory hurdles and increase costs. An analysis of market barriers for 2D semiconductors highlights manufacturing cost, defect control, and regulatory compliance as major challenges [247]. These aspects must be considered early in development.

Economic viability is another key factor. For adoption, 2D materials must offer better cost-to-performance ratios than existing technologies. An economic assessment shows that without major reductions in production cost and improvements in yield, performance gains alone will not lead to commercial uptake [248]. Techno-economic analysis should therefore accompany material development from an early stage. In summary, commercialization of 2D materials beyond graphene requires coordinated progress in manufacturing, cost control, industry collaboration, regulation, and sustainability. The field must move beyond isolated performance reports toward full value-chain readiness. Early integration of these considerations can enable successful transition from laboratory research to scalable energy technologies.

10.4 Grand Challenges

As research on 2D materials beyond graphene advances, several grand challenges must be addressed to enable large-scale energy applications. One major challenge is the scalable synthesis of large-area, high-quality 2D films with precise control over thickness, uniformity, surface chemistry, and crystal structure. Although laboratory results are promising, scale-up remains a key bottleneck, as highlighted in reviews of emerging graphene-like materials [249]. Without reliable industrial production, commercial deployment remains difficult. Long-term stability under real operating conditions is another critical challenge. Many 2D materials show excellent initial performance but degrade under high loading, temperature variation, humidity, or mechanical stress. Structural damage, interface failure, and chemical corrosion reduce device lifetime. A meta-analysis in aqueous ammonium-ion batteries points out that stability under extended cycling remains insufficiently studied for many 2D systems [250]. Achieving durable performance at device level is therefore essential.

Integration into complete energy systems presents further challenges. This includes interface design with current collectors and electrolytes, mechanical and thermal reliability, scalable processing, cost control, and recycling. Many studies stop at half-cell or proof-of-concept stages, which do not reflect real-world requirements.

Table 2. Grand Challenges and Future Roadmap for 2D Materials in Energy Applications

S.NO	Challenge Area	Key Bottlenecks	Target Metrics	Emerging Strategies	Outlook (Short < 2027 / Mid 2027–2032 / Long > 2032)	References
1	Scalable Synthesis of MXenes	Harsh HF-based etching, batch-to-batch variability, defect control	≥10 cm^2 uniform films, <5% defect density, HF-free methods	LiF/HCl etching, molten salt methods, Lewis acidic molten salts	Mid-term	[252]
2	MXene Oxidation Stability	Ambient degradation, water/oxygen sensitivity, performance loss	>1000 h ambient stability, <10% capacity fade	Surface functionalization, protective coatings, controlled oxidation	Short to Mid-term	[253]
3	MXene Interlayer Restacking	Sheet aggregation reduces accessible surface area and ion transport	Maintain >80% theoretical capacitance, <20% restacking	Pillar molecules, spacer insertion, 3D architectures	Short-term	[254]
4	Wafer-Scale 2D Synthesis	Poor uniformity in CVD, limited area coverage, high cost	≥4-inch wafer, single-crystal domains >1 cm^2	Roll-to-roll CVD, epitaxial growth, liquid-phase methods	Mid to Long-term	[255]
5	TMD Phase Stability (1T vs 2H)	Metastable 1T phase converts to 2H, loss of metallic conductivity	>70% 1T phase retention, 100% phase purity	Electron injection, plasma treatment, heteroatom doping	Mid-term	[256]
6	TMD Structural Aggregation	Layer restacking during cycling, conversion reaction irreversibility	>5000 cycles @ >80% capacity retention	Interlayer expansion, phase engineering, carbon scaffolds	Mid-term	[257]
7	Black Phosphorus Degradation	Rapid oxidation in air/water, photo-assisted degradation	>100 days ambient stability, <5% oxidation	Covalent functionalization, encapsulation, surface passivation	Short to Mid-term	[258]
8	BP Anisotropic Properties	Direction-dependent performance, mechanical fragility	Isotropic performance, flexible substrates	Composite architectures, cross-linking, hybrid structures	Mid-term	[259]
9	Electrocatalyst Stability (HER/OER)	Dissolution, oxidation, structural reconstruction under operation	>10,000 h @ constant overpotential, <5 mV decade^{-1} drift	Operando characterization, protective layers, alloy catalysts	Mid to Long-term	[260]
10	OER Catalyst Degradation	Morphological changes, metal leaching, phase	>5000 h stability @ 500 mA cm^{-2}, <10% performance loss	Surface stabilization, corrosion-resistant supports, bimetallics	Mid-term	[261]

		transformation				
11	HER Catalyst Activation	Low basal plane activity, edge-site limitations	Pt-like activity (<50 mV @ 10 mA cm^{-2}), >95% active sites	Defect engineering, single-atom catalysts, strain engineering	Short to Mid-term	[262]
12	2D Material Delamination	Weak catalyst-substrate adhesion, gas bubble detachment	>90% adhesion retention, <5% delamination	Covalent anchoring, 3D conductive scaffolds, binder optimization	Short-term	[263]
13	Interface Contact Resistance	High resistance at 2D-metal contacts limits device performance	<100 Ω·µm contact resistance, <10 mV voltage drop	Graphene interlayers, phase-engineered contacts, doping	Mid-term	[264]
14	Performance Metric Reporting	Incomplete data (loading, electrolyte volume, cell configuration)	Mandatory reporting standards, peer-reviewed checklists	Standardized cell architectures, automated data validation	Short to Mid-term	[265]
15	Multivalent Battery Performance	Sluggish Mg^{2+}/Zn^{2+}/Al^{3+} kinetics, narrow voltage windows	>200 mAh g^{-1}, >1000 cycles, >1.5 V operating window	Interlayer engineering, hybrid electrolytes, surface modification	Mid to Long-term	[266]
16	Li-S Battery Polysulfide Shuttling	Capacity fade, coulombic efficiency loss	>500 cycles @ >80% retention, >99.5% efficiency	MXene/TMD separators, polar interlayers, catalytic conversion	Short to Mid-term	[267]
17	Supercapacitor Energy Density	Low energy density vs batteries	>50 Wh kg^{-1}, >10,000 W kg^{-1} simultaneously	Hybrid capacitors, redox-active electrolytes, MXene films	Short-term	[268]
18	Flexible Energy Storage	Mechanical degradation under bending, limited scalability	>10,000 bend cycles @ <10% capacity loss	Freestanding films, textile integration, 3D printing	Short to Mid-term	[269]
19	Photocatalyst Charge Separation	Rapid electron-hole recombination, low quantum efficiency	>10% solar-to-hydrogen efficiency, >100 h stability	Z-scheme heterostructures, plasmonic enhancement, cocatalysts	Mid to Long-term	[270]
20	CO_2 Reduction Selectivity	Multi-carbon product selectivity, competing HER	>80% Faradaic efficiency for C2+ products, <10% H_2	Defect-rich surfaces, bimetallic sites, ionic liquid electrolytes	Long-term	[271]
21	Nitrogen Reduction (NRR) Efficiency	Competing HER, low NH_3 yield rates, contamination issues	>20% Faradaic efficiency, >10 µg h^{-1} $mgcat^{-1}$	Vacancy engineering, hydrophobic surfaces, Li-mediation	Long-term	[272]
22	Machine Learning Integration	Limited training data, model transferability, experimental validation	>90% prediction accuracy, <10% validation error	Neural network potentials, active learning, closed-loop systems	Short to Mid-term	[273]

23	AI-Guided Synthesis Optimization	Complex parameter spaces, synthesis-structure-property gaps	Autonomous synthesis platforms, real-time feedback	Bayesian optimization, reinforcement learning, robotic labs	Mid-term	[274]
24	High-Throughput Screening	Computational cost, descriptor identification, database gaps	Screen >10,000 compositions/month, validated descriptors	DFT+ML hybrid methods, materials genome databases	Short to Mid-term	[275]
25	Computational-Experimental Gap	DFT predictions don't match experimental observations	<15% deviation between theory and experiment	Multiscale modeling, operando validation, uncertainty quantification	Mid-term	[276]
26	Operando Characterization	Limited real-time monitoring, instrument accessibility, data interpretation	In-situ techniques for all key reactions, temporal resolution <1 s	Synchrotron XAS, environmental TEM, spectroelectrochemistry	Short to Mid-term	[277]
27	Toxicity & Environmental Impact	Unknown long-term toxicity of MXenes/TMDs, recycling challenges	Complete lifecycle assessment, >90% recyclability	Green synthesis routes, biodegradation studies, circular economy	Mid to Long-term	[278]
28	Cost-Effective Production	High precursor costs (Ti, Mo, V), energy-intensive synthesis	<$100/kg for MXenes, <$50/kg for TMDs	Earth-abundant alternatives, electrochemical synthesis, recycling	Mid to Long-term	[279]
29	Technology Readiness Level	Most 2D materials at TRL 3–4, limited pilot demonstrations	TRL 6–7 demonstrations, commercial partnerships	Industry collaboration, pilot-scale facilities, standardized testing	Mid to Long-term	[280]
30	Regulatory & Safety Standards	No established safety protocols for nanomaterials in energy devices	ISO standards, safety certifications, regulatory approval	Multi-stakeholder frameworks, risk assessment protocols	Long-term	[281]
31	Market Entry Barriers	High capital costs, established competitor technologies, risk aversion	Cost parity with incumbents, demonstrated reliability	Niche applications first, value chain integration, policy support	Long-term	[282]
32	Heterostructure Interface Control	Lattice mismatch, interface defects, thermal stability	Atomically sharp interfaces, <1% lattice mismatch	Van der Waals assembly, transfer-free growth, interface engineering	Mid-term	[283]
33	High-Entropy 2D Materials	Synthesis complexity, phase stability prediction	Stable compositions, tailored properties	Computational prediction, combinatorial synthesis	Long-term	[284]

Bridging the gap between material discovery and system integration is necessary for meaningful impact. Theoretical understanding and benchmarking also remain limited. Predictive models often lack multi-scale coupling and realistic environmental inputs. Standardised benchmarking protocols are missing, which restricts comparison and validation across studies. Reviews on 2D material metrology emphasise that inconsistent reporting of mass loading, cycling conditions, and stress testing limits reproducibility [251].

Sustainability and supply-chain issues form another long-term challenge. Large-scale use of 2D materials must align with environmental regulations, resource availability, and life-cycle management. Reducing hazardous chemicals, improving yield, ensuring material availability, and designing for recycling are essential steps. Without addressing these aspects, even high-performance materials may fail economic and sustainability evaluations. In conclusion, the grand challenges for 2D materials beyond graphene extend beyond material properties. They include scalable synthesis, long-term stability, system-level integration, reliable theory and benchmarking, and sustainable manufacturing. Addressing these interconnected challenges is essential to realise the full potential of 2D materials in future energy storage and conversion technologies. Table 2 lists the challenges and emerging strategies for 2D materials in energy applications.

11. Conclusions

Two-dimensional materials beyond graphene have developed into a rich and diverse materials platform for next-generation energy storage and conversion technologies. Over the past decade, research has expanded from graphene to a wide range of 2D systems, including MXenes, transition metal dichalcogenides, black phosphorus, metal oxides and hydroxides, layered double hydroxides, and other emerging materials. These systems provide enhanced chemical flexibility, tunable electronic structures, large accessible surface areas, and short ion and electron transport paths, which are essential for high-performance energy devices. Significant progress has been achieved in understanding synthesis routes, defect engineering, heterostructure construction, and interface design. These advances have enabled impressive performance in batteries, supercapacitors, electrocatalysis, and photoelectrochemical energy conversion. However, many reported results are based on small-scale laboratory demonstrations under ideal conditions. In practical applications, challenges related to material stability, electrode architecture, interfacial resistance, and large-area manufacturing remain unresolved. Bridging the gap between material discovery and device-level reliability is therefore a critical requirement.

Recent developments in advanced characterisation techniques and computational modelling have improved insight into reaction mechanisms and degradation processes. Machine learning and artificial intelligence have further accelerated material screening and optimisation. Nevertheless, predictive accuracy depends strongly on data quality, realistic modelling conditions, and experimental validation. Without robust synthesis pathways, standardised testing protocols, and long-term durability assessment, theoretical predictions cannot fully translate into technological impact. Future progress in this field requires a shift toward system-oriented research. Scalable and environmentally responsible synthesis methods must be prioritised. Interface engineering should focus on maintaining stable performance under realistic mechanical, thermal, and electrochemical stress. Universal benchmarking standards are needed to ensure reproducibility and meaningful comparison across studies. In parallel, techno-economic analysis and life-cycle assessment must guide material selection and device design. In conclusion, 2D materials beyond graphene hold strong potential to reshape the energy landscape. Realising this potential will depend on coordinated efforts across materials science, device engineering, computation, and industry. With sustained interdisciplinary collaboration, these atomically thin materials can become key components of efficient, durable, and sustainable energy technologies.

References

[1] F.R. Fan, R. Wang, H. Zhang, W. Wu, Emerging beyond-graphene elemental 2D materials for energy and catalysis applications. Chemical Society Reviews, 50(19), (2021) 10983–11031. https://doi.org/10.1039/C9CS00821G

[2] T. Li, T. Jing, D. Rao, S. Mourdikoudis, Y. Zuo, M. Wang, Two-dimensional materials for electrocatalysis and energy storage applications. Inorganic Chemistry Frontiers, 9(23), (2022) 6008–6046. https://doi.org/10.1039/D2QI01911F

[3] P.A. Shinde, A.M. Patil, S. Lee, E. Jung, S. Chan Jun, Two-dimensional MXenes for electrochemical energy storage applications. Journal of Materials Chemistry A. 10, (2022) 1105–1149. https://doi.org/10.1039/D1TA04642J

[4] T. Nawz, A. Safdar, M. Hussain, D. Sung Lee, M. Siyar, Graphene to Advanced MoS_2: A Review of Structure, Synthesis, and Optoelectronic Device Application. Crystals, 10(10), (2020) 902. https://doi.org/10.3390/cryst10100902

[5] X. Shen, X. Lin, Y. Peng, Y. Zhang, F. Long, Q. Han, Y. Wang, L. Han, Two-Dimensional Materials for Highly Efficient and Stable Perovskite Solar Cells, Nano-micro Letters, 16(1), (2024) 201. https://doi.org/10.1007/s40820-024-01417-1

[6] D. Lemian, F. Bode, Battery-Supercapacitor Energy Storage Systems for Electrical Vehicles: A Review, Energies, 15(15), (2022) 5683. https://doi.org/10.3390/en15155683

[7] M. Şahin, F. Blaabjerg, A. Sangwongwanich, A Comprehensive Review on Supercapacitor Applications and Developments, Energies, 15(3), (2022) 674. https://doi.org/10.3390/en15030674

[8] J.M. Lim, Y.S. Jang, H. Van T. Nguyen, J.S. Kim, Y. Yoon, B.J. Park, D.H. Seo, K.-K. Lee, Z. Han, K. (Ken) Ostrikov, S.G. Doo, Advances in High-Voltage Supercapacitors for Energy Storage Systems: Materials and Electrolyte Tailoring to Implementation, Nanoscale Advances, 5(3), (2023) 615–626. https://doi.org/10.1039/D2NA00863G

[9] J. Zhang, M. Gu, X. Chen, Supercapacitors for renewable energy applications: A review. Micro and Nano Engineering, 21, (2023) 100229. https://doi.org/10.1016/j.mne.2023.100229.

[10] M.F. Iqbal, F. Nasir, F. Shabbir, Z.U.D. Babar, M.F. Saleem, K. Ullah, N. Sun, F. Ali, Supercapacitors: an emerging energy storage system. Advanced Energy and Sustainability Research, 6(8), (2025). https://doi.org/10.1002/aesr.202400412.

[11] K.R. Ngoy, V.T. Lukong, K.O. Yoro, J.B. Makambo, N.C. Chukwuati, C. Ibegbulam, O. Eterigho-Ikelegbe, K. Ukoba, T.C. Jen, Lithium-ion Batteries and the Future of Sustainable Energy: A comprehensive Review. Renewable and Sustainable Energy Reviews, 223, (2025) 115971. https://doi.org/10.1016/j.rser.2025.115971

[12] S.V. Sadavar, S. Lee, S. Park, Advancements in Asymmetric Supercapacitors: From Historical Milestones to Challenges and Future Directions. Advanced Science, 11(34), (2024) 2403172. https://doi.org/10.1002/advs.202403172

[13] A.K. Bojarajan, S.S. Gunasekaran, S.K. Ravi, A.H. Al-Marzouqi, F.M. Hassan, S. Sangaraju, Advances in two dimensional materials for supercapacitor applications: From metal carbides to metal borides and beyond. Renewable and Sustainable Energy Reviews, 226, (2026) 116278. https://doi.org/10.1016/j.rser.2025.116278

[14] J. Chen, H. Chen, T. Yu, R. Li, Y. Wang, Z. Shao, S. Song, Recent Advances in the Understanding of the Surface Reconstruction of Oxygen Evolution Electrocatalysts and Materials Development. Electrochemical Energy Reviews, 4, (2021) 566–600. https://doi.org/10.1007/s41918-021-00104-8

[15] L. Zhu, Y. Li, J. Zhao, J. Liu, L. Wang, J. Lei, Recent Advanced Development of Stabilizing Sodium Metal Anodes. Green Energy & Environment, 8(5), (2023) 1279–1307. https://doi.org/10.1016/j.gee.2022.06.010

[16] S. Das, M. Baumann, M. Weil, Comprehensive Performance Evaluation and Sustainability Ranking of Battery Technologies based on Hesitant Intuitionistic Fuzzy Linguistic Decision-Making. Energy Conversion and Management, 328, (2025) 119594. https://doi.org/10.1016/j.enconman.2025.119594

[17] S. Jangra, B. Kumar, J. Sharma, S. Sengupta, S. Das, R. Brajpuriya, A. Ohlan, Y.K. Mishra, Goyat, A review on overcoming challenges and pioneering advances: MXene-based materials for energy storage applications. Journal of Energy Storage, 101, (2024) 113810. https://doi.org/10.1016/j.est.2024.113810.

[18] T. Rasheed, MXenes as an Emerging Class of Two-Dimensional Materials for Advanced Energy Storage Devices. Journal of Materials Chemistry A, 10(9), (2022) 4558–4584. https://doi.org/10.1039/D1TA10083A

[19] O. Samy, A. El Moutaouakil, A Review on MoS_2 Energy Applications: Recent Developments and Challenges. Energies, 14(15), (2021) 4586. https://doi.org/10.3390/en14154586

[20] H. Wang, D. Tran, J. Qian, F. Ding, D. Losic, MOS2/Graphene composites as promising materials for energy storage and conversion applications. Advanced Materials Interfaces, 6(20), (2019). https://doi.org/10.1002/admi.201900915.

[21] L. Liang, J. Wang, W. Lin, B.G. Sumpter, V. Meunier, M. Pan, Electronic bandgap and edge reconstruction in phosphorene materials. Nano Letters, 14(11), (2014) 6400–6406. https://doi.org/10.1021/nl502892t.

[22] Y. Zhang, H. Xu, S. Lu, Preparation and Application of Layered Double Hydroxide Nanosheets. RSC Advances, 11, (2021) 24254–24281. https://doi.org/10.1039/D1RA03289E

[23] W. Gao, Z. Zheng, P. Wen, N. Huo, J. Li, Novel two-dimensional monoelemental and ternary materials: growth, physics and application. Nanophotonics, 9(8), (2020) 2147–2168. https://doi.org/10.1515/nanoph-2019-0557.

[24] A.J. Borah, V. Natu, A. Biswas, A. Srivastava, A Review on Recent Progress in Synthesis, Properties, and Applications of MXenes. Oxford Open Materials Science, 5(1), (2025) itae017. https://doi.org/10.1093/oxfmat/itae017

[25] C.-X. Hu, Y. Shin, O. Read, C. Casiraghi, Dispersant-Assisted Liquid-Phase Exfoliation of 2D Materials beyond Graphene. Nanoscale, 13(2), (2021) 460–484. https://doi.org/10.1039/D0NR05514J

[26] T.M. Alharbi, C.L. Raston, High Conversion Continuous Flow Exfoliation of 2D MoS_2, Nanoscale Advances, 5(23), (2023) 6405–6409. https://doi.org/10.1039/D3NA00880K

[27] N. Anwar, G. Jiang, Y. Wen, M. Ahmed, H. Zhong, S. Ao, Z. Li, Y. Ling, G.F. Schneider, W. Fu, Z. Zhang, Evaluating the potential of two-dimensional materials for innovations in multifunctional electrochromic biochemical sensors: a review. Moore and More, 1(1), (2024) 12. https://doi.org/10.1007/s44275-024-00013-0

[28] X. Zhang, J. Lai, T. Gray, Recent Progress in Low-Temperature CVD Growth of 2D Materials. Oxford Open Materials Science, 3(1), (2023) itad010. https://doi.org/10.1093/oxfmat/itad010

[29] R. Kumar, N. Goel, D.K. Jarwal, Y. Hu, J. Zhang, M. Kumar, Strategic review on chemical vapor deposition technology-derived 2D material nanostructures for room-temperature gas sensors. Journal of Materials Chemistry C, 11(3), (2023) 774–801. https://doi.org/10.1039/D2TC04188J

[30] K. Choudhary, K.F. Garrity, S.T. Hartman, G. Pilania, F. Tavazza, Efficient computational design of two-dimensional van der Waals heterostructures: Band alignment, lattice mismatch, and machine learning. Physical Review Materials, 7(1), (2023) 014009. https://doi.org/10.1103/PhysRevMaterials.7.014009

[31] T.T. Xuan, L.N. Long, T. Van Khai, Effect of reaction temperature and reaction time on the structure and properties of MoS_2 synthesized by hydrothermal method. Vietnam Journal of Chemistry 58(1), (2020) 92–100. https://doi.org/10.1002/vjch.2019000144

[32] F. Liu, Z. Fan, Defect engineering of two-dimensional materials for advanced energy conversion and storage. Chemical Society Reviews, 52(5), (2023) 1723–1772. https://doi.org/10.1039/D2CS00931E

[33] Y. Xia, S. Sevim, J.P. Vale, J. Seibel, D. Rodríguez-San-Miguel, D. Kim, S. Pané, T.S. Mayor, S. De Feyter, J. Puigmartí-Luis, Covalent transfer of chemical gradients onto a graphenic surface with 2D and 3D control, Nature Communications,13(1), (2022) 7006. https://doi.org/10.1038/s41467-022-34684-w

[34] M.M. Cruz-Benítez, P. Gónzalez-Morones, E. Hernández-Hernández, J. R. Villagómez-Ibarra, J. Castro-Rosas, E. Rangel-Vargas, H. A. Fonseca-Florido, C. A. Gómez-Aldapa, Covalent functionalization of graphene oxide with fructose, starch, and micro-cellulose by sonochemistry. Polymers, 13(4), (2021) 490. https://doi.org/10.3390/polym13040490.

[35] Z. Zhao, H. Chen, W. Zhang, S. Yi, H. Chen, Z. Su, B. Niu, Y. Zhang, D. Long, Defect engineering in Carbon Materials for Electrochemical Energy Storage and Catalytic Conversion, Materials Advances, 4(3), (2023) 835–867.

https://doi.org/10.1039/D2MA01009G

[36] Y. Wang, Z. Ding, N. Arif, W.C. Jiang, Y.J. Zeng, 2D Material based Heterostructures for Solar Light Driven Photocatalytic H_2 Production. Materials Advances, 3(8), (2022) 3389–3417. https://doi.org/10.1039/D2MA00191H

[37] F. Bibi, I.A. Soomro, A. Hanan, M.N. Lakhan, A. Khan, N.R. Goraya, Z.U. Rehman, I. Hussain, K. Zhang, Advances in 2D/2D MXenes-based heterostructures for energy storage/conversion applications, Journal of Materials Science & Technology, 202, (2024) 82–118. https://doi.org/10.1016/j.jmst.2024.03.005

[38] X. Long, L. Zhang, Z. Tan, B. Zhou, Progress on 2D–2D Heterostructured Hybrid Materials for Efficient Electrocatalysis. Energy Advances, 2, (2023) 280–292. https://doi.org/10.1039/D2YA00318J

[39] T.H. Mai, R. Kumar, V. Soni, P. Singh, T. Iqbal, A.S.K. Kumar, V.H. Nguyen, P. Raizada, P. V. Pham, 2D Heterostructures in Photocatalysis for Emerging Applications: Current Status, Challenges, and Prospectives. Journal of Catalysis, 439, (2024) 115744. https://doi.org/10.1016/j.jcat.2024.115744

[40] J. Hao Ran Huang, S.W. Tseng, I.W. Peter Chen, In-Situ Electrochemical XRD and Raman Probing of Ion Transport Dynamics in Ionic Liquid-Etched Ti3C2Tx MXene for Energy Storage Applications. Chemical Engineering Journal, 503, (2025) 158232. https://doi.org/10.1016/j.cej.2024.158232

[41] N. Anjum, M.M. Rahman, A. Elattar, A. Sijuade, E.E. Kalu, O.I. Okoli, High-Yield MILD Synthesis of $Ti_3C_2T_x$ MXene: Characterization and Application in Developing Energy Storage Device. Advanced Sustainable Systems, 9(8), (2025) 2500402. https://doi.org/10.1002/adsu.202500402

[42] L. Dai, H. Yu, Y. Wang, X. Zhang, F. Xu, X. Pan, J.T. Luo, A. Zhong, $Ti_3C_2T_x$ MXene Composite with Much Improved Stability for Superior Humidity Sensors. Langmuir, 41(2), (2025) 1368–1376. https://doi.org/10.1021/acs.langmuir.4c04107

[43] J. Liu, J. Fu, Q. Xia, M. Xia, M. Ji, C. Yang, N.M. Shinde, Tin oxide/MXene nanocomposite for energy storage devices. Dalton Transactions, 54(29), (2025) 11349–11361. https://doi.org/10.1039/D5DT00617A

[44] L. Qin, J. Zhong, J. Li, In Situ Selenization of $Ti_3C_2T_x$ Assisted by Cu^{2+} with Superior Performance for Aluminum Ion Batteries. Energy & Fuels, 37(8), (2023) 6220–6229. https://doi.org/10.1021/acs.energyfuels.3c00323

[45] Y. Bhat, W.A. Adeosun, K. Prenger, Y.A. Samad, K. Liao, M. Naguib, S. Mao, A. Qurashi, Frontiers of MXenes-based Hybrid Materials for Energy Storage and Conversion Applications. Advanced Composites and Hybrid Materials, 8(1), (2025) 52. https://doi.org/10.1007/s42114-024-01121-z

[46] Z. Said, M.A. Sohail, H. Tabassum, I.H. Sajid, H.M. Ali, F. Jamil, Y.K. Mishra, A.K. Pandey, MXenes at the forefront: advances in energy storage and nanofluidic applications, Advanced Composites and Hybrid Materials, 8(4), (2025) 320. https://doi.org/10.1007/s42114-025-01404-z

[47] A. Gentile, N. Pianta, M. Fracchia, S. Pollastri, C. Ferrara, S. Marchionna, G. Aquilanti, S. Tosoni, P. Ghigna, R. Ruffo, $Ti_3C_2T_x$ MXenes as Anodes for Sodium-Ion Batteries: the In Situ Comprehension of the Electrode Reaction. ACS Applied Energy Materials, 8(4), (2025) 2229–2238. https://doi.org/10.1021/acsaem.4c02777

[48] J. Rahmatinejad, Z. Ye, Advanced MoS2 nanocomposites for post-lithium-ion batteries, Chemical Engineering Journal 500 (2024) 156872. https://doi.org/10.1016/j.cej.2024.156872

[49] S. Das, G. Swain, K. Parida, One step towards the 1T/2H-MoS_2 Mixed Phase: a Journey from Synthesis to Application. Materials Chemistry Frontiers, 5(5), (2021) 2143–2172. https://doi.org/10.1039/D0QM00802H

[50] Y. Teng, H. Zhao, Z. Zhang, L. Zhao, Y. Zhang, Z. Li, Q. Xia, Z. Du, K. Świerczek, MoS_2 Nanosheets Vertically Grown on Reduced Graphene Oxide via Oxygen Bonds with Carbon Coating as Ultrafast Sodium Ion Batteries Anodes. Carbon, 119, (2017) 91–100. https://doi.org/10.1016/j.carbon.2017.04.017

[51] I.T. Bello, D. Tsotetsi, B. Shaku, O. Adedokun, D. Chen, M.S. Dhlamini, Advances in MoS2-based nanomaterials for supercapacitors, batteries and photovoltaics applications,

Journal Energy Storage, 103, (2024) 114355. https://doi.org/10.1016/j.est.2024.114355

[52] Y. Huang, Y. Sun, X. Zheng, T. Aoki, B. Pattengale, J. Huang, X. He, W. Bian, S. Younan, N. Williams, J. Hu, J. Ge, N. Pu, X. Yan, X. Pan, L. Zhang, Y. Wei, J. Gu, Atomically Engineering Activation Sites onto Metallic 1T-MoS2 Catalysts for Enhanced Electrochemical Hydrogen Evolution. Nature Communications, 10(1), (2019) 982. https://doi.org/10.1038/s41467-019-08877-9

[53] L. Zhang, G. Zhao, X. Wu, Al/P doped MoS2 with High Conductivity toward High-Performance Asymmetric Supercapacitor, Journal of Alloys and Compounds, 1032, (2025) 181073. https://doi.org/10.1016/j.jallcom.2025.181073

[54] P.C. Kumar, S.M. Jeong, R. Naik, C.S. Rout, Rhombohedral 3R MoS_2 Polytype: A Promising Fundamental Material for Next-Generation Device Applications, Small, 21(41), (2025) e2504644. https://doi.org/10.1002/smll.202504644

[55] S.A. Getaneh, A.G. Temam, G.A. Workneh, A.C. Nwanya, P.M. Ejikeme, F.I. Ezema, Advances in MoS2-Based Ternary Nanocomposites for High-Performance Electrochemical energy storage, Hybrid Advances, 7 (2024) 100333. https://doi.org/10.1016/j.hybadv.2024.100333

[56] Y.-Y. Yeh, W.-H. Chiang, W.-R. Liu, Synthesis of few-layer WS2 by jet cavitation as anode material for lithium ion batteries. Journal of Alloys and Compounds, 775, (2019) 1251–1258. https://doi.org/10.1016/j.jallcom.2018.10.273

[57] M.B. Askari, P. Salarizadeh, P. Veisi, E. Samiei, H. Saeidfirozeh, M.T. Tourchi Moghadam, A. Di Bartolomeo, Transition-Metal Dichalcogenides in Electrochemical Batteries and Solar Cells. Micromachines, 14(3), (2023) 691. https://doi.org/10.3390/mi14030691

[58] H. Jin, S. Xin, C. Chuang, W. Li, H. Wang, J. Zhu, H. Xie, T. Zhang, Y. Wan, Z. Qi, W. Yan, Y.-R. Lu, T.-S. Chan, X. Wu, J.B. Goodenough, H. Ji, X. Duan, Black Phosphorus Composites with Engineered Interfaces for High-Rate High-Capacity Lithium Storage. Science, 370(6513), (2020)192–197. https://doi.org/10.1126/science.aav5842

[59] N. Sultana, A. Degg, S. Upadhyaya, T. Nilges, N. Sen Sarma, Synthesis, modification, and application of black phosphorus, few-layer black phosphorus (FLBP), and phosphorene: a detailed review. Materials Advances, 3(14), (2022) 5557–5574. https://doi.org/10.1039/d1ma01101d 5557–5574

[60] X. Xin, Y. Xu, Q. Liu, Y. Zhu, H. Chen, W. Chen, L. Gao, X. Song, Overcoming Volumetric Capacitance-Rate Performance Tradeoff with 0D/2D Conductive Carbon Nitride/Phosphorene Heterostructure for Flexible Supercapacitor. Chemical Engineering Journal, 499, (2024) 156522. https://doi.org/10.1016/j.cej.2024.156522

[61] O. Yilmaz, H.Y. Kalyon, M. Gencten, Y. Sahin, One Step Production of Phosphorene from Red Phosphorus and Investigation of their Supercapacitor Applications with Conducting Polymers, Journal of Energy Storage,79 (2024) 110133. https://doi.org/10.1016/j.est.2023.110133

[62] X. Wu, Y. Xu, Y. Hu, G. Wu, H. Cheng, Q. Yu, K. Zhang, W. Chen, S. Chen, Microfluidic-Spinning Construction of Black-Phosphorus-Hybrid Microfibres for Non-Woven Fabrics toward a High Energy Density Flexible Supercapacitor, Nature Communications, 9, (2018) 4573. https://doi.org/10.1038/s41467-018-06914-7

[63] J. Mei, T. Liao, Z. Sun, Opportunities and Challenges of Black Phosphorus for Electrocatalysis and Rechargeable Batteries. Advanced Sustainable Systems, 6(12), (2022). https://doi.org/10.1002/adsu.202200301

[64] A. Rabiei Baboukani, I. Khakpour, V. Drozd, C. Wang, Liquid-Based Exfoliation of Black Phosphorus into Phosphorene and Its Application for Energy Storage Devices, Small Structures, 2(5), (2021) 2000148. https://doi.org/10.1002/sstr.202000148

[65] J. Zhu, G. Xiao, X. Zuo, Two-Dimensional Black Phosphorus: An Emerging Anode Material for Lithium-Ion Batteries, Nano-Micro Letters, 12, (2020) 120. https://doi.org/10.1007/s40820-020-00453-x

[66] S.A. Thomas, Layered two-dimensional black phosphorous-based hybrid electrodes for

rechargeable batteries. Journal of Energy Storage, 73, (2023) 109068. https://doi.org/10.1016/j.est.2023.109068

[67] M. Fortunato, A. Sarapulova, B. Schwarz, A.M. Cardinale, S. Dsoke, NiFe-NO$_3$ Layered Double Hydroxide as a Novel Anode for Sodium Ion Batteries. Batteries & Supercaps, 8(3), (2025) e202400451. https://doi.org/10.1002/batt.202400451

[68] W.H. Wang, C.H. Han, W.X. Hong, Y.C. Chiu, I.H. Tseng, Y.H. Chang, H. Pourzolfaghar, Y.Y. Li, NiFe Layered Double Hydroxide (LDH) Anchored, Fe Single Atom and Nanoparticle Embedded on Nitrogen-Doped Carbon-CNT (carbon nanotube) framework as a Bifunctional Catalyst for Rechargeable Zinc-Air Batteries, Journal of Energy Storage 85, (2024) 111058. https://doi.org/10.1016/j.est.2024.111058

[69] Y. Ma, D. Liu, H. Wu, M. Li, S. Ding, A.S. Hall, C. Xiao, Promoting Bifunctional Water Splitting by Modification of the Electronic Structure at the Interface of NiFe Layered Double Hydroxide and Ag, ACS Applied Materials & Interfaces, 13(22), (2021) 26055–26063. https://doi.org/10.1021/acsami.1c05123

[70] H. Cui, S. Jia, T. Du, J. Liu, X. Lin, X. Zhang, F. Yang, p–n-Type LaCoO$_3$ /NiFe LDH Heterostructures for Enhanced Photogenerated Carrier-Assisted Electrocatalytic Oxygen Evolution Reaction, ACS Applied Materials & Interfaces, 16(51), (2024) 70477–70488. https://doi.org/10.1021/acsami.4c13756

[71] Y. Zhou, J. Si, H. Wang, X. Li, S. Zhang, C. Deng, Co$_9$S$_8$ @NiFe-LDH Bifunctional Electrocatalysts as High-Efficiency Cathodes for Zn–Air Batteries, Energy & Fuels, 37(13), (2023) 9619–9625. https://doi.org/10.1021/acs.energyfuels.3c00938

[72] F. Wang, T. Wang, S. Sun, Y. Xu, R. Yu, H. Li, One-step synthesis of nickel iron-layered double hydroxide/reduced graphene oxide/carbon nanofibres composite as electrode materials for asymmetric supercapacitor. Scientific Reports, 8(1), (2018) 8908. https://doi.org/10.1038/s41598-018-27171-0

[73] M. Sreenivasulu, N.K.V. Hiremath, M.A. Alshehri, N.P. Shetti, A green solvent-free approach synthesis for rational designing of a NiFe-layered double hydroxide (NiFe-LDH) electrocatalyst for hydrogen generation. Energy & Fuels, 38(21), (2024) 20791–20806. https://doi.org/10.1021/acs.energyfuels.4c03780

[74] R. Xu, X. Wang, Z. Yang, Y. Chang, X. Chen, J. Wang, H. Li, Electrodeposition fabrication of La-doped NiFe layered double hydroxide to improve conductivity for efficient overall water splitting. ACS Applied Energy Materials, 7(9), (2024)3866–3875. https://doi.org/10.1021/acsaem.4c00246

[75] S. Iqbal, J.C. Ehlers, I. Hussain, K. Zhang, C. Chatzichristodoulou, Trends and industrial prospects of NiFe-layered double hydroxide for the oxygen evolution reaction. Chemical Engineering Journal, 499, (2024) 156219. https://doi.org/10.1016/j.cej.2024.156219

[76] D. Yang, P. Dai, X. Jiang, S.M. Alshehri, T. Ahamad, Y. Bando, X. Wang, Methods for preparation of hexagonal boron nitride nanomaterials. Chemistry of Materials, 36(20), (2024) 10008–10053. https://doi.org/10.1021/acs.chemmater.4c00582

[77] W. Zhang, Y. Liang, D. Yue, Y. Feng, Hexagonal boron nitride nanosheets: Fabrication, thermal properties and application in polymers. High Performance Polymers, 36(4), (2024) 211–229. https://doi.org/10.1177/09540083241238774

[78] C. Ma, Y. Zhang, S. Yan, B. Liu, Carbon-doped boron nitride nanosheets: A high-efficient electrocatalyst for ambient nitrogen reduction. Applied Catalysis B: Environmental, 315, (2022) 121574. https://doi.org/10.1016/j.apcatb.2022.121574

[79] X. Zhang, L. An, C. Bai, L. Chen, Y. Yu, Hexagonal boron nitride quantum dots: Properties, preparation and applications. Materials Today Chemistry, 20, (2021) 100425. https://doi.org/10.1016/j.mtchem.2021.100425

[80] D. Krishnamoorthy, R. Chaudhary, V. Chaudhary, A.K. Singh, Development of cohesive exfoliated h-BN-CuS nanosheets through an ultrasonic approach for hybrid supercapacitors. CrystEngComm, 27(25), (2025) 4389–4403. https://doi.org/10.1039/D5CE00267B

[81] D.P. Rai, B. Chettri, P.K. Patra, S. Sattar, Hydrogen storage in bilayer hexagonal boron nitride: A first-principles study. ACS Omega, 6(45), (2021) 30362–30370. https://doi.org/10.1021/acsomega.1c03443

[82] S. Mishra, B.K. Jena, Review and perspectives on multifunctional applications of hexagonal boron nitride nanosheets and quantum dots in energy conversions. Energy & Fuels, 39(9), (2025) 4119–4150. https://doi.org/10.1021/acs.energyfuels.4c05473

[83] S. Angizi, M.H. Azar, A. Hatamie, A. Simchi, Two-dimensional hexagonal boron nitride (2D h-BN) and its hybrid structures for electrochemical sensing. In: 2D Materials-Based Electrochemical Sensors. Elsevier, (2023) 253–280. https://doi.org/10.1016/B978-0-443-15293-1.00008-2

[84] R.N. Muthu, S. Rajashabala, R. Kannan, Hydrogen storage performance of lithium borohydride decorated activated hexagonal boron nitride nanocomposite for fuel cell applications. International Journal of Hydrogen Energy, 42(23), (2017) 15586–15596. https://doi.org/10.1016/j.ijhydene.2017.04.240

[85] Q. Ji, C. Li, J. Wang, J. Niu, Y. Gong, Z. Zhang, Q. Fang, Y. Zhang, J. Shi, L. Liao, X. Wu, L. Gu, Z. Liu, Y. Zhang, Metallic vanadium disulfide nanosheets as a platform material for multifunctional electrode applications. Nano Letters, 17(8), (2017) 4908–4916. https://doi.org/10.1021/acs.nanolett.7b01914

[86] Sharma, S. Kapse, A. Verma, S. Bisoyi, G.K. Pradhan, R. Thapa, C.S. Rout, All-Solid-State Supercapacitor based on Advanced 2D Vanadium Disulfide/Black Phosphorus Hybrids for Wearable Electronics. ACS Applied Energy Materials, 5(8), (2022) 10315–10327. https://doi.org/10.1021/acsaem.2c02116

[87] A.B. Nandana, R.B. Rakhi, Exploring Vanadium Disulfide (VS_2) Nanosheets as High-Efficiency Supercapacitor Electrodes. Energy Technology, 13(5), (2025) e202402153. https://doi.org/10.1002/ente.202402153

[88] L. Wang, H. Dang, T. He, R. Liu, R. Wang, F. Ran, Dual-Functional and Polydopamine-Coated Vanadium disulfide for Fast-Charging Lithium-Ion Batteries. Battery Energy, 3(4), (2024) e20240001. https://doi.org/10.1002/bte2.20240001

[89] S. Feng, J. Chen, L. Ma, J. Wu, J. Lin, L. Liao, X. Lu, X. Yan, S. Zeng, Y. Xi, Hierarchical nanoarchitecture of vanadium disulfide decorated 3D porous carbon skeleton with improved electrochemical performance toward Li-ion battery and supercapacitor. Ceramics International, 48(14), (2022) 20020–20032. https://doi.org/10.1016/j.ceramint.2022.03.277

[90] M. Liu, Z. Zhao, W. Zhang, W. Zheng, Perspective of Vanadium Disulfide: A Rising Star Finds plenty of room in Single and Multielectron Energy Storage. Energy & Fuels, 36(23), (2022) 13931–13955. https://doi.org/10.1021/acs.energyfuels.2c02642

[91] L. Li, Z. Li, A. Yoshimura, C. Sun, T. Wang, Y. Chen, Z. Chen, A. Littlejohn, Y. Xiang, P. Hundekar, S.F. Bartolucci, J. Shi, S.F. Shi, V. Meunier, G.C. Wang, N. Koratkar, Vanadium disulfide flakes with nanolayered titanium disulfide coating as cathode materials in lithium-ion batteries. Nature Communications, 10(1), (2019) 1764. https://doi.org/10.1038/s41467-019-09400-w

[92] L. Zhuang, J. Zhang, Y. Liu, G. Ma, C. Lin, Y. Wu, X. Lin, MOF-derived NiS_2/V_2O_3 spherical heterostructures for high-performance supercapacitors. Journal of Physics and Chemistry of Solids, 209, (2026) 113237. https://doi.org/10.1016/j.jpcs.2025.113237

[93] S. Chinnasamy, A. Mani, Electrochemical stability and superior capacitance of bismuth cobalt metal-organic framework incorporated with vanadium disulfide nanosheet for supercapacitor application. Journal of Alloys and Compounds, 1002, (2024) 175266. https://doi.org/10.1016/j.jallcom.2024.175266

[94] A. Mandal, A.K. Yadav, S.K. Pandey, S. Chakrabarti, Fabrication of 1T VS_2 electrode-based in-plane micro-supercapacitor using a cost-effective mask-assisted printing technique. Physica Status Solidi A, 220(20), (2023) e202300274. https://doi.org/10.1002/pssa.202300274

[95] P. Naveenkumar, J. Yesuraj, M. Maniyazagan, N. Kang, H.W. Yang, K. Kim, S.J. Kim, Heterostructured SnSe-MnSe@rGO as a

composite electrode for Li-ion batteries and high energy density asymmetric supercapacitors. Chemical Engineering Journal, 488, (2024) 150937. https://doi.org/10.1016/j.cej.2024.150937

[96] J. Zhou, L. Wang, M. Yang, J. Wu, F. Chen, W. Huang, N. Han, H. Ye, F. Zhao, Y. Li, Y. Li, Hierarchical VS_2 nanosheet assemblies: A universal host material for the reversible storage of alkali metal ions. Advanced Materials, 29(35), (2017) 1702061. https://doi.org/10.1002/adma.201702061

[97] J. Barnett, K.G. Wirth, R. Hentrich, Y.C. Durmaz, M.A. Rose, F. Gunkel, T. Taubner, Low temperature near-field fingerprint spectroscopy of 2D electron systems in oxide heterostructures and beyond. Nature Communications, 16(1), (2025) 4417. https://doi.org/10.1038/s41467-025-59633-1

[98] J. Gao, J. Li, Q. Wang, C. Zou, Progress of MXene-based materials in the field of rechargeable batteries. Materials, 18(10), (2025) 2386. https://doi.org/10.3390/ma18102386

[99] L. Li, G. Jiang, C. An, Z. Xie, Y. Wang, L. Jiao, H. Yuan, Hierarchical Ti_3C_2@TiO_2 MXene hybrids with tunable interlayer distance for highly durable lithium-ion batteries. Nanoscale, 12(18), (2020) 10369–10379. https://doi.org/10.1039/D0NR01222J

[100] U. Kalsoom, S. Khan, M. Kashif, H.S. Yaseen, S.A. Hussain, S. Azizi, M. Maaza, MXene-based hybrid composites for lithium-ion batteries: Advances in synthesis strategies and electrochemical performance. Ionics, 31(10), (2025) 10053–10073. https://doi.org/10.1007/s11581-025-06628-z

[101] A. M. Amani, M. Abbasi, A. Najdian, F. Mohamadpour, S. R. Kasaee, H. Kamyab, S. Chelliapan, M. Shafiee, L. Tayebi, A. Vaez, A. Najafian, E. Vafa, S. Mosleh-Shirazi, MXene-based materials for enhanced water quality: Advances in remediation strategies. Ecotoxicology and Environmental Safety, 291, (2025) 117817. https://doi.org/10.1016/j.ecoenv.2025.117817.

[102] H.Y. Zhou, L.W. Lin, Z.Y. Sui, H.Y. Wang, B.H. Han, Holey Ti_3C_2 MXene-derived anode enables boosted kinetics in lithium-ion capacitors. ACS Applied Materials & Interfaces, 15, (2023) 12161–12170. https://doi.org/10.1021/acsami.2c21327.

[103] H. Chen, G. Lu, Z. Cao, Q. Zhu, Y. Ye, Y. Gao, Y. Shi, Q. Zhao, B. Li, Z. Du, X. Tao, S. Yang, MXene-configured graphite towards long-life lithium-ion batteries under extreme conditions. Nature Communications, 16, (2025) 8493. https://doi.org/10.1038/s41467-025-63443-w

[104] J. Zhao, N. Ma, T. Wang, Y. Wang, B. Liang, Y. Zhang, S. Luo, Y. Xiong, Q. Wang, J. Fan, Theoretical insights and design of MXene for aqueous batteries and supercapacitors: Status, challenges, and perspectives. Nanoscale Horizons, 10, (2025) 78–103. https://doi.org/10.1039/D4NH00305E

[105] M.B. Askari, P. Salarizadeh, P. Veisi, E. Samiei, H. Saeidfirozeh, M.T. Tourchi Moghadam, A. Di Bartolomeo, Transition-metal dichalcogenides in electrochemical batteries and solar cells. Micromachines, 14, (2023) 691. https://doi.org/10.3390/mi14030691

[106] P. Chong, Z. Zhou, K. Wang, W. Zhai, Y. Li, J. Wang, M. Wei, The stabilizing of 1T-MoS_2 for all-solid-state lithium-ion batteries. Batteries, 9, (2022) 26. https://doi.org/10.3390/batteries9010026

[107] Z.J. Yang, Y. Wang, M. Chhowalla, Metallic-phase two-dimensional transition-metal dichalcogenides for electrochemical applications. MRS Bulletin, 50, (2025) 1243–1251. https://doi.org/10.1557/s43577-025-00983-y

[108] Y. Zhang, H. Ponnuru, Q. Jiang, H. Shan, H. Maleki Kheimeh Sari, W. Li, J. Wang, J. Hu, J. Peng, X. Li, Toward layered MoS_2 anode for harvesting superior lithium storage. RSC Advances, 12, (2022) 9917–9922. https://doi.org/10.1039/D1RA08255H

[109] A. Roy, S. Dey, G. Singh, MoS_2, WS_2, and $MoWS_2$ flakes as reversible host materials for sodium-ion and potassium-ion batteries. ACS Omega, 9, (2024) 24933–24947. https://doi.org/10.1021/acsomega.4c01966

[110] J. Zhu, G. Xiao, X. Zuo, Two-dimensional black phosphorus: An emerging anode material for lithium-ion batteries. Nano-Micro Letters, 12, (2020) 120. https://doi.org/10.1007/s40820-020-00453-x

[111] L. Liu, X. Gao, X. Cui, B. Wang, F. Hu, T. Yuan, J. Li, L. Zu, H. Lian, X. Cui, Chemical vapor transport synthesis of fibrous red phosphorus crystal as anodes for lithium-ion batteries. Nanomaterials, 13, (2023) 1060. https://doi.org/10.3390/nano13061060

[112] X. Huang, Y. Li, G. Qu, X.F. Yu, D. Cao, Q. Liu, G. Jiang, Molecular-level degradation pathways of black phosphorus revealed by mass spectrometry fingerprinting. Chemical Science, 14, (2023) 6669–6678. https://doi.org/10.1039/D2SC06297F

[113] Z.L. Xu, S. Lin, N. Onofrio, L. Zhou, F. Shi, W. Lu, K. Kang, Q. Zhang, S.P. Lau, Exceptional catalytic effects of black phosphorus quantum dots in shuttling-free lithium sulfur batteries. Nature Communications, 9, (2018) 4164. https://doi.org/10.1038/s41467-018-06629-9

[114] Y. Wei, Z. Chen, X. Guo, H. Xie, Z. Sun, S. Osman, J. Xiao, T. Chen, K.S. Hui, H. Cheng, K.N. Hui, MOF glass confined black phosphorus via Co–P anchoring for advanced lithium-ion battery anodes. Advanced Science, 12, (2025) e202511772. https://doi.org/10.1002/advs.202511772

[115] W. Liang, X. Zhou, B. Zhang, Z. Zhao, X. Song, K. Chen, L. Wang, Z. Ma, J. Liu, The versatile establishment of charge storage in polymer solid electrolyte with enhanced charge transfer for LiF-rich SEI generation in lithium metal batteries. Angewandte Chemie International Edition, 63, (2024) e202320149. https://doi.org/10.1002/anie.202320149

[116] Z.L. Xu, S. Lin, N. Onofrio, L. Zhou, F. Shi, W. Lu, K. Kang, Q. Zhang, S.P. Lau, Exceptional catalytic effects of black phosphorus quantum dots in shuttling-free lithium sulfur batteries. Nature Communications, 9, (2018) 4164. https://doi.org/10.1038/s41467-018-06629-9

[117] Y. Shen, Z. Zhu, Z. Xu, Y. Li, Recent progress in 2D inorganic non-conductive materials for alkali metal-based batteries. Energy Advances, 3, (2024) 1844–1868. https://doi.org/10.1039/D4YA00209A

[118] P. Ma, Z. Zhang, J. Wang, H. Li, H.Y. Yang, Y. Shi, Self-assembled 2D VS_2/Ti_3C_2Tx MXene nanostructures with ultrafast kinetics for superior electrochemical sodium-ion storage. Advanced Science, 10, (2023) e202304465. https://doi.org/10.1002/advs.202304465

[119] L. Tang, L. Zhang, G. Yin, X. Tao, L. Yu, X. Wang, C. Sun, Y. Sun, E. Hong, G. Zhao, G. Zhu, 2D porous Ti_3C_2 MXene as anode material for sodium-ion batteries with excellent reaction kinetics. Molecules, 30, (2025) 1100. https://doi.org/10.3390/molecules30051100

[120] J. Zheng, Y. Wu, Y. Sun, J. Rong, H. Li, L. Niu, Advanced anode materials of potassium ion batteries: From zero dimension to three dimensions. Nano-Micro Letters, 13, (2021) 12. https://doi.org/10.1007/s40820-020-00541-y

[121] S. Kalluri, M. Yoon, M. Jo, S. Park, S. Myeong, J. Kim, S.X. Dou, Z. Guo, J. Cho, Surface engineering strategies of layered $LiCoO_2$ cathode material to realize high-energy and high-voltage Li-ion cells. Advanced Energy Materials, 7, (2017) 1601507. https://doi.org/10.1002/aenm.201601507

[122] X. Wang, L. Bannenberg, Design and characterization of 2D MXene-based electrode with high-rate capability. MRS Bulletin, 46, (2021) 755–766. https://doi.org/10.1557/s43577-021-00150-z

[123] M. Hu, L. Chen, Y. Jing, Y. Zhu, J. Dai, A. Meng, C. Sun, J. Jia, Z. Li, Intensifying electrochemical activity of Ti_3C_2Tx MXene via customized interlayer structure and surface chemistry. Molecules, 28, (2023) 5776. https://doi.org/10.3390/molecules28155776

[124] Y. Shen, Z. Zhu, Z. Xu, Y. Li, Recent progress in 2D inorganic non-conductive materials for alkali metal-based batteries. Energy Advances, 3, (2024) 1844–1868. https://doi.org/10.1039/D4YA00209A

[125] A.K. Bojarajan, S.S. Gunasekaran, S.K. Ravi, A.H. Al-Marzouqi, F.M. Hassan, S. Sangaraju, Advances in two-dimensional materials for supercapacitor applications: From metal carbides to metal borides and beyond. Renewable and Sustainable Energy Reviews, 226, (2026) 116278. https://doi.org/10.1016/j.rser.2025.116278

[126] T. Gao, C.W. Lai, S.M. Rangappa, S. Siengchin, F. Gapsari, Y. Li, I.A. Badruddin, MXene-based materials for supercapacitors: Trends and opportunities. Journal of Materials Science:

Materials in Electronics, 36, (2025) 1877. https://doi.org/10.1007/s10854-025-15850-4

[127] J. Tang, X. Huang, T. Qiu, X. Peng, T. Wu, L. Wang, B. Luo, L. Wang, Interlayer space engineering of MXenes for electrochemical energy storage applications. Chemistry – A European Journal, 27, (2021) 1921–1940. https://doi.org/10.1002/chem.202002283

[128] W. Cheng, J. Fu, H. Hu, D. Ho, Interlayer structure engineering of MXene-based capacitor-type electrode for hybrid micro-supercapacitor toward battery-level energy density. Advanced Science, 8, (2021) 2100775. https://doi.org/10.1002/advs.202100775

[129] M.S. Ali, M.S. Ali, S. Bhandari, S. Saini, S. Karmakar, D. Chattopadhyay, Recent progress on MXene-polymer nanocomposites and their applications. Sustainable Materials and Technologies, 45, (2025) e01563. https://doi.org/10.1016/j.susmat.2025.e01563

[130] S.A. Kadam, K.P. Kadam, N.R. Pradhan, Advancements in 2D MXene-based supercapacitor electrodes: Synthesis, mechanisms, electronic structure engineering, flexible wearable energy storage for real-world applications, and future prospects. Journal of Materials Chemistry A, 12, (2024) 17992–18046. https://doi.org/10.1039/D4TA00328D

[131] X. Xu, L. Yang, W. Zheng, H. Zhang, F. Wu, Z. Tian, P. Zhang, Z. Sun, MXenes with applications in supercapacitors and secondary batteries: A comprehensive review. Materials Reports: Energy, 2, (2022) 100080. https://doi.org/10.1016/j.matre.2022.100080

[132] S.R.K.A. S.R.K.A., K. Pramoda, C.S. Rout, Assembling a high-performance asymmetric supercapacitor based on pseudocapacitive S-doped VSe_2/CNT hybrid and 2D borocarbonitride nanosheets. Journal of Materials Chemistry C, 11, (2023) 2565–2573. https://doi.org/10.1039/D2TC04600H.

[133] T. Yuan, Z. Zhang, Q. Liu, X.T. Liu, Y.N. Miao, C. Yao, MXene (Ti_3C_2Tx)/cellulose nanofiber/polyaniline film as a highly conductive and flexible electrode material for supercapacitors. Carbohydrate Polymers, 304, (2023) 120519. https://doi.org/10.1016/j.carbpol.2022.120519

[134] H.H. Hegazy, J. Khan, N. Shakeel, E.A. Alabdullkarem, M.I. Saleem, H. Alrobei, I.S. Yahia, 2D-based electrode materials for supercapacitors – status, challenges, and prospects. RSC Advances, 14, (2024) 32958–32977. https://doi.org/10.1039/D4RA05473C

[135] A. Inman, T. Hryhorchuk, L. Bi, R. Wang, B. Greenspan, T. Tabb, E.M. Gallo, A. VahidMohammadi, G. Dion, A. Danielescu, Y. Gogotsi, Wearable energy storage with MXene textile supercapacitors for real world use. Journal of Materials Chemistry A, 11, (2023) 3514–3523. https://doi.org/10.1039/D2TA08995E

[136] S. Iravani, R.S. Varma, MXene-based wearable supercapacitors and their transformative impact on healthcare, Materials Advances, 4, (2023) 4317–4332. https://doi.org/10.1039/D3MA00365E

[137] H. Zhu, R. Xu, T. Wan, W. Yuan, K. Shu, N. Boonprakob, C. Zhao, Nanocomposites of conducting polymers and 2D materials for flexible supercapacitors, Polymers, 16, (2024) 756. https://doi.org/10.3390/polym16060756

[138] Z. Yan, S. Luo, Q. Li, Z. Wu, S. Liu, Recent advances in flexible wearable supercapacitors: properties, fabrication, and applications, Advanced Science, 11, (2024) 2302172. https://doi.org/10.1002/advs.202302172

[139] S. Saifi, X. Xiao, S. Cheng, H. Guo, J. Zhang, P. Müller-Buschbaum, G. Zhou, X. Xu, H.-M. Cheng, An ultraflexible energy harvesting-storage system for wearable applications, Nature Communications, 15, (2024) 6546. https://doi.org/10.1038/s41467-024-50894-w

[140] R. Bulathsinghala, W. Ding, R. Dharmasena, Triboelectric nanogenerators for wearable sensing applications: A system level analysis. Nano Energy, 116, (2023) 108792. https://doi.org/10.1016/j.nanoen.2023.108792.

[141] Y.S. Cho, J. Kang, Two-dimensional materials as catalysts, interfaces, and electrodes for an efficient hydrogen evolution reaction, Nanoscale, 16, (2024) 3936–3950. https://doi.org/10.1039/D4NR00147H

[142] S.G. Peera, R. Koutavarapu, L. Chao, L. Singh, G. Murugadoss, G. Rajeshkhanna, 2D MXene nanomaterials as electrocatalysts for hydrogen evolution reaction (HER): a review,

Micromachines, 13, (2022) 1499. https://doi.org/10.3390/mi13091499

[143] S. Bai, M. Yang, J. Jiang, Recent advances of MXenes as electrocatalysts for hydrogen evolution reaction. npj 2D Materials and Applications, 5, (2021) 78. https://doi.org/10.1038/s41699-021-00259-4.

[144] K. Ren, F. Wang, T. Liu, H. Qin, Y. Jing, Wrinkles in 2D TMD heterostructures: unlocking enhanced hydrogen evolution reaction catalysis, Journal of Materials Chemistry A, 13, (2025) 20859–20867. https://doi.org/10.1039/D5TA00681C

[145] S. Wei, Y. Fu, M. Liu, H. Yue, S. Park, Y.H. Lee, H. Li, F. Yao, Dual-phase MoS_2/MXene/CNT ternary nanohybrids for efficient electrocatalytic hydrogen evolution, npj 2D Materials and Applications, 6, (2022) 25. https://doi.org/10.1038/s41699-022-00300-0

[146] Y. Li, Y. Deng, D. Liu, Q. Ji, X. Cai, Two-dimensional oxides for oxygen evolution reactions and related device applications, Materials Chemistry Frontiers, 8, (2024) 880–902. https://doi.org/10.1039/D3QM00848G

[147] X. Lu, H. Xue, H. Gong, M. Bai, D. Tang, R. Ma, T. Sasaki, 2D layered double hydroxide nanosheets and their derivatives toward efficient oxygen evolution reaction, Nano-Micro Letters, 12, (2020) 86. https://doi.org/10.1007/s40820-020-00421-5

[148] B.R. Anne, J. Kundu, M.K. Kabiraz, J. Kim, D. Cho, S. Choi, A review on MXene as promising support materials for oxygen evolution reaction catalysts, Advanced Functional Materials, 33, (2023) 2306100. https://doi.org/10.1002/adfm.202306100

[149] R. Raj, S.K. Paswan, L. Kumar, G.P. Singh, K.K. Haldar, Ti_3C_2Tx nanosheet/$NiFe_2O_4$ nanoparticle composites for electrocatalytic water splitting, ACS Applied Nano Materials, 8, (2025) 1649–1662. https://doi.org/10.1021/acsanm.4c06758

[150] D. Gogoi, R.S. Karmur, M.R. Das, N.N. Ghosh, 2D-Ti_3C_2Tx MXene-supported Cu_2S nanoflakes for supercapacitors and electrocatalytic oxygen evolution reaction, Journal of Materials Chemistry A, 11, (2023) 23867–23880. https://doi.org/10.1039/D3TA05104H

[151] K. Zhang, X. Liang, Y. Wang, Y. Zou, X. Zhao, H. Chen, X. Zou, Support-tuned iridium reconstruction with crystalline phase dominating acidic oxygen evolution, Nature Communications, 16, (2025) 8164. https://doi.org/10.1038/s41467-025-63541-9

[152] J. Liu, J. Mouallem, M. Ghadban, M. Secanell, Determination of anode and cathode overpotentials in AEMFCs using multiple edge-type reference electrodes: Experiments and simulations. International Journal of Hydrogen Energy, 184, (2025) 151887. https://doi.org/10.1016/j.ijhydene.2025.151887

[153] Y. Zhou, L. Sheng, L. Chen, Q. Luo, W. Zhao, W. Zhang, J. Yang, Two-dimensional conductive metal–organic frameworks as efficient electrocatalysts for oxygen evolution and reduction reactions, Inorganic Chemistry Frontiers, 10, (2023) 5044–5052. https://doi.org/10.1039/D3QI01112G

[154] K.N. Khattak, Y. Shao, J. Zhou, Recent development and challenges in TMD-based 2D materials towards OER/ORR electrocatalysis, Reaction Chemistry & Engineering, 11, (2026) 11–41. https://doi.org/10.1039/D5RE00328H

[155] Y. Yang, Y. Yang, Y. Liu, S. Zhao, Z. Tang, Metal–organic frameworks for electrocatalysis: beyond their derivatives, Small Science, 1, (2021) 2100015. https://doi.org/10.1002/smsc.202100015

[156] C. Xu, M. Zhang, X. Yin, Q. Gao, S. Jiang, J. Cheng, X. Kong, B. Liu, H.-Q. Peng, Recent advances in two-dimensional nanomaterials as bifunctional electrocatalysts for full water splitting, Journal of Materials Chemistry A, 11, (2023) 18502–18529. https://doi.org/10.1039/D3TA02293E

[157] M. Shah, U. Abdullah, E. Pervaiz, M. Ali, 2D bifunctional tungsten disulfide-embedded UiO-66 (WS_2@UiO-66) as a highly active electrocatalyst for water splitting, Energy Advances, 3, (2024) 459–470. https://doi.org/10.1039/D3YA00348E

[158] S. Swain, B. Sirichandana, P. Bhol, K.S. Anantharaju, G. Hegde, 2D bifunctional materials: unlocking innovations for efficient water splitting, Sustainable Energy & Fuels, 9, (2025)2870–2899. https://doi.org/10.1039/D5SE00080G

[159] A. Raza, J.Z. Hassan, U. Qumar, A. Zaheer, Z.U.D. Babar, V. Iannotti, A. Cassinese, Strategies for robust electrocatalytic activity of 2D materials: ORR, OER, HER, and CO_2RR, Materials Today Advances, 22, (2024) 100488. https://doi.org/10.1016/j.mtadv.2024.100488

[160] H. Li, Y. Lin, J. Duan, Q. Wen, Y. Liu, T. Zhai, Stability of electrocatalytic OER: from principle to application, Chemical Society Reviews, 53, (2024) 10709–10740. https://doi.org/10.1039/D3CS00010A

[161] J. Zhang, Q. Cao, X. Yu, H. Yao, B. Su, X. Guo, Interface synergistic effect of NiFe-LDH/3D GA composites on efficient electrocatalytic water oxidation, Nanomaterials, 14, (2024) 1661. https://doi.org/10.3390/nano14201661

[162] A. Saeidfar, A.C. Kirlioglu, S.A. Gursel, S. Yesilyurt, Role of catalyst layer composition in the degradation of low platinum-loaded proton exchange membrane fuel cell cathodes: an experimental analysis, Journal of Power Sources, 625, (2025) 235676. https://doi.org/10.1016/j.jpowsour.2024.235676

[163] J. Song, Q. Ye, K. Wang, Z. Guo, M. Dou, Degradation investigation of electrocatalyst in proton exchange membrane fuel cell at a high energy efficiency, Molecules, 26, (2021) 3932. https://doi.org/10.3390/molecules26133932

[164] T. A. Rafei, N. Y. Steiner, E. Pahon, D. Hissel, Toward a representative accelerated stress test for PEMFC stacks in automotive applications. Applied Energy, 401, (2025) 126790. https://doi.org/10.1016/j.apenergy.2025.126790.

[165] G. Dastgeer, M.W. Zulfiqar, S. Nisar, R. Zulfiqar, M. Imran, S. Panchanan, S. Dutta, K. Akbar, A. Vomiero, Z. Wang, Emerging role of 2D materials in photovoltaics: efficiency enhancement and future perspectives, Nano-Micro Letters, 18, (2026) 32. https://doi.org/10.1007/s40820-025-01869-z.

[166] S. A. Elrafei, L. M. Heijnen, R. H. Godiksen, A. G. Curto, Monolayer semiconductor superlattices with high optical absorption. ACS Photonics, 11(7), (2024) 2587–2594. https://doi.org/10.1021/acsphotonics.4c00277.

[167] F. Ren, X. Liu, R. Chen, Z. Jiang, Z. Sun, Q. Zhou, X. Cai, J. Zhou, J. Wang, S. Liu, G. Zheng, W. Liang, Z. Liu, P. A. Troshin, Y. Qi, W. Chen, Crosslinker-stabilized quasi-two-dimensional perovskite for solar modules with certified stability. Joule, 9(2), (2024) 101793. https://doi.org/10.1016/j.joule.2024.11.010.

[168] M. Liang, A. Ali, A. Belaidi, M.I. Hossain, O. Ronan, C. Downing, N. Tabet, S. Sanvito, F. El-Mellouhi, V. Nicolosi, Improving stability of organometallic-halide perovskite solar cells using exfoliated two-dimensional molybdenum chalcogenides, *NPJ 2D Mater. Appl.* 4 (2020) 40. https://doi.org/10.1038/s41699-020-00173-1

[169] M. E. Sonawane, K. P. Gattu, D. A. Tonpe, V. V. Kutwade, I. M. Mohammed, F. M. Khan, P. S. Gajbar, S. F. Shaikh, R. B. Sharma, MoS2 augmentation in CZTS solar cells: Detailed experimental and simulation analysis. Nano-Structures & Nano-Objects, 39, (2024) 101268. https://doi.org/10.1016/j.nanoso.2024.101268.

[170] S.E. Jun, J.K. Lee, H.W. Jang, Two-dimensional materials for photoelectrochemical water splitting, *Energy Adv.* 2 (2023) 34–53. https://doi.org/10.1039/D2YA00231K

[171] A. Yang, J. Blancon, W. Jiang, H. Zhang, J. Wong, E. Yan, Y. Lin, J. Crochet, M. G. Kanatzidis, D. Jariwala, T. Low, A. D. Mohite, H. A. Atwater, Giant enhancement of photoluminescence emission in WS2-two-dimensional perovskite heterostructures. Nano Letters, 19(8), (2019) 4852–4860. https://doi.org/10.1021/acs.nanolett.8b05105.

[172] T. L. Leung, I. Ahmad, A. A. Syed, et al., Stability of 2D and quasi-2D perovskite materials and devices. Communications Materials, 3 (2022) 63. https://doi.org/10.1038/s43246-022-00285-9.

[173] L. Schumacher, R. Marschall, Recent advances in semiconductor heterojunctions and Z-schemes for photocatalytic hydrogen generation. Topics in Current Chemistry, 380(6), (2022) 53. https://doi.org/10.1007/s41061-022-00406-5

[174] X. Huang, Z. Cui, X. Shu, H. Dong, Y. Weng, Y. Wang, Z. Yang, First-principles study on the electronic properties of GeC/BSe van der Waals heterostructure: a direct Z-scheme photocatalyst for overall water splitting. Physical Review Materials, 6(3), (2022) 034010.

https://doi.org/10.1103/PhysRevMaterials.6.034010

[175] Y. Wang, Z. Ding, N. Arif, W.-C. Jiang, Y.-J. Zeng, 2D material-based heterostructures for solar light driven photocatalytic H_2 production. Materials Advances, 3(8), (2022) 3389–3417. https://doi.org/10.1039/D2MA00191H

[176] Y. Li, J. Wang, 2D/2D Z-scheme WO_3/g-C_3N_4 heterojunctions for photocatalytic organic pollutant degradation and nitrogen fixation. Materials Advances, 5(2), (2024) 749–761. https://doi.org/10.1039/D3MA00915G

[177] H. Fang, C. Battaglia, C. Carraro, S. Nemsak, B. Ozdol, J.S. Kang, H.A. Bechtel, S.B. Desai, F. Kronast, A.A. Unal, G. Conti, C. Conlon, G.K. Palsson, M.C. Martin, A.M. Minor, C.S. Fadley, E. Yablonovitch, R. Maboudian, A. Javey, Strong interlayer coupling in van der Waals heterostructures built from single-layer chalcogenides. Proceedings of the National Academy of Sciences of the United States of America, 111(17), (2014) 6198–6202. https://doi.org/10.1073/pnas.1405435111

[178] S.E. Jun, J.K. Lee, H.W. Jang, Two-dimensional materials for photoelectrochemical water splitting. Energy Advances, 2(1), (2023) 34–53. https://doi.org/10.1039/D2YA00231K

[179] J. Ke, F. He, H. Wu, S. Lyu, J. Liu, B. Yang, Z. Li, Q. Zhang, J. Chen, L. Lei, Y. Hou, K. Ostrikov, Nanocarbon-enhanced 2D photoelectrodes: a new paradigm in photoelectrochemical water splitting. Nano-Micro Letters, 13(1), (2021) 24. https://doi.org/10.1007/s40820-020-00545-8

[180] R.K. Ye, S.S. Sun, L.Q. He, S.R. Yang, X.Q. Liu, M.D. Li, P.P. Fang, J.Q. Hu, Surface engineering of hematite nanorods by 2D Ti_3C_2 MXene: suppressing electron–hole recombination for enhanced photoelectrochemical performance. Applied Catalysis B: Environmental, 291, (2021) 120107. https://doi.org/10.1016/j.apcatb.2021.120107

[181] K.R. Wijaya, L.J. Diguna, A. Tsalsabila, I.J. Budiarso, H. Judawisastra, A. Arramel, F.A.A. Nugroho, M.D. Birowosuto, A. Wibowo, 2D transition metal dichalcogenides for photovoltaics, hydrogen production, and CO_2 photoreduction. RSC Sustainability, 3(11), (2025) 4887–4910. https://doi.org/10.1039/D5SU00494B

[182] Z. Huang, J. Wu, C. Yang, F. Yan, G. Yuan, Surfactant-free 2D/2D Pd/g-C_3N_4 for enhanced photocatalytic CO_2 reduction. Catalysis Science & Technology, 14(3), (2024) 615–623. https://doi.org/10.1039/D3CY01623D

[183] F. Zhao, Y. Feng, Y. Wang, X. Zhang, X. Liang, Z. Li, F. Zhang, T. Wang, J. Gong, W. Feng, Two-dimensional gersiloxenes with tunable bandgap for photocatalytic H_2 evolution and CO_2 photoreduction to CO. Nature Communications, 11(1), (2020) 1443. https://doi.org/10.1038/s41467-020-15262-4

[184] Y. Ruan, Z.H. He, Z.T. Liu, W. Wang, L. Hao, L. Xu, A.W. Robertson, Z. Sun, Emerging two-dimensional materials for electrocatalytic nitrogen reduction reaction to yield ammonia. Journal of Materials Chemistry A, 11(42), (2023) 22590–22607. https://doi.org/10.1039/D3TA04848A

[185] M. Xu, Y. Ji, Y. Qin, H. Dong, Y. Li, A universal descriptor for two-dimensional carbon nitride-based single-atom electrocatalysts toward nitrogen reduction reaction. Journal of Materials Chemistry A, 12(41), (2024) 28046–28055. https://doi.org/10.1039/D4TA05067C

[186] R. Mehmood, Z. Ahmad, M.B. Hussain, M. Athar, G. Akbar, Z. Ajmal, S. Iqbal, R. Razaq, M.A. Ali, A. Qayum, A.N. Chishti, F. uz Zaman, R. Shah, S. Zaman, Adnan, 2D–2D heterostructure g-C_3N_4-based materials for photocatalytic H_2 evolution: progress and perspectives. Frontiers in Chemistry, 10, (2022) 1063288. https://doi.org/10.3389/fchem.2022.1063288

[187] K. Zhu, X. Luan, K. Matras-Postolek, P. Yang, 2D/2D MoS_2/g-C_3N_4 layered heterojunctions with enhanced interfacial electron coupling effect. Journal of Electroanalytical Chemistry, 893, (2021) 115350. https://doi.org/10.1016/j.jelechem.2021.115350

[188] K. Niu, L. Chi, J. Rosen, J. Björk, Termination-accelerated electrochemical nitrogen fixation on single-atom catalysts supported by MXenes. Journal of Physical Chemistry Letters, 13(12), (2022) 2800–2807. https://doi.org/10.1021/acs.jpclett.2c00195

[189] P. Baskaran, M. Rajasekar, Recent trends and future perspectives of thermoelectric materials and their applications. RSC Advances, 14(30), (2024) 21706–21744. https://doi.org/10.1039/D4RA03625E

[190] K. Manibalan, M.-Y. Ho, Y.-C. Du, H.-W. Chen, H.-J. Wu, Enhanced room-temperature thermoelectric performance of 2D-SnSe alloys via electric-current-assisted sintering. Materials, 16(2), (2023) 509. https://doi.org/10.3390/ma16020509

[191] M.H. Kalantari, X. Zhang, Thermal transport in 2D materials. Nanomaterials, 13(1), (2023) 117. https://doi.org/10.3390/nano13010117

[192] V.C.S. Theja, V. Karthikeyan, D.S. Assi, H. Huang, V. Kannan, Y. Chen, C. Shek, V.A.L. Roy, 2D MXene Interface Engineered Bismuth Telluride Thermoelectric module with Improved Efficiency for Waste Heat Recovery. Advanced Materials Technologies, 9(21), (2024) 2301722. https://doi.org/10.1002/admt.202301722

[193] K. Li, J. Wang, H. Wang, Recent advances of 2D conductive metal–organic frameworks in thermoelectrics. Journal of Materials Chemistry A, 12(24), (2024) 14245–14267. https://doi.org/10.1039/D4TA01820F

[194] B. Lee, H. Cho, K.T. Park, J.-S. Kim, M. Park, H. Kim, Y. Hong, S. Chung, High-performance Compliant Thermoelectric Generators with Magnetically Self-Assembled Soft Heat Conductors for Self-Powered Wearable Electronics. Nature Communications, 11(1), (2020) 5948. https://doi.org/10.1038/s41467-020-19756-z

[195] A.A. Nikitina, F.V. Lavrentev, V.Yu. Yurova, D.Yu. Piarnits, O.O. Volkova, E.V. Skorb, D.G. Shchukin, Layered nanomaterials for renewable energy generation and storage. Materials Advances, 5(2), (2024) 394–408. https://doi.org/10.1039/D3MA00924F

[196] D. Jiang, Z. Liu, Z. Xiao, Z. Qian, Y. Sun, Z. Zeng, R. Wang, Flexible electronics based on 2D transition metal dichalcogenides. Journal of Materials Chemistry A, 10(1), (2022) 89–121. https://doi.org/10.1039/D1TA06741A

[197] J. Hu, M. Dong, Recent advances in two-dimensional nanomaterials for sustainable wearable electronic devices. Journal of Nanobiotechnology, 22(1), (2024) 63. https://doi.org/10.1186/s12951-023-02274-7

[198] D. Akinwande, N. Petrone, J. Hone, Two-Dimensional Flexible Nanoelectronics. Nature Communications, 5(1), (2014) 5678. https://doi.org/10.1038/ncomms6678

[199] W. Sohn, M. Kim, H.W. Jang, Atomic-scale insights into 2D materials from aberration-corrected scanning transmission electron microscopy: progress and future. Small Science, 4(2), (2024) 2300073. https://doi.org/10.1002/smsc.202300073

[200] O.O. Barah, M. David, M. Joseph, Atomic-scale characterization: a review of advances in microscopy, spectroscopy, and machine learning. Journal of Materials Science: Composites, 6(1), (2025) 6. https://doi.org/10.1186/s42252-025-00073-x

[201] M. Barawi, C.A. Mesa, L. Collado, I.J. Villar-García, F. Oropeza, V.A. de la Peña O'Shea, M. García-Tecedor, Latest advances in in situ and operando X-ray-based techniques for the characterisation of photoelectrocatalytic systems. Journal of Materials Chemistry A, 12(35), (2024) 23125–23146. https://doi.org/10.1039/D4TA03068K

[202] Z. Xue, W. Zeng, K. Zhou, C. Shen, Z. Yang, J. Zhu, S. Wang, Probing two-dimensional materials by advanced atomic force microscopy. Chinese Science Bulletin, 68(31), (2023) 4152–4169. https://doi.org/10.1360/TB-2023-0354

[203] J. Zhao, J. Lian, Z. Zhao, X. Wang, J. Zhang, A review of in situ techniques for probing active sites and mechanisms of electrocatalytic oxygen reduction reactions. Nano-Micro Letters, 15(19), (2023). https://doi.org/10.1007/s40820-022-00984-5

[204] H. Jiang, J. Chen, X. Li, Z. Jin, T. Chen, J. Liu, D. Li, A comprehensive review of in situ measurement techniques for evaluating electro-chemo-mechanical behaviors of battery electrodes. Molecules, 29(8), (2024) 1873. https://doi.org/10.3390/molecules29081873

[205] M. Matsui, Y. Orikasa, T. Uchiyama, N. Nishi, Y. Miyahara, M. Otoyama, T. Tsuda, Electrochemical in situ/operando spectroscopy and microscopy Part 2: battery applications. Electrochemistry, 90(10), (2022) 22–66109.

https://doi.org/10.5796/electrochemistry.22-66109

[206] D. Mastrippolito, M. Cavallo, D. Borowski, E. Bossavit, C. Gureghian, A. Colle, T. Gemo, A. Khalili, H. Zhang, A. Ram, E. Dandeu, S. Ithurria, J. Biscaras, P. Dudin, J.-F. Dayen, J. Avila, E. Lhuillier, D. Pierucci, Operando photoemission imaging of the energy landscape from a 2D material-based field-effect transistor. ACS Nano, 19(9), (2025) 9241–9249. https://doi.org/10.1021/acsnano.5c00256

[207] B.M. Abraham, P. Sinha, P. Halder, J.K. Singh, Fusing a machine learning strategy with density functional theory to hasten the discovery of 2D MXene-based catalysts for hydrogen generation. Journal of Materials Chemistry A, 11, (2023) 8091–8100. https://doi.org/10.1039/D3TA00344B

[208] K. Choudhary, K.F. Garrity, S.T. Hartman, G. Pilania, F. Tavazza, Efficient computational design of two-dimensional van der Waals heterostructures: band alignment, lattice mismatch, and machine learning. Physical Review Materials, 7(1), (2023) 014009. https://doi.org/10.1103/PhysRevMaterials.7.014009

[209] X. Meng, C. Qin, X. Liang, G. Zhang, R. Chen, J. Hu, Z. Yang, J. Huo, L. Xiao, S. Jia, Deep learning in two-dimensional materials: characterization, prediction, and design. Frontiers of Physics, 19(5), (2024) 53601. https://doi.org/10.1007/s11467-024-1394-7

[210] Galashev, Computational modeling of doped 2D anode materials for lithium-ion batteries. Materials, 16(2), (2023) 704. https://doi.org/10.3390/ma16020704

[211] H. Sibi, J. Biju, C. Chowdhury, Advancing 2D material predictions: superior work function estimation with atomistic line graph neural networks. RSC Advances, 14(51), (2024) 38070–38078. https://doi.org/10.1039/D4RA07703B

[212] S. Yang, W. Choi, B.W. Cho, F.O. Agyapong-Fordjour, S. Park, S.J. Yun, H. Kim, Y. Han, Y.H. Lee, K.K. Kim, Y. Kim, Deep learning-assisted quantification of atomic dopants and defects in 2D materials. Advanced Science, 8(16), (2021) 2101099. https://doi.org/10.1002/advs.202101099

[213] K.R. Abidi, P. Koskinen, Optimizing density-functional simulations for two-dimensional metals. Physical Review Materials, 6(12), (2022) 124004. https://doi.org/10.1103/PhysRevMaterials.6.124004

[214] J. K. Abifarin, Y. Lu, Statistics in enabling 2D materials: Optimization, predictive modelling, and data-driven discovery. Materials Today Physics, 57 (2025) 101814. https://doi.org/10.1016/j.mtphys.2025.101814.

[215] L. Liu, W. An, F. Gu, L. Cui, X. He, M. Fan, 2D layered materials: structures, synthesis, and electrocatalytic applications. Green Chemistry, 25, (2023) 6149–6169. https://doi.org/10.1039/D3GC01822A

[216] W. Bao, H. Shen, G. Zeng, Y. Zhang, Y. Wang, D. Cui, J. Xia, K. Jing, H. Liu, C. Guo, F. Yu, K. Sun, J. Li, Engineering the next generation of MXenes: challenges and strategies for scalable production and enhanced performance. Nanoscale, 17(11), (2025) 6204–6265. https://doi.org/10.1039/D4NR04560B

[217] Z. Liu, X. Gong, J. Cheng, L. Shao, C. Wang, J. Jiang, R. Cheng, J. He, Wafer-scale synthesis of two-dimensional materials for integrated electronics. Chip, 3(1), (2024) 100080. https://doi.org/10.1016/j.chip.2023.100080

[218] T. Hossain, Md.R. Repon, Md.A. Shahid, A. Ali, T. Islam, Progress, prospects and challenges of MXene-integrated optoelectronic devices. ChemElectroChem, 11(8), (2024) e202400008. https://doi.org/10.1002/celc.202400008

[219] V. Shukla, A. Stone, M. McGrath, A. Kane, R. Hurt, Chemical degradation kinetics for two-dimensional materials in natural and biological environments: a data-driven review. Environmental Science: Nano, 9(7), (2022) 2297–2319. https://doi.org/10.1039/D1EN01171E

[220] Lee, M. Shekhirev, M. Anayee, Y. Gogotsi, Multi-year study of environmental stability of $Ti_3C_2T_x$ MXene films. Graphene and 2D Materials, 9(1), (2024) 77–85. https://doi.org/10.1007/s41127-024-00076-8

[221] F. Liu, J. Zhou, Y. Wang, Y. Xiong, F. Hao, Y. Ma, P. Lu, J. Wang, J. Yin, G. Wang, J. Yu, Y. Yan, Z. Zhu, J. Zeng, Z. Fan, Rational engineering of 2D materials as advanced

catalyst cathodes for high-performance metal–carbon dioxide batteries. Small Structures, 4(9), (2023) 202300025. https://doi.org/10.1002/sstr.202300025

[222] S. He, G. Xu, Z. Yan, H. Hu, X. Li, K. Huang, G. Wang, L. Yang, J. Huang, Z. Ren, D. Cui, B. Xu, Y. Wang, S. Dou, Y. Liang, W. Lai, Adaptive stress response in 2D graphene@Se composite toward ultra-stable all-solid-state lithium-selenium batteries. Advanced Materials, 37(38), (2025) e2507782. https://doi.org/10.1002/adma.202507782.

[223] X. Shen, X. Lin, Y. Peng, Y. Zhang, F. Long, Q. Han, Y. Wang, L. Han, Two-dimensional materials for highly efficient and stable perovskite solar cells. Nano-Micro Letters, 16(201), (2024) 201. https://doi.org/10.1007/s40820-024-01417-1

[224] L. Tao, Y. Zhao, Y. Deng, Editorial: Interface engineering in two-dimensional material based electronic and optoelectronic devices. Frontiers in Materials, 10, (2023) 1305802. https://doi.org/10.3389/fmats.2023.1305802

[225] L. Qiu, G. Si, X. Bao, J. Liu, M. Guan, Y. Wu, X. Qi, G. Xing, Z. Dai, Q. Bao, G. Li, Interfacial engineering of halide perovskites and two-dimensional materials. Chemical Society Reviews, 52, (2023) 212–247. https://doi.org/10.1039/D2CS00218C

[226] J. Datta, D. Datta, Electro-chemo-mechanical properties of 2D materials for energy storage: computational frontiers. Journal of the Indian Institute of Science, (2025). https://doi.org/10.1007/s41745-025-00485-5

[227] Y. Oh, S. Song, J. Bae, A review of bandgap engineering and prediction in 2D material heterostructures: a DFT perspective. International Journal of Molecular Sciences, 25(23), (2024) 13104. https://doi.org/10.3390/ijms252313104

[228] S. Mohammed, L. Budach, M. Feuerpfeil, N. Ihde, A. Nathansen, N. Noack, H. Patzlaff, F. Naumann, H. Harmouch, The effects of data quality on machine learning performance on tabular data. Information Systems, 132, (2025) 102549. https://doi.org/10.1016/j.is.2025.102549.

[229] T. Hickel, A. Waske, A. Tehranchi, B. Bhattacharya, T. M. Stawski, T. Fellinger, A. Mehmood, J. Witt, O. Ozcan, A. G. Buzanich, S. Kumar, R. K. Mishra, M. Holzer, A. S. S. De Camargo, L. A. Jácome, A. Manzoni, A. Fantin, E. John, V. Hodoroaba, et al., Chemically complex materials enable sustainable high-performance materials. Current Opinion in Solid State and Materials Science, 42, (2026) 101256. https://doi.org/10.1016/j.cossms.2026.101256.

[230] U. Celano, D. Schmidt, C. Beitia, G. Orji, A.V. Davydov, Y. Obeng, Metrology for 2D materials: a perspective review from the international roadmap for devices and systems. Nanoscale Advances, 6, (2024) 2260–2269. https://doi.org/10.1039/D3NA01148H

[231] M. Lanza, Q. Smets, C. Huyghebaert, L.-J. Li, Yield, variability, reliability, and stability of two-dimensional materials based solid-state electronic devices. Nature Communications, 11(5689), (2020). https://doi.org/10.1038/s41467-020-19053-9

[232] D. Lutomia, R. Poria, D. Kala, P. Garg, R. Nagraik, A. Kaushal, S. Gupta, D. Kumar, 2D nanomaterials in biosensing: synthesis, characterization, integration in biosensors and their applications. Biosensors and Bioelectronics X, 24, (2025) 100615. https://doi.org/10.1016/j.biosx.2025.100615

[233] G. Tom, S. P. Schmid, S. G. Baird, Y. Cao, K. Darvish, H. Hao, S. Lo, S. Pablo-García, E. M. Rajaonson, M. Skreta, N. Yoshikawa, S. Corapi, G. D. Akkoc, F. Strieth-Kalthoff, M. Seifrid, A. Aspuru-Guzik, Self-driving laboratories for chemistry and materials science. Chemical Reviews, 124(16), (2024) 9633–9732. https://doi.org/10.1021/acs.chemrev.4c00055.

[234] Md.M. Uddin, M.H. Kabir, Md.A. Ali, Md.M. Hossain, M.U. Khandaker, S. Mandal, A. Arifutzzaman, D. Jana, Graphene-like emerging 2D materials: recent progress, challenges and future outlook. RSC Advances, 13(47), (2023) 33336–33375. https://doi.org/10.1039/D3RA04456D

[235] R.K. Mishra, J. Sarkar, I. Chianella, S. Goel, H.Y. Nezhad, Black phosphorus: the rise of phosphorene in 2D materials applications. Next Materials, 4, (2024) 100217. https://doi.org/10.1016/j.nxmate.2024.100217

[236] Q. Li, W. Zhou, X. Wan, J. Zhou, Strain effects on monolayer $MoSi_2N_4$: Ideal strength and failure mechanism. Physica E: Low-Dimensional Systems and Nanostructures, 131, (2021) 114753. https://doi.org/10.1016/j.physe.2021.114753

[237] F.R. Fan, R. Wang, H. Zhang, W. Wu, Emerging beyond-graphene elemental 2D materials for energy and catalysis applications. Chemical Society Reviews, 50(19), (2021) 10983–11031. https://doi.org/10.1039/C9CS00821G

[238] B. Ryu, L. Wang, H. Pu, M.K.Y. Chan, J. Chen, Understanding, discovery, and synthesis of 2D materials enabled by machine learning. Chemical Society Reviews, 51(6), (2022) 1899–1925. https://doi.org/10.1039/D1CS00503K

[239] V. Venturi, H.L. Parks, Z. Ahmad, V. Viswanathan, Machine learning enabled discovery of application dependent design principles for two-dimensional materials. Machine Learning: Science and Technology, 1(3), (2020) 035015. https://doi.org/10.1088/2632-2153/aba002

[240] Y. Song, E.M.D. Siriwardane, Y. Zhao, J. Hu, Computational discovery of new 2D materials using deep learning generative models. ACS Applied Materials & Interfaces, 13(45), (2021) 53303–53313. https://doi.org/10.1021/acsami.1c01044

[241] W. Xia, L. Tang, H. Sun, C. Zhang, K.-M. Ho, G. Viswanathan, K. Kovnir, C.-Z. Wang, Accelerating materials discovery using integrated deep machine learning approaches. Journal of Materials Chemistry A, 11(47), (2023) 25973–25982. https://doi.org/10.1039/D3TA03771A

[242] N. Han, B.-L. Su, AI-driven material discovery for energy, catalysis and sustainability. National Science Review, 12(5), (2025) nwaf110. https://doi.org/10.1093/nsr/nwaf110

[243] P. Gupta, B. Ding, C. Guan, D. Ding, Generative AI: A systematic review using topic modelling techniques. Data and Information Management, 8(2), (2024) 100066. https://doi.org/10.1016/j.dim.2024.100066

[244] Z. U. D. Babar, V. Iannotti, G. Rosati, A. Zaheer, R. Velotta, B. Della Ventura, R. Álvarez-Diduk, A. Merkoçi, MXenes in healthcare: Synthesis, fundamentals and applications. Chemical Society Reviews, 54(7), (2025) 3387–3440. https://doi.org/10.1039/d3cs01024d.

[245] Pandey, Shreya, P. Phogat, MXene as high-performance 2D materials for next-generation photovoltaic cells. Sustainable Materials and Technologies, 45, (2025) e01530. https://doi.org/10.1016/j.susmat.2025.e01530

[246] S. Thomas, An industry view on two-dimensional materials in electronics. Nature Electronics, 4(12), (2021) 856–857. https://doi.org/10.1038/s41928-021-00690-x

[247] X. Shen, X. Lin, Y. Peng, Y. Zhang, F. Long, Q. Han, Y. Wang, L. Han, Two-dimensional materials for highly efficient and stable perovskite solar cells. Nano-Micro Letters, 16(201), (2024). https://doi.org/10.1007/s40820-024-01417-1

[248] J. K. Abifarin, J. F. Torres, Y. Lu, 2D materials for enabling hydrogen as an energy vector. Nano Energy, 129, (2024) 109997. https://doi.org/10.1016/j.nanoen.2024.109997

[249] H. Singh, H. A. Budiarto, B. Singh, K. Kumar, R. Gupta, A. Bhowmik, A. J. Santhosh, Graphene for next-generation technologies: advances in properties, applications, and industrial integration. Results in Engineering, 27, (2025) 106865. https://doi.org/10.1016/j.rineng.2025.106865.

[250] J. Xu, T. Liu, X. Dong, X. Dong, W. Zhou, X. Li, D. Chao, Z. Zhou, R. Zhao, Challenges and opportunities in 2D materials for high-performance aqueous ammonium ion batteries. National Science Review, 12(2), (2025) nwae433. https://doi.org/10.1093/nsr/nwae433

[251] U. Celano, D. Schmidt, C. Beitia, G. Orji, A.V. Davydov, Y. Obeng, Metrology for 2D materials: A perspective review from the international roadmap for devices and systems. Nanoscale Advances, 6, (2024) 2260–2269. https://doi.org/10.1039/D3NA01148H

[252] M. Mim, K. Habib, S.N. Farabi, S.A. Ali, M.A. Zaed, M. Younas, S. Rahman, MXene: A roadmap to sustainable energy management, synthesis routes, stabilization, and economic assessment. ACS Omega, 9(30), (2024) 4c04849. https://doi.org/10.1021/acsomega.4c04849

[253] I. Hussain, F. Bibi, S. Pandiyarajan, A. Hanan, H.-C. Chuang, K. Zhang, Partially oxidized

MXenes for energy storage applications. Progress in Materials Science, 147, (2025) 101351. https://doi.org/10.1016/j.pmatsci.2024.101351

[254] A.M. Abraham, S.C. George, A review of MXene's retroactive development in energy storage applications. ChemPlusChem, 10(30), (2025) 202502846. https://doi.org/10.1002/slct.202502846

[255] Z. Said, M.A. Sohail, H. Tabassum, I.H. Sajid, H.M. Ali, F. Jamil, Y.K. Mishra, A.K. Pandey, MXenes at the forefront: Advances in energy storage and nanofluidic applications. Advanced Composites and Hybrid Materials, 8(320), (2025) 320. https://doi.org/10.1007/s42114-025-01404-z

[256] M. Gu, A.M. Rao, J. Zhou, B. Lu, Molecular modulation strategies for two-dimensional transition metal dichalcogenide-based high-performance electrodes for metal-ion batteries. Chemical Science, 15, (2024) 2323–2350. https://doi.org/10.1039/D3SC05768B

[257] J. Edgington, L.C. Seitz, Advancing the rigor and reproducibility of electrocatalyst stability benchmarking and intrinsic material degradation analysis for water oxidation. ACS Catalysis, 13(5), (2023) 3379–3394. https://doi.org/10.1021/acscatal.2c06282

[258] G. Abellán, S. Wild, V. Lloret, N. Scheuschner, R. Gillen, U. Mundloch, J. Maultzsch, M. Varela, F. Hauke, A. Hirsch, Fundamental insights into the degradation and stabilization of thin layer black phosphorus. Journal of the American Chemical Society, 139(30), (2017) 10432–10440. https://doi.org/10.1021/jacs.7b04971

[259] H. Zhang, C. Shan, K. Wu, M. Pang, Z. Kong, J. Ye, W. Li, L. Yu, Z. Wang, Y.L. Pak, J. An, X. Gao, J. Song, Modification strategies and prospects for enhancing the stability of black phosphorus. ChemPlusChem, 90(1), (2025) 202400552. https://doi.org/10.1002/cplu.202400552

[260] H. Li, Y. Lin, J. Duan, Q. Wen, Y. Liu, T. Zhai, Stability of electrocatalytic OER: From principle to application. Chemical Society Reviews, 53(21), (2024) 10709–10740. https://doi.org/10.1039/D3CS00010A

[261] D.T. Tran, P.K.L. Tran, D. Malhotra, T.H. Nguyen, T.T.A. Nguyen, N.T.A. Duong, N.H. Kim, J.H. Lee, Current status of developed electrocatalysts for water splitting technologies: From experimental to industrial perspective. Nano Convergence, 12(9), (2025). https://doi.org/10.1186/s40580-024-00468-9

[262] S.C. Cho, J.H. Seok, H.N. Manh, J.H. Seol, C.H. Lee, S.U. Lee, Expanding the frontiers of electrocatalysis: Advanced theoretical methods for water splitting. Nano Convergence, 12(4), (2025). https://doi.org/10.1186/s40580-024-00467-w

[263] K. Wan, Y. Li, Y. Wang, G. Wei, Recent Advance in the Fabrication of 2D and 3D Metal Carbides-based Nanomaterials for Energy and environmental applications. Nanomaterials, 11(1), (2021) 246. https://doi.org/10.3390/nano11010246

[264] M. Houssa, K. Iordanidou, A. Dabral, A. Lu, G. Pourtois, V. Afanasiev, A. Stesmans, Contact Resistance at MoS_2-based 2D metal/semiconductor lateral heterojunctions. ACS Applied Nano Materials, 2(2), (2019) 760–766. https://doi.org/10.1021/acsanm.8b01963

[265] E. Talaie, P. Bonnick, X. Sun, Q. Pang, X. Liang, L.F. Nazar, Methods and protocols for electrochemical energy storage materials research. Chemistry of Materials, 29(1), (2017) 90–105. https://doi.org/10.1021/acs.chemmater.6b02726

[266] V. Hoang Huy, Y. Ahn, J. Hur, Recent advances in transition metal dichalcogenide cathode materials for aqueous rechargeable multivalent metal-ion batteries. Nanomaterials, 11(6), (2021) 1517. https://doi.org/10.3390/nano11061517

[267] H. Yuan, J. Hua, W. Wei, M. Zhang, Y. Hao, J. Chang, Progress and prospect of flexible MXene-based energy storage. Carbon Energy, 7(1), (2025) 639. https://doi.org/10.1002/cey2.639

[268] J.-M. Chen, H.-L. Zhang, X. Peng, X. Shao, Y.F. Chai, M. Ma, Z.L. Li, S.-D. Liu, B. Ding, Heterostructure engineering of transition metal dichalcogenides for high-performance supercapacitors. Rare Metals, 44, (2025) 8198–8236. https://doi.org/10.1007/s12598-025-03484-8

[269] G. Zhang, Z. Gao, C. Zhu, F. Cui, Z. Jiang, R. Pan, J. Shen, L. Zhu, B. Jiang, L. Sun, K. Yin, Multifunctional flexible self-supporting film electrode for wearable energy-storage sensing system. Chemical Engineering Journal, 502, (2024) 157929. https://doi.org/10.1016/j.cej.2024.157929

[270] R. Yang, Y. Fan, Y. Zhang, L. Mei, R. Zhu, J. Qin, J. Hu, Z. Chen, Y.H. Ng, D. Voiry, S. Li, Q. Lu, Q. Wang, J.C. Yu, Z. Zeng, 2D transition metal dichalcogenides for photocatalysis. Angewandte Chemie International Edition, 62(13), (2023) e202218016. https://doi.org/10.1002/anie.202218016

[271] L. Chen, J. Chen, W. Fu, J. Chen, D. Wang, Y. Xiao, S. Xi, Y. Ji, L. Wang, Energy-efficient CO_2 conversion to multicarbon products at high rates on CuGa bimetallic catalyst. Nature Communications, 15(7053), (2024). https://doi.org/10.1038/s41467-024-51466-8

[272] F. Garnes-Portoles, V. Lloret, J.A. Vidal-Moya, M. Loffler, K.J.J. Mayrhofer, J.P. Ceron-Carrasco, G. Abellan, A. Leyva-Perez, Few-layer black phosphorus enables nitrogen fixation under ambient conditions. RSC Advances, 14, (2024) 4742–4747. https://doi.org/10.1039/D3RA07331A

[273] K.S. Kim, Machine learning for accelerating energy materials discovery: Bridging quantum accuracy with computational efficiency. Advanced Energy Materials, 16(2), (2026) 202503356. https://doi.org/10.1002/aenm.202503356

[274] K. Deshsorn, P. Chavalekvirat, S. Deepaisarn, H.-C. Chuang, P. Iamprasertkun, Historical data mining deep dive into machine learning-aided 2D materials research in electrochemical applications. ACS Materials Au, 6(1), (2026) 28–56. https://doi.org/10.1021/acsmaterialsau.5c00030

[275] B. Mortazavi, Recent advances in machine learning-assisted multiscale design of energy materials. Advanced Energy Materials, 15(9), (2025) 202403876. https://doi.org/10.1002/aenm.202403876

[276] Z. Yao, Y. Lum, A. Johnston, L.M. Mejia-Mendoza, X. Zhou, Y. Wen, A. Aspuru-Guzik, E.H. Sargent, Z.W. Seh, Machine learning for a sustainable energy future. Nature Reviews Materials, 8, (2022) 202–215. https://doi.org/10.1038/s41578-022-00490-5

[277] M. Dorri, A.K.M.R. M, K. Zaghib, In operando and in situ characterization tools for advanced rechargeable batteries: Effects of electrode origin and electrolyte. Journal of Power Sources, 658, (2025) 238188. https://doi.org/10.1016/j.jpowsour.2025.238188

[278] I.A. Vasyukova, O.V. Zakharova, D.V. Kuznetsov, A.A. Gusev, Synthesis, toxicity assessment, environmental and biomedical applications of MXenes: A review. Nanomaterials, 12(11), (2022) 1797. https://doi.org/10.3390/nano12111797

[279] A.K. Worku, M.A. Alemu, D.W. Ayele, M.Z. Getie, M.A. Teshager, Recent advances in MXene-based materials for high-performance metal-air batteries. Green Chemistry Letters and Reviews, 17(1), (2024) 2325983. https://doi.org/10.1080/17518253.2024.2325983

[280] R.R. Nilchiani, J. Caddell, H.B. Taramsari, The extended technology readiness level (eTRL): From deployment to obsolescence. IEEE Open Journal of Systems Engineering, 3, (2025) 1–9. https://doi.org/10.1109/OJSE.2025.3527288

[281] J. Allan, S. Belz, A. Hoeveler, M. Hugas, H. Okuda, A. Patri, H. Rauscher, P. Silva, W. Slikker, B. Sokull-Kluettgen, W. Tong, E. Anklam, Regulatory landscape of nanotechnology and nanoplastics from a global perspective. Regulatory Toxicology and Pharmacology, 122, (2021) 104885. https://doi.org/10.1016/j.yrtph.2021.104885

[282] L.L.J. Meijer, J.C.C.M. Huijben, A. van Boxstael, A.G.L. Romme, Barriers and drivers for technology commercialization by SMEs in the Dutch sustainable energy sector. Renewable and Sustainable Energy Reviews, 112, (2019) 114–126. https://doi.org/10.1016/j.rser.2019.05.050

[283] P. Wang, C. Jia, Y. Huang, X. Duan, van der Waals heterostructures by design: From 1D and 2D to 3D. Matter, 4(2), (2021) 552–581. https://doi.org/10.1016/j.matt.2020.12.015

[284] A. Kumar, N.K. Mukhopadhyay, T.P. Yadav, Recent progresses on high entropy alloy

development using machine learning: A review. Computational Materials Today, 8, (2025) 100038. https://doi.org/10.1016/j.commt.2025.100038

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Data will be available on request.

No new data were created or analyzed in this study. All data supporting the findings of this review are contained within the article and its reference list.

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