Machine Learning Applications in Materials Modeling and Optimization for Sustainable Energy Storage: A Systematic Approach

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Abstract

The study demonstrates that machine learning is becoming increasingly important in the modelling and optimisation of materials for sustainable energy storage. This field is growing rapidly, as evidenced by the diversity of applied techniques and the complexity of the materials analysed. The paper identifies the need for models capable of integrating multiple variables and scales, as well as the importance of advancing methods that overcome current limitations in accuracy, generalisation, and data availability. The text also underscores the significance of interdisciplinary approaches that integrate theory, experimentation, and industrial application to expedite the development of efficient and reliable solutions. The enhancement of the impact of machine learning on the design and improvement of materials is contingent on multisector collaboration and standardisation in data management. Such collaboration and standardisation are pivotal in ensuring the sustainability and competitiveness of future energy systems.

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Introduction

The importance of sustainable energy storage in facilitating the transition to low-carbon energy systems cannot be overstated. This is particularly true in the context of the increasing incorporation of renewable sources, such as solar and wind, which require effective storage solutions to ensure reliable and sustainable energy production. Despite their environmental benefits, these sources are characterised by their intermittent nature, necessitating the development of effective solutions for the storage and release of energy on demand. [1] The most relevant technologies include rechargeable batteries, such as lithium-ion batteries, supercapacitors, and hybrid systems. [2]

The performance of these technologies is contingent on the quality of the materials utilised in their fabrication. [3] The properties of these materials determine key parameters such as storage capacity, charge and discharge rates, thermal stability, and system lifetime. Consequently, the design and discovery of new functional materials is one of the main challenges for the sector. [2] In this scenario, machine learning (ML) emerges as an effective tool in materials science. Its capacity to process substantial quantities of data, discern intricate relationships, and predict properties with a high degree of accuracy is effecting a transformation in the manner by which materials are modelled, designed, and optimized.[4] In contrast to the utilisation of computationally expensive experimental methods or simulations, the employment of ML based approaches has been demonstrated to accelerate materials development, reduce validation times, and facilitate technological innovation.[5]

Consequently, the integration of ML and energy storage emerges as a strategic domain for applied research and global sustainability. The proliferation of research employing ML techniques to engineer, model, and enhance materials for sustainable energy storage has been observed to occur without the concomitant development of a systematic framework to articulate the knowledge generated.[5], [6]

This has resulted in a fragmentation of the field, evident in the varied utilisation of algorithms, the diverse selection of materials, the differences in modelled properties, and the multiple optimization objectives.[7] This dispersion, although indicative of an expanding field, hinders the establishment of a shared foundation that would facilitate the identification of patterns, trends, gaps, and limitations. The extant literature on the subject typically focuses on specific cases, employing distinct methodologies, which makes it difficult to establish precise comparisons or transfer learning to other contexts.[8]

This absence of integration imposes limitations on the generation of valuable knowledge, thereby hindering the development of advanced materials for energy storage.[5] The issue of fragmentation also impacts the comprehensive understanding of the field and its practical application, especially in instances where rapid innovation is imperative to address the challenges of the energy transition. Moreover, a paucity of systematic reviews and comparative analyses is evident in the extant literature, with such analyses being instrumental in the organization of advances, the identification of common problems, and the proposal of clear directions for future research.

In this regard, the objective of this research is to explore and systematize the scientific evidence on the application of machine learning techniques in the modelling and optimization of materials for sustainable energy storage. In order to achieve this objective, a series of questions have been devised to guide the review and define the scope of the expected results.

- Which machine learning techniques have been most widely used to model materials in sustainable energy storage systems?
- Which types of materials have been most frequently studied using machine learning approaches for energy storage applications?
- Which material variables or properties have been most frequently modeled or predicted

using machine learning techniques?

- Which optimization objectives have guided the use of machine learning in the design of energy storage materials?

- What limitations have been documented in the application of machine learning in this field of research?

This study proffers an integrated and systematic overview of the extant scientific literature pertaining to the application of machine learning techniques to materials for sustainable energy storage. The text's added value lies in its identification of recurring patterns, thematic gaps, and development opportunities, providing a clear and structured framework that is useful for both researchers and developers of advanced energy technologies. This synthesis provides a valuable foundation for future research and the acceleration of innovation in this pivotal domain for the energy transition.

Methodology

A systematic approach was adopted to collect, evaluate, and synthesize scientific evidence on machine learning applications in sustainable energy storage materials. The PRISMA 2020 protocol, an international standard for conducting and reporting systematic reviews, was utilised. The protocol provides a structured framework that guarantees methodological rigor, transparency in the selection and analysis of studies, and reproducibility of results. The utilisation of this approach guarantees the uniformity and dependability of the presentation of findings, thereby facilitating the lucid identification of criteria, procedures, and results. The application of PRISMA 2020 has been demonstrated to enhance the scientific validity of research syntheses, thereby ensuring their reliability and utility for the research community.[9]

Eligibility criteria

The inclusion criteria were defined with the objective of selecting studies that applied machine learning and artificial intelligence techniques to sustainable energy storage materials. In order to ensure the currency of knowledge, it was necessary to consider only research in accessible languages that had been published in a recent period. Priority was given to articles focusing on the modelling, optimization, or design of energy materials using computational methods based on machine learning or artificial intelligence.

The selection process comprised three phases of exclusion in order to ensure the quality and relevance of the corpus. The initial phase involved the elimination of duplicate or irrelevant documents resulting from indexing errors, which did not align with the thematic objectives. In the second phase of the study, research papers that did not have full-text access due to restrictions on availability were excluded from the analysis. This decision was taken because a detailed evaluation of these papers would have been unfeasible. The third phase entailed the exclusion of studies based on their methodological quality, direct relevance, and the elimination of thematic duplicates or conceptual overlaps that did not add value. These phases enabled the refinement of the evidence, ensuring a rigorous and representative analysis that optimises validity and facilitates a clear and substantiated synthesis.

Sources of information

The Scopus and Web of Science databases were utilised to collate scientific information on machine learning applications in materials for sustainable energy storage. Scopus encompasses a wide range of academic disciplines, including the applied sciences, engineering, and energy, thus providing access to recent and relevant studies in these fields. Web of Science offers a rigorous focus on indexed journals and international recognition in the natural sciences and technology, ensuring the quality and relevance of the sources consulted.[10]

It is evident that both databases provide advanced tools for systematic searching, including filters by date, language and document type, as well as Boolean operators for combining terms. This facilitates the creation of precise and reproducible search equations. Furthermore, they facilitate the export of references for subsequent analysis and processing with dedicated software.

Search strategy

A search equation was designed for each database based on the defined inclusion criteria. In Scopus, the formula was: TITLE ("machine learning" OR "artificial intelligence") AND TITLE-ABS-KEY ("energy storage materials" OR "energy materials"). For Web of Science, the equation was adapted to the corresponding syntax: TS=("machine learning" OR "artificial intelligence") AND TS=("energy storage materials" OR "energy materials"), replacing TITLE with TS= and TITLE-ABS-KEY with TS=. The selection of Boolean terms and operators ensures the accurate retrieval of studies on machine learning applied to energy storage materials. The strategy was adjusted to the specific characteristics of each database to maximize coverage and relevance in the results.

Selection process

The selection process was initiated with the execution of the search equations in Scopus and Web of Science, thereby generating an initial set of records. Titles and abstracts were then screened to discard irrelevant studies. A full review was conducted on the remaining documents in order to evaluate their relevance in accordance with the established criteria. The selection process was conducted independently by two reviewers, who resolved any discrepancies through discussion and consensus. The organisation of references and facilitation of tracking was achieved through the implementation of bibliographic management software, thereby ensuring the integrity and control of the process from inception to completion.

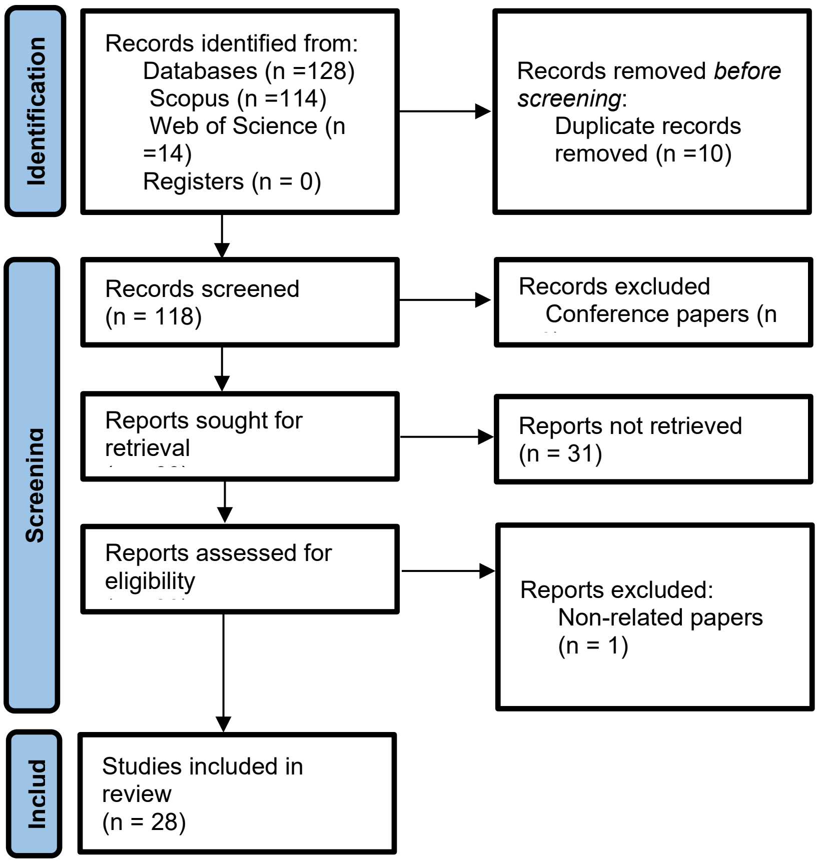

Figure 1. PRISMA flowchart. Prepared by the authors based on Scopus and Web of Science.

Data processing

Microsoft Excel was utilised to facilitate the organisation, coding, and preliminary analysis of the extracted data. The classification of key variables was conducted using machine learning techniques, with the variables themselves being categorised based on material types, modelled physicochemical properties, the objectives of optimisation, and the limitations that have been reported. Standardised procedures were applied in order to maintain consistency in data coding and management. Mechanisms were also implemented to ensure data traceability, allowing for clear tracking from extraction to final analysis. This strategy facilitated the rigorous systematization and synthesis of the collected evidence, thereby optimising the quality and reliability of the results obtained.

Risk of bias

Potential biases in data selection and extraction were identified due to the exclusive use of specific databases and narrow search terms, which may restrict the inclusion of relevant studies. In an effort to mitigate the influence of subjective factors, a set of uniform and objective criteria were implemented to guide the evaluation process. The implementation of independent peer review resulted in a reduction of errors and an enhancement of selection accuracy. The presence of reporting biases within the included studies was also taken into consideration. The procedure is delineated in meticulous detail in the accompanying flowchart (see Figure 1), thus ensuring optimal transparency and facilitating critical assessment of the management of risk of bias in research.

Results

The results have been organised according to the research questions in order to facilitate understanding and systematic analysis of the evidence collected. This structure methodically addresses the various dimensions of the use of machine learning techniques in the modelling and optimisation of materials for sustainable energy storage. Table 1 provides a concise overview of the selected studies and their analysis, which were subjected to a rigorous review process.

Table 1. Studies included in the research. Prepared by the authors based on Scopus and Web of Science.

Title	**Authors**
A Fast Forward Prediction Marco for Energy Materials Design Based on Machine Learning Methods	[11]
High Mechanical Energy Storage Capacity of Ultranarrow Carbon Nanowires Bundles by Machine Learning Driving Predictions	[12]
Accelerated Development of Perovskite-Inspired Materials via High-Throughput Synthesis and Machine-Learning Diagnosis	[13]
Actinide molten salts: A machine-learning potential molecular dynamics study	[14]
An accurate machine learning calculator for the lithium-graphite system	[15]
Applying machine learning to balance performance and stability of high energy density materials	[16]
Artificial intelligence is aiding the search for energy materials	[17]
Automated machine learning structure-composition- property relationships of perovskite materials for energy conversion and storage	[18]
Computation-accelerated discovery of the K2NiF4-type oxyhydrides combing density functional theory and machine learning approach	[19]
Exploring an accurate machine learning model to quickly estimate stability of diverse energetic materials	[20]
Frame spray pyrolysis optimization via statistics and machine learning	[21]
Green standard model using machine learning: identifying threats and opportunities facing the implementation of green building in Iran	[22]
Integrating Nanomaterial and High-Performance Fuzzy-Based Machine Learning Approach for Green Energy Conversion	[23]
Lattice dynamics and elastic properties of α-U at high-temperature and high-pressure by machine learning potential simulations	[24]
Leveraging composition-based energy material descriptors for machine learning models	[25]
Machine learning assisted prediction in the discharge capacities of novel MXene cathodes for aluminum ion batteries	[26]

Machine learning in the era of smart automation for renewable energy materials	[27]
Machine learning techniques to probe the properties of molten salt phase change materials for thermal energy storage	[28]
Machine learning-accelerated prediction of overpotential of oxygen evolution reaction of single-atom catalysts	[29]
Machine learning-accelerated quantum mechanics-based atomistic simulations for industrial applications	[30]
Machine learning-assisted prediction, screen, and interpretation of porous carbon materials for high performance supercapacitors-	[31]
Machine-Learning Aided First-Principles Prediction of Earth-Abundant Pnictogen Chalcohalide Solid Solutions for Solar-Cell Devices	[32]
Many-body physics and machine learning enabled discovery of promising solar materials	[33]
MH-PCTpro: A machine learning model for rapid prediction of pressure-composition-temperature (PCT) isotherms	[34]
Noble metal catalyst detection in rocks using machine-learning: The future to low-cost, green energy materials?	[35]
Phase Prediction Study of High-Entropy Energy Alloy Generation Based on Machine Learning	[36]
Superior polymeric gas separation membrane designed by explainable graph machine learning	[37]
UV-Visible Absorption Spectra of Solvated Molecules by Quantum Chemical Machine Learning	[38]

As demonstrated in Figure 2, the frequency of machine learning technique utilisation in the modelling and optimisation of materials for sustainable energy storage is evident. Regression algorithms are the most prevalent, with seven entries. Subsequent to this, machine learning potentials, assembly models, and statistical analysis tools are presented, each with six entries. It is evident that both deep neural networks and feature selection techniques are represented by four entries. Convolutional neural networks and cross-validation strategies are recorded on three occasions. It is notable that Bayesian optimization techniques are employed on two separate occasions.

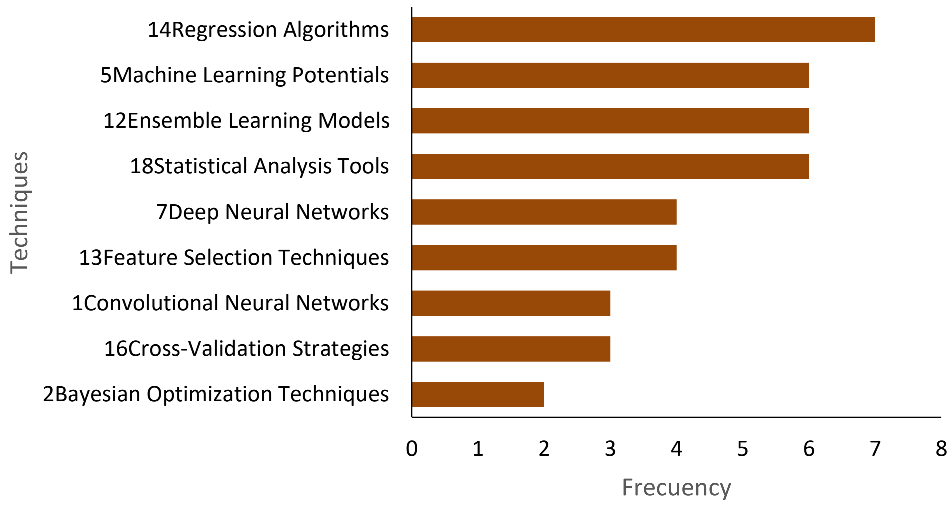

Figure 2. Distribution of machine learning techniques. Prepared by the authors based on Scopus and Web of Science.

As illustrated in Figure 3, the distribution of materials most frequently addressed with machine learning in the study of sustainable energy storage is presented. Carbon-based materials, high-energy materials, general energy materials, and catalytic materials account for the highest frequency, with three entries. Subsequent entries are categorised as multivalent ion materials, perovskite-inspired materials, and molten salt systems, with each category containing two entries. Lithium-ion materials are identified with a single entry.

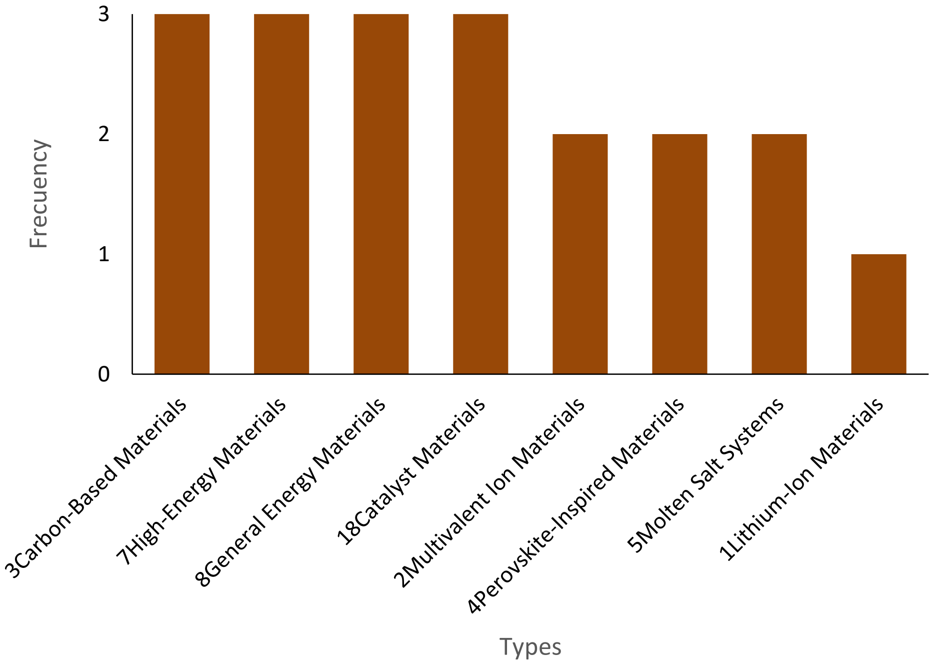

Figure 3. Types of materials studied. Prepared by the authors based on Scopus and Web of Science.

As illustrated in Figure 4, the frequency of properties that are modelled or predicted by machine learning in materials for sustainable energy storage is represented, with stability indicators at the forefront, having been mentioned five times, followed by mechanical properties, structural descriptors, and thermodynamic properties, which have each been mentioned four times. Electrochemical properties, energy storage metrics, catalytic activity indicators, and hydrogen storage properties have each been mentioned three times, while crystallographic characteristics have been mentioned two times.

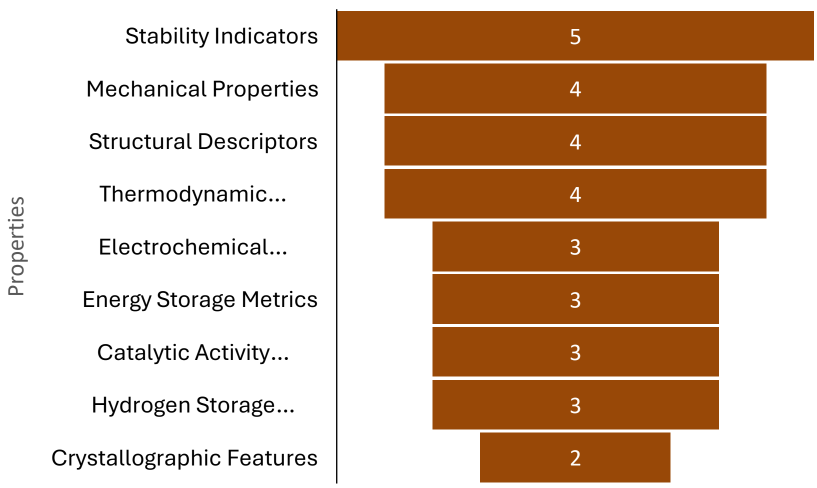

Figure 4. Modeled or predicted properties. Prepared by the authors based on Scopus and Web of Science.

As illustrated in Figure 5, the distribution of the primary optimisation objectives applied through machine learning in materials for sustainable energy storage is presented. It is evident that feature selection optimisation and material discovery acceleration are of particular significance, with each being mentioned on eight occasions. The accuracy of stability predictions and the efficiency of DFT simulations are also frequently discussed. Other relevant categories include descriptor-based modelling, catalytic performance evaluation, and optoelectronic property prediction. The application of high-throughput screening methodologies in the context of environmental sustainability is a subject that merits further consideration.

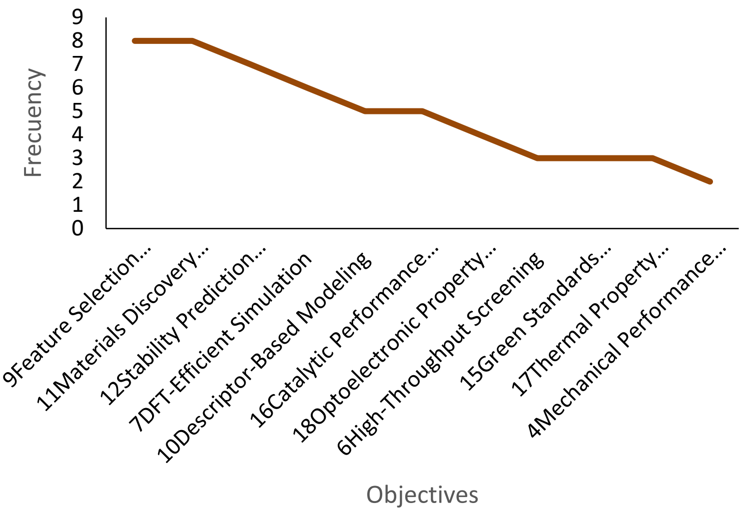

Figure 5. Applied optimization objectives. Prepared by the authors based on Scopus and Web of Science.

As illustrated in Figure 6, the distribution of documented limitations in machine learning applications for modelling and optimisation of materials in sustainable energy storage has been examined. The most prevalent categories are limits on prediction accuracy and domain-specific constraints, with thirteen records each. The text goes on to note methodological assumptions, a paucity of experimental data, and validation and reproducibility issues. It is important to note that there are several limitations that must be considered. These include model generalisation restrictions, difficulties with data access, small sample sizes, gaps in descriptor coverage, and challenges with feature selection.

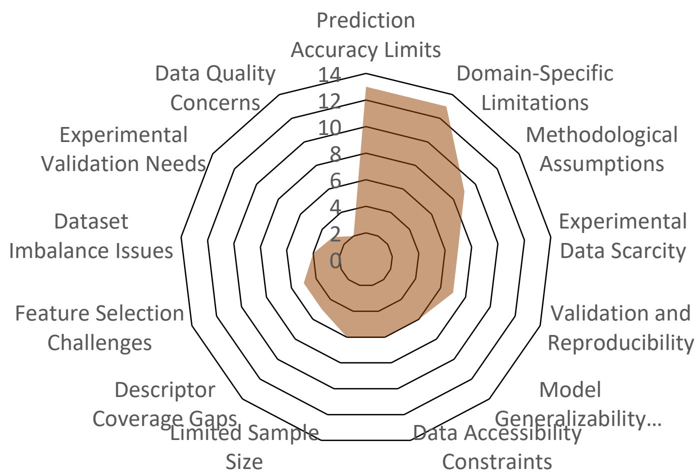

Figure 6. Documented limitations in ML for materials. Prepared by the authors based on Scopus and Web of Science.

The results were then organised according to the research questions, thereby providing a comprehensive overview of machine learning applications in materials for sustainable energy storage. The most commonly used techniques, types of materials studied, modeled properties, optimization objectives, and documented limitations were identified. This configuration facilitates the identification of prevailing trends and the discernment of areas that present both challenges and opportunities, while circumventing the reiteration of particulars. This provides a clear and organised view of the current state of the field.

Discussion

The discussion has been organised in order to present a comprehensive analysis of the results on machine learning applications in the modelling and optimisation of materials for sustainable energy storage. A comparison with previous studies is made to contextualize the findings, followed by the proposal of a conceptual framework that synthesizes the main contributions. Furthermore, the theoretical, policy, and practical implications are analysed. The limitations of the study are presented, and future research lines are proposed to address the identified gaps and challenges.

Analysis of results

The findings indicate a diverse utilisation of machine learning methodologies in the modelling and optimisation of materials for sustainable energy storage, with a predominance of regression methods and learning potentials. This tendency signifies a predilection for models that exhibit both high accuracy and low computational cost, a propensity that is particularly advantageous in scenarios characterised by a paucity of data. Gou et al. [20] demonstrated that the incorporation of data-augmented regression techniques enhances the accuracy of prediction in the estimation of dissociation energies. In a similar vein, [24] demonstrated that learning potentials facilitate the simulation of elastic properties under extreme conditions with a high degree of reliability.

The results demonstrate a diverse selection of materials modelled with machine learning in the context of sustainable energy storage. The focus of this research is materials with complex properties, including carbon-based and high-energy materials, which are of interest due to their storage capacity and structural efficiency. Zhao et al. [12] demonstrate that carbon nanowires exhibit high mechanical storage density when simulated with learning potentials. As demonstrated by Huang et al. [16], predictive models have been shown to facilitate the concurrent enhancement of performance and stability in high-density energy materials.

The findings demonstrate a heterogeneity in the properties modelled through machine learning in materials for sustainable energy storage. The primary focus of the studies is on stability indicators and mechanical properties, with a subsequent emphasis on structural descriptors and thermodynamic variables. Furthermore, the model encompasses the electrochemical properties and storage metrics, including capacity and efficiency. In their 2024 study, Liu et al. propose a predictive approach that facilitates the selection of materials based on multiple functional attributes. In the study undertaken by Nguyen et al. [14], the efficacy of models in accurately representing structural and dynamic properties in complex systems, including actinide molten salts, under varying conditions, was validated.

The findings suggest that machine learning is predominantly employed for the optimisation of feature selection and the acceleration of materials discovery, resulting in reduced development times. The application of the aforementioned concept is twofold. Firstly, it is employed to enhance the accuracy of stability prediction. Secondly, it is utilised to optimise the efficiency of density functional theory (DFT)-based simulations. The prediction of optoelectronic and catalytic properties is an additional objective. These applications illustrate the capacity of machine learning to circumvent the constraints imposed by conventional methodologies, a phenomenon that aligns with the observations made by [17], [26].

The primary constraints on the utilisation of ML for modelling materials intended for sustainable energy storage pertain to predictive accuracy and domain limitations. These results are consistent with those of previous studies [13], [15], which demonstrate a discrepancy between theoretical prediction and experimental validation, exacerbated by limited datasets and issues with generalisation. Moreover, methodological, access, and reproducibility difficulties have been identified, indicating that the effectiveness of ML depends on data quality, feature selection, and the coordination between theory and experimentation.

Comparison of results with other studies

The present study offers a methodical examination of the implementation of ML techniques in the modelling and optimisation of materials for sustainable energy storage. The most commonly used techniques, types of materials analysed, modelled properties, optimisation objectives, and reported limitations are addressed. This organisation facilitates the identification of predominant trends and areas of challenge, aligning with the current state of the literature.

In accordance with [39], both works acknowledge the advancements in the utilisation of ML to expedite the design and discovery of energy materials. The study emphasises the identification and classification of techniques and limitations, while Mortazavi highlights developments in high-precision interatomic potentials, generative models, and the integration of ML platforms for autonomous laboratories. The observed discrepancy can be attributed to the structural approach adopted in this study, in contrast to Mortazavi's technological and prospective perspective.

[40] concentrate on the integration of ML with computational fluid dynamics (CFD) to optimise modular thermal storage systems. As with the study, they emphasise computational efficiency as a key advantage, demonstrating significant reductions in computational time and cost for thermal predictions. However, Singh et al. operate within a distinct domain of research, namely thermal modular design, while the present study encompasses a more extensive range of materials and methodologies. This specialisation delineates the discrepancies in methodological profundity and applicative specificity.

In their 2025 study, Korkua et al. utilised simulations to enhance the efficacy of $SrCl_2$-based thermochemical systems. This was achieved by implementing parametric adjustments, thereby demonstrating a notable enhancement in energy efficiency. In contrast, the study emphasises the general limitations of ML, such as data scarcity and the gap between theory and experimentation. [41] however, offer specific solutions through advanced simulations. This divergence is indicative of the fact that the present study offers a panoramic view, whilst Korkua et al. offer a practical approach for specific systems.

[42] conducted an analysis of decentralised optimisation based on reinforcement learning and demand response, demonstrating advances in the robust management of distributed energy systems. The two studies under consideration both highlight the importance of ML for energy optimisation. However, Martínez and Arévalo broaden the focus to include flexibility and scalability in peer-to-peer markets, emphasising regulatory and uncertainty aspects, which are rarely addressed in this study. This discrepancy is indicative of a divergence in the level of analysis: materials versus distributed energy systems.

In their review of ML applications for optimising battery energy storage systems (BESS), [43] address both security and dynamic management. There is a consensus on the increasing integration of ML to enhance performance and management. However, Dong et al. focus on specific technologies and various scales, while the present study presents a general perspective on materials modelling and optimisation, demonstrating complementarity across scales and applications.

Proposed conceptual framework

As illustrated in Figure 7, a conceptual framework has been developed to integrate the primary dimensions of the study. The diagram summarises the most commonly used machine learning techniques, the types of materials evaluated, the properties modelled, the optimisation objectives, and the identified limitations. The figure illustrates the relationships between these elements, thereby providing a clear perspective on the current state and supporting future research in the modelling and optimisation of materials for energy storage using ML.

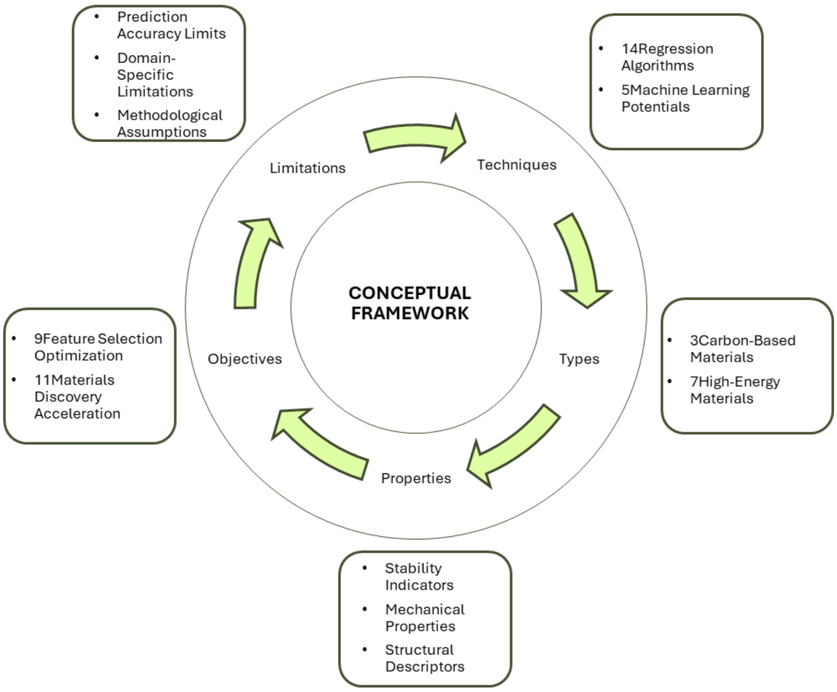

Figure 7. Conceptual framework for ML applications in energy materials. Prepared by the authors.

Implications

The findings of this research on the utilisation of ML applications in the modelling and optimisation of materials for sustainable energy storage hold significant implications for theoretical, policy, and practical domains. These interrelated dimensions provide insight into the scope and importance of ML in the transition to efficient and sustainable energy technologies. From a theoretical perspective, the findings serve to strengthen and expand the conceptual foundations for the integration of ML techniques in materials science. The present study confirms the increasing effectiveness of algorithms such as neural networks, regression, and generative models for predicting critical physical and chemical properties in energy materials.

However, limitations have been identified, including issues related to data quality and availability, the difficulty of generalising models outside of training sets, and the discrepancy between computational predictions and experimental validation. In order to address these factors, there is a necessity to develop theories capable of robustly integrating theoretical modelling, experimental data acquisition, and algorithmic optimisation. Moreover, it is proposed that the theoretical framework be expanded to incorporate multidisciplinary approaches, including computational chemistry, materials physics, advanced statistics, and explainable artificial intelligence. This approach is intended to enhance the interpretability and reliability of ML models.

In terms of policy, the results suggest that public and sector policymakers should promote strategic support for projects that generate high-quality, openly accessible data. Data scarcity and fragmentation have been identified as significant barriers to technological advancement and reduced competitiveness in the energy sector. Policies that encourage collaboration between academic institutions, technology centres, and industry can facilitate the creation of common repositories and standards for managing experimental and simulated data. In a similar vein, governments and regulatory bodies must establish regulatory frameworks that incentivise the responsible implementation of ML in energy materials, ensuring transparency, reproducibility, and safety.

It is imperative that the technical capacities of public institutions are strengthened in order to ensure that regulation is able to keep pace with advances without hindering the adoption of innovations. In summary, it is imperative that public policies are aligned with technological dynamics in order to facilitate the sustainable energy transition and ensure technological sovereignty in the domain of energy storage materials. The findings of this study demonstrate that, in practical and industrial settings, there is a significant impact on materials development and optimisation methodologies. The utilisation of ML has been demonstrated to expedite the design of materials characterised by specific properties, enhance energy efficiency, and reduce the economic burden associated with conventional experimental methodologies.

However, the practical implementation of such systems faces several challenges, including the effective integration of experimental data, the continuous validation of models, and the training of specialised personnel. In the context of energy and technology companies, ML facilitates the optimisation of synthesis and scaling processes, and the design of more robust and durable storage systems. The integration of ML within autonomous laboratories and integrated platforms holds the potential to transform the domain of research and development, facilitating rapid iteration cycles between simulation and testing. From a scientific perspective, the present study proposes a systematic framework to guide future research in addressing knowledge gaps.

The development of hybrid methods that combine machine learning with physical simulations and experimental data is promoted, with the objective of obtaining more accurate and applicable models. The integration of theoretical, policy, and practical implications demonstrates the multidimensionality of the challenge posed by the incorporation of machine learning into energy storage materials. The development of integrative theories, the formulation of policies that encourage collaboration and data generation, and the adoption of innovative industrial practices are identified as fundamental pillars for progress in this field. It is imperative to emphasise that interdisciplinary and multisectoral cooperation will be crucial to overcome current limitations and realise the potential of machine learning in sustainable and efficient energy solutions.

Limitations

The study presents methodological limitations that affect the interpretation of the results. The paucity of data available for the training and validation of machine learning models had a detrimental effect on the generalisation capacity and robustness of the algorithms. It is posited that this restriction may engender bias and consequently diminish the accuracy of material property prediction, a phenomenon that is especially salient in cases with limited experimental representation. The heterogeneity of materials and modeled properties impeded the uniform selection and comparison of ML techniques, thereby limiting the depth of the comparative analysis. Moreover, the overreliance on public databases and literature resulted in constrained access to unpublished or specialised information, which had the potential to influence the identification of limitations and opportunities. The discrepancy between computational simulations and experimental validation persists as an unresolved challenge, impacting the practical applicability of the models. In conclusion, the overarching methodology of the study precluded the investigation of particular applications and the formulation of bespoke methodologies. These limitations underscore the necessity for future research to be conducted with more comprehensive experimental data and hybrid methods.

Lines of future research

It is recommended that future lines of research concentrate on the generation and consolidation of broad, homogeneous, and accessible experimental databases. This will enhance the quality and quantity of information for the training and validation of ML models. The integration of data from diverse sources, including autonomous laboratories and advanced simulations, will facilitate the development of robust and generalizable models.

The promotion of common standards for the collection, normalisation, and storage of data on energy storage materials is imperative, as is the fostering of interdisciplinary and multisector collaboration. It is recommended that advances be made in hybrid methods combining ML with physical simulations and experimental techniques in order to bridge the gap between computational predictions and practical validation. The development of algorithms that are both explainable and transparent will increase the interpretability and confidence of results, facilitating their adoption in industrial and regulatory contexts. The exploration of generative models and reinforcement learning offers the potential to accelerate discovery and design with specific objectives, such as energy efficiency and durability. It is recommended that future research place a priority on the application of ML to technologically relevant materials, including thermochemical and electrochemical compounds. The identification of critical properties and mechanisms that favour optimisation is of paramount importance in this field.

This will overcome limitations derived from general analyses and promote methodological proposals adapted to specific contexts. It is imperative to address the challenges associated with the scalability and reproducibility of ML models in real-life experimental settings. In order to ensure relevance and applicability, continuous validation and updating with new data is required. The development of specialised talent and the strengthening of technical capacities in academic institutions and companies will enhance research and transfer to the productive sector.

Finally, the development of public policies and regulatory frameworks that foster cooperation between academia, industry, and government should be encouraged, along with investment in infrastructure for data management and generation. These actions will facilitate the responsible and efficient implementation of ML in the development of energy storage materials, contributing to sustainable and competitive energy systems. Collectively, these proposals form a comprehensive strategy to surmount current limitations and optimise the impact of machine learning in this domain.

Conclusions

This study underscores the expanding role of ML in the modelling and optimisation of materials for sustainable energy storage, unveiling a multifaceted and intricate landscape. The diversity of applied techniques indicates an expanding field, where the convergence of traditional and emerging algorithms points to solutions that balance accuracy, efficiency, and predictive capacity. The range of materials examined illustrates the possibilities and difficulties involved in adapting ML to particular contexts, emphasising the necessity for methodologies that take into account chemical and structural particularities.

The intricacy of the modelled properties necessitates models that are capable of integrating multiple scales and data types. The objectives of optimization are oriented towards the enhancement of processes and materials, with the aim of accelerating the cycle between discovery and application. Nevertheless, the documented limitations suggest that model robustness and generalisation persist as considerable challenges, underscoring the necessity to integrate rigorous experimental data with methodological advancements.

This analysis, in accordance with recent studies, suggests that the future of ML in this field is contingent on technical innovations, as well as interdisciplinary integration and multisector collaboration. In order to optimise the impact of ML on energy storage materials, it is imperative to formulate frameworks that seamlessly integrate theory, experimentation and industrial application in a coherent and sustainable manner.

Acknowledgements

Not applicable

Data Availability Statement

The data support the findings will be available upon reasonable request

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