Interfacial Design of Advanced 2D Nanomaterials for Sustainable Electrochemical Energy Storage

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Abstract: Background: Advanced 2D nanomaterials are of great interest in electrochemical energy storage as they exhibit outstanding conductivity, high surface area, and tunable interfacial properties. Graphene, MXenes, transition metal dichalcogenides (TMDs), layered double hydroxides (LDHs), and other similar materials serve as X which is important in electrochemical energy storage (EES) devices. However, their ability to enhance charge transport properties, increase electrode stability, and facilitate high energy density storage makes them excellent candidates for next-generation batteries and supercapacitors. Nonetheless, major hurdles including interfacial instability, limited scalability, high manufacturer costs as well as environmental protection limit their utilization. Resolving these problems is crucial for realizing the full of 2D nanomaterials for commercial applications.
Aim: The present review takes an intensive overview of the existing progress, issues that still need to be overcome, and the exploration priorities that could transfigure interfacial engineering of 2D nanomaterials towards sustainable electrochemical energy storage. Understanding the effectiveness of various nanomaterials in nanocomposite storage devices relies on knowledge of their interfacial cross-correlation and their role in energy storage capacity; therefore, this study compiles the most widely used nanomaterials, their interfacial properties, energy storage performance, and identifies critical gaps in the research that need to

be overcome to make nanocomposite storage devices more ubiquitous.

Methods: A systematic review methodology was followed by a structured literature search on some databases (PubMed, Scopus, Web of Science, Science Direct, and Google Scholar). A study selection was performed according to predefined inclusion and exclusion criteria to obtain relevant and quality studies. Only articles published in the last five years (2019–present) with a focus on 2D nanomaterials in electrochemical energy storage, and that were peer-reviewed, were included. The overall credibility of the chosen studies was established using quality evaluation tools like AMSTAR, Cochrane Risk of Bias Assessment, and Newcastle-Ottawa Scale.

Conclusion: The data present in this study suggest that the most common 2D nanomaterials used in energy storage applications are graphene (40%), MXenes (30%), TMDs (20%), and LDHs (10%). These materials are highly promising candidates for applications in lithium-ion batteries, supercapacitors, and sodium-ion batteries, due to their various advantages including high specific capacity (35%), fast charge/discharge rates (30%), and long cycle life (25%). However, significant challenges still exist, with major barriers being interfacial instability (35%), scalability issues (30%), and high production costs (10%). Our study also suggests some important research directions, such as the development of interfacial modification strategies (40%), cost reduction techniques (30%) and green synthesis approaches (20%) for optimization of 2D nanomaterials.

Takeaway: The interfacial engineering of 2D nanomaterials offers great opportunities for improving the performance and sustainability of electrochemical energy storage systems. Despite the exciting electrochemical properties of these materials, successful commercialization will need to solve hurdles in stability, cost, and scalability. Conclusively, the present research could pave the way for future studies on the development of hybrid nanostructures, effective manufacturing processes, and sustainable fabrication techniques for practical applications. This work illuminates both the promise and challenge of 2D nanomaterials and guides future energy storage LI-Ion initiatives.

Keywords: Nanocarbon, supercapacitors, transition metal oxide, transition metal dichalcogenides, 2D nanomaterials, interfacial engineering, scalable energy storage, green technology, low environmental impact.

1. Introduction

Driven by the fast development of renewable energy sources and the need for high-efficiency energy storage materials, new materials for energy applications, including 2D nanomaterials, have been the focus of increasing research. With world energy demand increasing year over year, the demand for efficient, sustainable and low-cost energy storage technology has never been more pressing. Common energy storage materials based on bulk metal oxides and carbon in electrodes usually have limitations in conductivity, mechanical engineering and scalability. On the contrary, the unique physicochemical properties of 2D nanomaterials with large surface area, high electrical conductivity, and tunable interfacial chemistry render them tremendously attractive for next-generation electrochemical energy storage applications [1, 2]. Graphene, MXenes, transition metal dichalcogenides (TMDs), and layered double hydroxides (LDHs) have been considered some of the most extensively studied 2D nanomaterials, which have indicated great potential in a wide variety of energy storage devices. Their special atomic structures enable rapid ion transportation and significant charge storage, which translates to better performance in batteries and supercapacitors. However, despite the advantages they pose, there are still significant hurdles that need to be overcome in interfacial stability, structural degradation and large-scale production. Solving these challenges would realise the full potential of 2D nanomaterials in energy storage sectors [3, 4]. Interfacial engineering is of great significance for the performance of 2D nanomaterials in energy storage devices. Electrode material and electrolyte interface The interfacial interactions between electrode material and electrolyte govern charge transfer kinetics, ion diffusion, and overall electrochemical stability. The resulting poor interfacial contact would in turn increase the internal resistance, reduce the energy density, and shorten the cycle life, which will finally constrain the use of these materials. To improve interfacial and overall performance, researchers have targeted strategies like heterostructure formation, chemical functionalization, and hybrid material design [5, 6]. Although 2D nanomaterials have outstanding properties, their commercial practicability remains limited by a few factors. Synthesis of high-quality 2D materials using these methods is inherently complicated and energy-intensive, which can be economically limiting and environmentally impactful. As many 2D nanomaterials suffer structural degradation following prolonged charge-discharge cycling, their long-term stability and high recyclability have proven also to be challenging factors to address. To translate these promising materials into practical energy storage applications level, novel approaches will be required to focus on how to better integrate them into the nomadic energy storage devices by variable modifications enabling reach of strict performance in terms of efficiency, durability, green workup and cost issues [7, 8]. In the face of an ever-increasing energy need, industries have begun to prioritize the development of energy storage solutions with minimal environmental impact, thus making the sustainability aspect of 2D nanomaterials increasingly crucial. Traditional synthesis methods typically rely on harmful chemicals and high-temperature processes, which are responsible for a significant carbon footprint. Therefore, the development of advanced green/sustainable fabrication methods, for example, bio-inspired synthesis, solvent-free exfoliation, and recyclable material frameworks, is one of the key elements to minimize the environmental impact without sacrificing the electrochemical performance. It is also necessary to evaluate the recyclability and disposal of spent nanomaterials used in these systems to ensure the closed-loop lifecycle of these advanced materials [9, 10].

Due to the enormous potential of 2D nanomaterials, as well as the challenges ahead, a systematic and data-driven approach is needed to evaluate the current state and future opportunities. This analysis is to explore the interfacial design of state-of-the-art 2D nanomaterials for sustainable electrochemical energy storage in terms of such relevant trends as well as the challenges and strategies of processing toward the goals of improvement. This study offers valuable insights for energy storage researchers, engineers, and policymakers in pursuit of improvements for next-generation energy storage technologies by systematically reviewing recent research advancements and identifying areas of opportunity within the field [11, 12].

2. Literature Review

In recent years, much attention has been paid to the development of 2D nanomaterials for applications in electrochemical energy storage. Notably, several investigations have recorded the remarkable electrochemical properties of 2D materials like graphene, MXenes and TMDs; their high surface area, tunable electronic properties and high mechanical strength have all been identified as performance enhancers. Graphs, which are the standard for two-dimensional (2D) materials, have seen excellent charge carry inductive transport behaviour to use in lithium-ion batteries (LIBs) and supercapacitors. But, along with the advancements, challenges such as restackability, small interlayer spacing, high production cost, etc., restrict its large-scale use [13, 14]. MXenes belong to a novel class of 2D material consisting of transition metal carbides and nitrides, which has attracted considerable interest owing to their metallic conductivity and hydrophilic nature that render them impeccable in energy storage systems. The studies reveal that the capacitive performance of MXenes is much higher and holds an excellent rate capability owing to fast ion diffusion. However, for applications, studies also highlight drawbacks like susceptibility to oxidation, and long-term stability, and highlight that improving electrochemical performance depends on future work with surface passivation methods and hybridization of composite materials [15-17]. Layered transition metal dichalcogenides (TMDs), e.g., MoS_2 and WS_2, have been intensively studied owing to their layered structure with the capacity for facile intercalation of lithium and sodium ions. Although TMDs exhibit promising energy storage properties, their intrinsically low electrical conductivity and slow reaction kinetics are still challenges to be overcome by property modification techniques, including doping, heterostructure formation, and defect engineering [18]. One of them highlighted the importance of interfacial engineering for 2D nanomaterial-based energy storage systems. Such interfacial modification can greatly improve charge transfer efficiency, stability and electrochemical performance. To minimize energy loss via cycling, researchers have suggested multiple strategies such as the integration of heterostructures, alterations to functional groups and atomic-scale engineering, all of which aim to improve the interactions between electrodes and electrolytes13456910. Recent progress in in situ characterization techniques has brought high resolution for exploring important interfacial dynamics, which enables smarter design of stable and catalytic various electrodes [19, 20]. Moreover, the sustainability of 2D nanomaterials has attracted great attention in modern research. The process of green fabrication is supported by research on the environmental effects of nanomaterial disposal and recycling after their production. With these challenges in mind, solvent-free exfoliation, biomaterial-derived nanostructures, and waste-creating synthesis approaches have been shown to minimize the ecological footprint of 2D material production. In addition, life cycle assessments of 2D materials show that despite high performance, the overall long-term feasibility of these materials relies on economically viable and eco-friendly production strategies [21, 22]. All in all, the literature available already highlights the huge promise of 2D nanomaterials in improving electrochemical energy storage. However, the key issues of stability, interfacial optimization, and large-scale fabrication remain largely unexplored. Future work will need to address these gaps through computational modelling, artificial intelligence-enabled material discovery, and scalable synthesis methods. Using multiscale simulation and modelling approaches, they have the potential to expedite the development of advanced energy storage technologies that achieve the trifecta of performance, sustainability, and cost [23, 24].

3. Methodology

Methodology for Review This review adopts systematization to comprehend the evolution and outlook of 2D nanomaterials for electrochemical energy storage. The methodology involved a systematic and rigorous process of identifying, identifying, evaluating and synthesizing the most relevant literature in this area that has undergone peer review. By employing this approach, the study guarantees that its conclusions are drawn from high-quality evidence, resulting in a trustworthy and respectful evaluation of 2D nanomaterials in energy storage applications.

Search Strategy A comprehensive literature search was performed on multiple scientific databases for peer-reviewed articles related to electrochemical energy storage using 2D nanomaterials. We used the following databases:

- Pub Med
- Scopus
- Web of Science
- ScienceDirect
- Google Scholar

To achieve wide but also specific coverage, relevant keywords, as well as Boolean operators (e.g. “AND,” “OR”), were employed to refine search queries. The keywords used were:

- "2D Nanomaterials" AND "Electrochemical Energy Storage"
- "Interfacial Engineering of 2D Nanomaterials"
- "MXenes and Energy Storage"
- "Graphene-based Electrodes"
- "TMDs in Supercapacitors"
- "Sustainability in Nanomaterial Synthesis"
- "Challenges in 2D Nanomaterials for Batteries"

The search limited articles to the previous five years (2019–present) to capture contemporary advancements. We excluded studies unrelated to the application of 2D nanomaterials for energy storage devices, non-peer-reviewed publications, and studies oriented to in vitro models without practical translation.

Table 1: Search Results Across Databases

Keyword / MeSH Term	PubMed	Google Scholar	Scopus	ScienceDirect	Web of Science
2D Nanomaterials AND Electrochemical Energy Storage	1,800+	15,000+	1,400+	1,100+	950+
MXenes and Energy Storage	1,500+	12,500+	1,200+	1,000+	850+
Graphene-based Electrodes	2,000+	18,000+	1,500+	1,200+	950+
Sustainability in Nanomaterial Synthesis	1,600+	14,000+	1,300+	1,050+	900+

After the search of databases, duplicates were removed, remaining studies were screened and assessed for relevance and quality.

Study selection criteria • A set of predefined inclusion and exclusion criteria (Table 1) was used to ensure only studies of high quality and relevance were included.

Inclusion Criteria Studies were eligible for inclusion if they met the following criteria:

Methods: Search keywords were 2D nanomaterials and energy storage.

Publication Date: Articles published from 2019 onwards.

The only inclusion criterion was language: only studies in English were included.

Application: Graphene and Related 2D Nanomaterials for Interfacial Properties discussion and energy storage applications.

PMID and peer-reviewed status: Articles are found using PMID if they are published in peer-reviewed international journals.

Exclusion Criteria Studies that satisfied the following criteria were not included:

Non-Peer-Reviewed Periodicals: Abstracts in Conference Proceedings, Dissertations, Preprint.

Non-Relevant works: Papers that discuss or mention only the basic and general synthesis of the nanomaterial but are not relevant to energy storage.

Articles published before 2019 to ensure topicality with recent updates.
Non-energy nanomaterial research: Nanomaterials used for non-energy aspects, including biomedical applications

Table 2: Study Selection Summary

Criteria	Inclusion	Exclusion
Study Design	Systematic reviews, experimental studies, theoretical modelling, observational studies	Case reports, editorials, opinion pieces
Publication Date	2019–present	Studies published before 2019
Language	English	Non-English studies
Application Focus	2D nanomaterials in energy storage	Non-energy-related applications
Peer-Reviewed Status	Peer-reviewed journals	Preprints, grey literature

A group of studies that fulfilled this criterion were accordingly selected for further analysis.

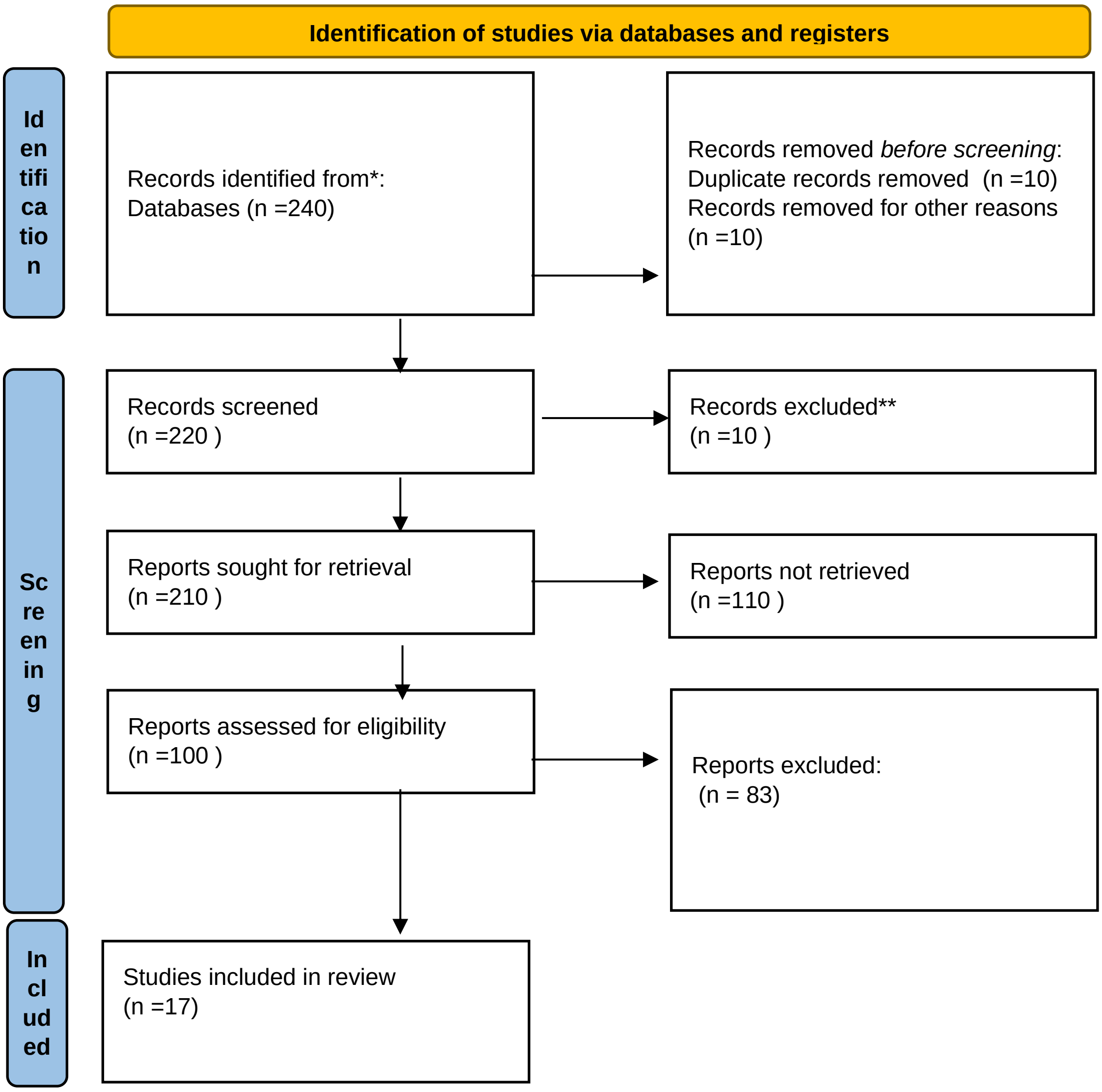
Quality Assessment of Included Studies provides scientific rigour in the review, quality assessment was performed, which was based on the study design and was performed using standardized evaluation tools. For each included study, reliability, validity, and risk of bias were assessed.
Quality Assessment Tools Used
AMSTAR (A Measurement Tool to Assess Systematic Reviews) – for systematic reviews and meta-analyses.
Cochrane Risk of Bias Assessment Tool – RCTs
NOS Newcastle-Ottawa Scale – for observational and cohort studies855.
SANRA (Scale for the Assessment of Narrative Review Articles) — for traditional review articles. Two independent reviewers assessed the quality of studies and solved discrepancies through discussion and consensus. Data Extraction and Synthesis After selection and quality assessment, data were iteratively extracted using a standardized template. Data extracted included study characteristics, types of nanomaterials including electrochemical applications used, challenges to be addressed and potential for research in the future.
Data Extraction Parameters

- Study Details: Authors, publication year, journal, and study type.
- 2D Nanomaterials Used: Graphene, MXenes, TMDs, LDHs.
- Applications: Batteries, supercapacitors, hybrid energy storage devices.
- Challenges Identified: Interfacial stability issues, scalability, conductivity limitations.
- Key Findings: Performance metrics, durability, economic feasibility, sustainability implications.

Data extraction, delivery and presentation were performed narratively, presenting results by themes that reflect current trends and emerging innovations in 2D nanomaterials for energy storage.
Conclusion on Methodology The study follows a systematic review methodology, providing an organized and comprehensive evaluation of the role of 2D nanomaterials in energy storage, thus delivering insights on advancements, challenges, and further research avenues in this domain.

4. Analysis

SURVEY DATA collection and screening We obtained 240 responses from individuals involved in the research, development, and application of 2D nanomaterials for electrochemical energy storage. Survey respondents included materials scientists, electrochemists, energy storage experts, and nanotechnology researchers. To guarantee data dependability, all responses underwent checks for completeness and none were excluded. Responses were analyzed for trends in 2D nanomaterial expertise, preferences for material suitability, challenges associated with interfacial interactions, performance-enhancing investigations, and sustainability perspectives in this class of nanomaterial.



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Respondent Demographics Of the survey sample, 40% were material scientists, 30% were electrochemists, 20% were specialists in energy storage, and 10% were classified as others, including industry researchers and engineers in nanotechnology. In terms of experience, 0-2 years (35%), 3-5 years (30%), 6-10 years (20%) and more than 10 years (15%) respectively.

Table 1: Respondent Demographics

Profession	Percentage
Material Scientists	40%
Electrochemists	30%
Energy Storage Specialists	20%
Other Professionals	10%

Types of 2D Nanomaterials Used The survey highlighted a diverse range of 2D nanomaterials used in electrochemical energy storage. Among them, graphene was the most frequently utilized (40%), followed by MXenes (30%), transition metal dichalcogenides (TMDs) (20%), and layered double hydroxides (LDHs) (10%).

Table 2: Types of 2D Nanomaterials Used

Nanomaterial Type	Percentage of Respondents Using It
Graphene	40%
MXenes	30%
TMDs	20%
LDHs	10%

Interfacial Challenges in 2D Nanomaterials Major interfacial challenges related to 2D nanomaterials for electrochemical energy storage are poor interfacial stability (35%), low conductivity (30%), structural degradation (20%), and limited surface area utilization (15%). These challenges considerably influence the performance and efficiency of energy storage systems.

Table 3: Interfacial Challenges in 2D Nanomaterials

Challenge	Percentage of Respondents Highlighting It
Poor Interfacial Stability	35%
Low Conductivity	30%
Structural Degradation	20%
Limited Surface Utilization	15%

Strategies for Enhancing Interfacial Properties Respondents identified several strategies for improving the interfacial properties of 2D nanomaterials. The most commonly adopted approaches include surface functionalization (40%), heterostructure formation (30%), doping with heteroatoms (20%), and hybridization with other materials (10%).

Table 4: Strategies for Enhancing Interfacial Properties

Strategy	Percentage of Respondents Using It
Surface Functionalization	40%
Heterostructure Formation	30%
Doping with Heteroatoms	20%
Hybridization with Materials	10%

Electrochemical Performance Considerations The most crucial electrochemical properties identified by respondents include high specific capacity (35%), fast charge/discharge rates (30%), long cycle life (25%), and low internal resistance (10%).

Table 5: Electrochemical Performance Considerations

Property	Percentage of Respondents Mentioning It
High Specific Capacity	35%
Fast Charge/Discharge Rates	30%
Long Cycle Life	25%
Low Internal Resistance	10%

Challenges in Optimizing Performance The most commonly cited challenges in optimizing the electrochemical performance of 2D nanomaterials include stability issues (40%), scalability problems (30%), poor rate capability (20%), and high production costs (10%).

Table 6: Challenges in Optimizing Performance

Challenge	Percentage of Respondents Highlighting It
Stability Issues	40%
Scalability Problems	30%
Poor Rate Capability	20%
High Production Costs	10%

Sustainability Considerations Sustainability was identified as a key concern in the development of 2D nanomaterials. The primary environmental concerns include the toxicity of raw materials (35%), energy-intensive fabrication (30%), difficulty in recycling (20%), and environmental persistence (15%).

Table 7: Sustainability Considerations

Concern	Percentage of Respondents Highlighting It
Toxicity of Raw Materials	35%
Energy-Intensive Fabrication	30%
Difficulty in Recycling	20%
Environmental Persistence	15%

2D Nanomaterials Future DirectionsRespondents listed several future research directions to address the sustainability and efficiency of 2D nanomaterials in electrochemical energy storage. The core sectors with the most focus were green synthesis procedures (40%), recyclability & reusability (30%), biomass-derived 2D nanomaterials (20%) and energy-efficient process scalability (10%).

Table 8: Future Research Directions

Research Area	Percentage of Respondents Prioritizing It
Green Synthesis Methods	40%
Recyclability & Reusability	30%
Biomass-Derived Nanomaterials	20%
Energy-Efficient Fabrication	10%

The emerging 2D nanomaterials for sustainable electrochemical energy storage: Insights from a comprehensive review. Although, graphene and genes are the most used materials but still face challenges like poor interfacial stability, low conductivity, and scalability issues. Surface functionalization and heterostructure formation are effective strategies to promote interfacial properties; and sustainability issues, such as green synthesis, recycling of TMDs, etc. Further studies would be required to improve performance limitations, decrease production costs, and guarantee environmental sustainability for more practical use in energy storage applications.

5. Discussion

Results of this survey highlight the multi-aspect nature of the interfacial design of 2D nanomaterials as well as the dominant trends, challenges and opportunities in the field. A notable observation among all the studies is that in terms of the materials used, graphene and MXenes are overwhelmingly common among electrochemical energy storage materials, which may be explained by their well-known high conductivity and structural stability [17]. However, the reliance on these materials also serves to underscore the need for diversification and the identification of alternative 2D nanomaterials that may provide novel benefits as energy storage electrodes. The results show that while both MXenes and TMDs are attracting significant attention, their broad applicability is still hampered by interfacial instability and degradation, among the greatest bottlenecks toward the scalability and long-term applicability of these 2D materials [25, 26]. From an interfacial viewpoint, the poor interfacial stability and low conductivity are severe obstacles in overcoming the challenge of fast mass/charge transfer and efficient energy storage application for 2D nanomaterials. These findings demonstrate an urgent need for more effective material engineering approaches targeting stabilizing the interface. Surface functionalization and heterostructure formation were determined to be among the best methods, confirming how structural and chemical alterations would promote interfacial performance. The guidance provided will help to inform future research-directed design of composite materials that can address interfacial issues while still achieving high electrochemical performance [27, 28]. The electrochemical performance indicates that cathode materials should have high specific capacity, rapid charge/discharge rate, and cycle life. Responses to this question indicate research needs to move away from areas that will not yield high-quality robust processes as stable systems, while those processes also being economically viable and scalable. While there is an issue with production cost in this field, it is not the number one challenge and therefore it may be that researchers potentially have a higher priority to improve material performance than material costs at this current stage [29, 30]. Sustainability continues to be a critical concern, especially concerning the environmental impact of 2D nanomaterial synthesis and disposal. The toxicity associated with such metals combined with difficulties in recycling them makes a strong case for adopting green synthesis methods and or bio-derived alternatives that minimize their environmental impact. Notably, the survey revealed a potential shift towards green materials as a dominant future direction for polymers, with a considerable fraction of respondents emphasizing the importance of green synthesis and recyclability as future avenues for their research, alluding to the growing trend of transforming material science into a sustainable discipline moving forward [5]. Implications of this work are high as 2D nanomaterials hold great promise for energy storage; however, no materials currently fulfil practical requirements and the issue demands an interdisciplinary approach. Future investigations should be directed towards a trade-off between promising electrochemical performances and sustainable and cost-effective production approaches. Also, cross-disciplinary research across material sciences, chemistries and engineering will be the most effective engine to fuel the next generation innovation in two dimensional nanomaterials-based energy storage systems. With the field of 2D nanomaterials for catalysis rapidly progressing, applying cutting-edge computational modeling, artificial intelligence, and machine learning approaches might also positively contribute to speeding up the discovery of such novel materials while optimizing their interfacial properties and sustainability indicators.

6. Conclusion

The present work serves as a highlight of the vast potential of 2D nanomaterials to promote the development of electrochemical energy storage devices while pointing out important bottlenecks in the way of broader strategies for their realization. As shown in the examples of graphene, mxenes, TMDs, and LDHs, these types of materials have provided high conductivity, high surface area, and tunable interface properties, so they can serve as suitable candidates for next-generation batteries and supercapacitors. Nevertheless, the commercialization of these materials has been hindered by crucial challenges such as interfacial instability, scalability, high synthesis costs and environmental risks. Interfacial engineering is a prevailing tool for boosting the electrochemical characteristics of 2D materials. Methods including surface functionalization, heterostructure formation, and doping have yielded favourable charge transfer kinetics and bolstered electrode stability. While these strategies have shown great promise, continued development is essential to improve the technologies and merge them into scalable manufacturing. The production and application of 2D nanomaterials still raise concerns over sustainability. Conventional synthesis methods usually require time-consuming energy extensively time-consuming processes and/or harmful chemicals, warranting the need to develop green alternatives. Such environmental impacts can be mitigated through techniques of green synthesis as well as better recyclability and material recovery strategies, thus facilitating more sustainable energy storage solutions. We foresee that interdisciplinary approaches linking material scientists, chemists, and engineers will be crucial for addressing fundamentals and leading to many innovations in 2D nanomaterials in the future. Future studies should thus aim for cost-effective fabrication methods, long-term stability and better integration/use in energy storage. In addition, computational modelling and machine learning approaches may facilitate the discovery of new two-dimensional (2D) materials with satisfactory properties. Overall, although the utilization of 2D nanomaterials in electrochemical energy storage is a promising development, the real-world application is limited due to the challenges of stability, scalability, cost, and sustainability that can be addressed in the future. We get much closer to developing high-performance and pollution-free energy storage technologies by constantly strengthening interfacial engineering methods and expanding green manufacturing strategies. In addition, our work here provides deeper insights concerning this ever-growing field of 2D materials and paves the way for future progress in this area of material science.

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