Journal of Computational Systems and Applications

https://jcsa.cultechpub.com/jcsa

Cultech Publishing

Review

AI-Driven Computational Insights into Electrochemical Energy Storage: A Review of Emerging Trends in Battery Chemistry

Ansar B. Adam[1,*], Raymond B. Donatus[1], Emmanuel B. Attahdaniel[1], Hyelalibiya Ataitiya[1], Oluwadolapo J. Ewenifa[2], Musa Y. Abubakar[2], Abubakar M. Shittu[3]

[1]Department of Chemistry, Federal University Wukari, Wukari, Nigeria

[2]Department of Inustrial Chemistry, Federal University Wukari, Wukari, Nigeria

[3]Department of Chemistry, University of Jos, Jos, Nigeria

[*]Corresponding author: Ansar B. Adam, ansarbilyamin@gmail.com

Abstract

Modern battery technologies depend on electrochemical storage systems. However, the performance of such systems is limited by complicated multi-scale processes. These processes include transport of ions, interfacial reactions, and degradation processes. These coupled physicochemical dynamics across scales cannot be captured accurately by traditional computational methods. This review analyzes more than 150 recently published studies (2018-2025) on the seamless integration of artificial intelligence like machine learning and deep learning and physics-informed hybrid models with standard computational chemistry frameworks. As materials discovery and performance optimization are increasingly accelerated by AI-powered methods, this review provides a systematic overview of their applications, successes, and challenges in electrochemical energy storage. AI-powered techniques are speeding the discovery of high-performing electrode materials (Ni-rich cathodes, solid-state electrolytes). AI can increase battery lifetime prediction accuracy by 30-50%. It can also lead to the development of digital twins for real-time monitoring and optimization of systems. Also, the review notes developing trends towards autonomous laboratories and self-optimizing battery systems, where AI connects data-driven insights to fundamental chemical understanding. Our study reveal the immense potential of AI in developing next-generation, sustainable, and circular electrochemical energy storage technologies. Further, they also highlight the challenges and research directions for effective deployment.

Keywords

Artificial intelligence, Battery chemistry, Computational modeling, Electrochemical energy storage, Digital twins

Article History

Received: 30 September 2025 Revised: 17 November 2025

Accepted: 27 November 2025 Available Online: 05 December 2025

1. Introduction

The consumption of energy worldwide has been ever-growing since industrialization and urbanization, a trend enhanced by technology. Conventional fossil fuels can no longer fulfill the demand due to greenhouse gas (GHG) emissions, climate change, and environmental degradation [1]. Renewable and low-carbon energy systems guarantee the long-term security of energy supply with minor damage to the environment [2].

The greatest challenge for renewable energy sources, such as wind and solar energy, is their intermittent nature. The electrochemical energy storage systems (battery, supercapacitor) are responsible for storing high levels of excessive energy during times of high generation and releasing it during times of less production [3]. These technologies ensure the stability of grids, enable the incorporation of renewable energy into existing systems, and power e-mobility and smart gadgets on the go.

The performance of the electric energy storage system (EESS) is determined mainly by the battery chemistry that governs energy density, lifetime, and efficiency. New battery designs for lithium-sulfur, sodium-ion, and solid-state storage devices explore innovative electrode and electrolyte designs. We must make these processes more efficient, not only to meet sustainability objectives but also to meet the evolving technology needs of applications like electric vehicles and decentralized microgrids [4].

In the coming years, artificial intelligence (AI) and machine learning (ML) are expected to play an important role in making our research work more effective and efficient. Chemical science discoveries are being driven by technology, which can be used to analyze large datasets and allow the identification of relationships that would not otherwise be observable, according to [5,6].

The Figure 1 aboveillustrates a multiscale modeling framework that connects materials-level phenomena to device-level behavior in electrochemical energy storage systems, with AI integrated across all scales. At the materials scale, quantum-chemical methods (e.g., Density Functional Theory (DFT), ab initio) capture active sites, electronic structure, and bonding. Molecular- and nanoscale processes, including ion solvation, electrolyte composition, and solid electrolyte interphase (SEI) formation, are resolved using molecular dynamics (MD). Micro-/mesoscale aspects such as electrode architecture, porosity, and interfacial contact are represented through continuum and multiphysics models. These outputs feed into AI- and machine-learning-based digital twins, which enable system-level predictions of full-cell behavior, thermal effects, and grid integration. Across scales, the integrated framework supports analysis of key degradation mechanisms--including thermal runaway, capacity fade, and voltage instability--thereby providing a unified platform for navigating materials development, modeling complexity, and performance degradation.

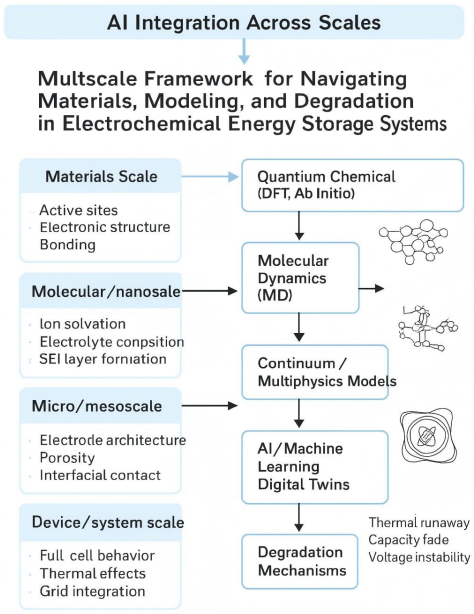

Figure 1. Multiscale framework for navigating materials, modeling, and degradation in electrochemical energy storage systems.

The diagram shows the hierarchy between material scales, modeling frameworks, and degradation mechanisms. The article discusses the integration of quantum chemical, MD, and continuum multiphysics models across atomic to system levels, with AI as a cross-scale bridge for AI-driven prediction and optimization.

In electrochemistry, applications refer to the optimization of electrode architecture, performance prediction when vital operating circumstances of batteries occur, and discovery of new catalysts for energy conversion systems [7]. Moreover, artificial neural networks and support vector machines enable researchers to evade inefficient trial-and-error experiments [8,9].

The study focuses on the advanced exploration of electrochemical energy storage systems and their AI-powered developments for energy transition. That review argues that interdisciplinary strategies for next-gen energy technologies like AI can simplify tech Research and Development pipelines (R&D pipelines), battery chemistries, and real-time performance management. AI will help shape solutions to global energy issues. It will improve efficiency for heat loss, irreversible reactions, and others. We will reach sustainable energy infrastructures through the technology.

2. Methodology

2.1 Research Design

This systematic review study seeks to summarize and discuss the intersection of AI and computational chemistry in improving electrochemical energy storage research. By means of qualitative synthesis and quantitative trend analysis, this method assesses the rising use of AI for new battery chemistries, modelling frameworks, and material design. A well-defined and reproducible method was adopted to ensure rigor and comprehensive coverage of the literature landscape as per Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) 2020 guidelines.

2.2 Literature Search Strategy

Relevant peer-reviewed publications were obtained through a multi-database search, which includes Scopus, Web of Science, IEEE Xplore, ScienceDirect, and Google Scholar. The search took place between 2018 and 2025, which indicates the rapid incorporation of AI in battery science.

Search terms included combinations of keywords such as: Boolean operators (AND, OR) and truncation were applied. Searches like “artificial intelligence AND battery chemistry” and “machine learning OR deep learning AND electrochemical storage” guaranteed broad coverage while being highly relevant. The reference lists of important reviews were also searched for any additional studies.

The Figure 2 illustrates the yearly number of publications over an eight-year period. Research output shows a steady increase from 2018 to 2023, peaking sharply in 2024 before declining in 2025. This pattern reflects growing scientific interest followed by a slight correction or stabilization in the most recent year.

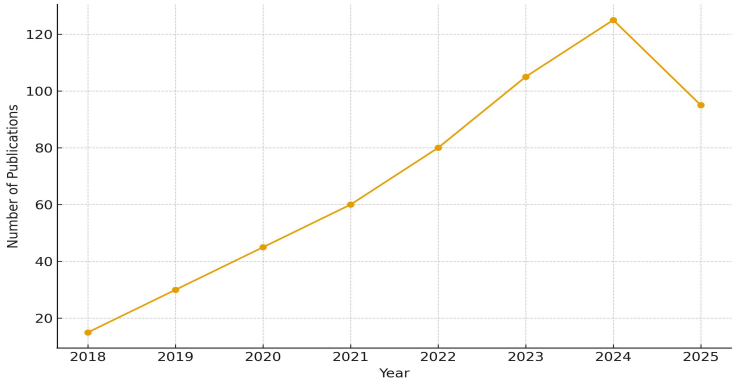

Figure 2. Trend on AI electrochemicalenergy storage (2018-2025).

2.3 Inclusion and Exclusion Criteria

The studies were selected based on the following criteria to maintain focus and quality.

Inclusion criteria: Articles, conference papers, and systematic reviews published in scientific or peer-reviewed journals. It involves using AI or a computer to check batteries. Concentrate on discovering materials, modeling degradation, or optimizing performance. Insights found in either quantitative or qualitative form related to electrochemical energy storage.

Exclusion criteria: Non-English publications. Studies not related to energy storage or lacking methodological transparency. Reports lacking usable data or insufficient talk about AI use.

After screening and re-screening stage-wise, forty-eight core publications were shortlisted for final analysis.

2.4 Data Extraction and Analysis

Data extraction followed a structured template, recording: publication details (authors, year, source); battery type or chemistry investigated; techniques used, Neural Networks, Random Forest, Support Vector Machine (SVM), etc.; types of computational Frameworks for thermodynamic calculations; essential outcomes that connected with material design, performance prediction, and degradation.

There was a repetition of the themes with a similar method. The frequency of AI technique use, through time series analysis, and modeling use and expert number, through descriptive statistics, was summarized by trend analysis. The analyses were visualized through trend figures and comparative charts, respectively.

2.5 Quality Assurance and Validation

A two-level review was done to ensure reliability and avoid bias.

(1) Independent screening of titles, abstracts, and full texts for relevance.

(2) Methodological quality assessment based on adapted PRISMA criteria evaluating transparency, completeness, and reproducibility.

Table 1 presents a summary of the literature screening and selection process conducted according to the PRISMA guidelines. The table details the number of records identified through the initial search, duplicates removed, records excluded at title/abstract and full-text stages, and the final number of studies included in the systematic review.

Table 1. Summary of literature screening and inclusion based on PRISMA framework.

Screening Stage	Records Identified	Records Excluded	Records Included
Initial database search	412	-	-
Duplicates removed	48	-	364
Title/abstract screening	-	212	152
Full-text assessment	-	84	68
Final included studies	-	-	68

2.6 Conceptual Framework and Integration

The extracted data were synthesized into a conceptual framework illustrating how AI integrates across computational hierarchies from quantum chemical modeling to digital twin systems. This framework underpins the organization of subsequent sections, each corresponding to a specific modeling level (quantum, molecular, continuum, and system optimization). The fusion of data-driven and physics-based approaches forms the central analytical perspective of this review.

2.7 Ethical and Sustainability Considerations

Given the environmental and ethical discourse surrounding AI deployment, the review also incorporated sustainability assessments. Studies were evaluated for discussions on data ethics, computational energy efficiency, and environmental impacts of AI-driven material discovery. This ensured alignment with broader principles of sustainable innovation and responsible research within the circular energy economy.

3. Fundamentals of Battery Chemistry

Now that we've discussed how we searched the literature and how we analyzed what we found, we turn our attention to the chemistry of batteries, the subject of the application of AI and computational approaches. To understand how AI can help optimize electrochemical energy storage processes and predict performance over time, it's important to first understand the battery types, reactions, and degradation mechanisms involved. The next section presents a comprehensive view of the electrochemical storage systems with respect to design and operation.The creation of effective and long-lasting systems for storing energy through electrochemical processes is one of the most critical areas of research in modern energy science. These systems can transform chemical energy into electric energy and opposite way. This can offer solutions to the intermittency challenges of renewable energy sources like solar and wind.

3.1 Types of Electrochemical Storage Systems

The modern strategy for electrification and decarbonization depends on energy storage technologies. The growing needs for portable electronics, electric mobility, and large-scale grid stabilization motivated their development. Today, several battery chemistries dominate the well-established and developing technology. Each chemistry offers its own unique advantages and challenges.

3.1.1 Lithium-Ion Batteries

Lithium-ion batteries (LIBs) are the most used storage devices for their high energy density, long cycle life, and relatively high efficiency [10,11].

LIBs are so successful precisely because lithium ions are lightweight and highly reactive, and they can quickly intercalate into layered electrode materials. This has helped LIBs run mobile phones, laptops, and electric motors and work on storage projects on the grid.

Although LIBs have achieved commercial maturity and wide adoption, their critical challenges remain prominent. Thermal runaway is a serious safety problem: fast charging generates too much heat and can lead to other kinds of destructive failure [12]. Furthermore, the short supply of critical raw materials such as cobalt and nickel raises sustainability, ethics, and cost turbulence issues [13]. It is not cost-effective and is technologically difficult to recycle LIBs at an industrial scale.

3.1.2 Sodium-Ion Batteries

Sodium-ion batteries (SIBs) are rising as a good alternative option for LIBs because sodium is cheap, abundant, and well distributed. No lithium resources are concentrated in geopolitically sensitive areas. This makes SIBs attractive for global deployment.

The electrochemistry of SIBs is similar to that of LIBs since sodium ions shuttle between their cathode and anode. The large ionic radius of sodium leads to poor Na^+ diffusion and intercalation capacity. This is the reason for the low energy density in SIBs [14]. In contrast, SIBs are seen as ideal for stationary grid-scale storage, where cost and sustainability trump size and weight.

3.1.3 Solid-State Batteries

Solid-state batteries (SSBs) use solid electrolytes which makes them much safer than LIBs. The use of non-volatile organic solvents minimizes fire hazards while the use of lithium metal anodes can achieve much higher theoretical capacities than graphite.

However, SSBs still have unsolved issues involving interfacial resistance, dendrite formation, and mechanical instability at electrode-electrolyte boundaries [15]. The commercial use of solid state battery technology has been delayed due to technical challenges but automakers and research institutions are working on it.

3.1.4 Flow Batteries

Flow batteries, like the vanadium redox flow batteries (VRFBs), differ from conventional designs in that energy capacity and power capacity are decoupled. Liquid electrolytes are contained in external tanks where energy is stored, and the power output depends on the size of the electrochemical cell stack.

Flow batteries are ideal for larger-scale renewable integration, where size, efficiency, and cost are notably less important than scalability, safety, and long operational life [16]. The application of these batteries in mobile and portable devices is limited due to their low energy density and higher system complexity.

Table 2 provides an overview of four major electrochemical energy-storage technologies—LIBs, SIBs, SSBs, and redox Flow Batteries (e.g., VRFBs). For each system, the table summarizes the operating mechanism, key advantages, performance limitations, and typical application domains. The comparison highlights differences in sustainability, safety, energy density, and scalability, offering a foundational context for evaluating next-generation storage solutions. Values and descriptions reflect general characteristics reported across contemporary literature.

Table 2. Comparative summary of electrochemical storage systems.

Battery Type	Mechanism	Advantages	Challenges	Applications	Ref.
LIBs	Lithium ions shuttle between cathode and anode through liquid (or hybrid) electrolyte; widely used 'intercalation' chemistry.	High energy density; Long cycle life; High efficiency; Well-established manufacturing base.	Thermal runaway and safety risks; Degradation; Dependence on cobalt and nickel; Recycling challenges.	Portable electronics, Electric Vehicles(EVs), grid storage.	[17-19].
SIBs	Sodium ions (Na^+) intercalate in similar electrode hosts; cheaper, more abundant sodium rather than lithium.	Low cost and abundant sodium; Geopolitically stable; Environmentally sustainable.	Lower energy density due to larger ionic radius; Slower diffusion; Limited intercalation capacity.	Stationary energy storage, grid-scale balancing, renewable integration.	[20,21]
SSBs	Replace liquid electrolytes with solid ones; enable lithium or sodium metal anodes for enhanced energy density.	Enhanced safety; Higher theoretical capacity; Longer lifespan potential.	High interfacial resistance; Dendrite formation; Mechanical instability; High production cost.	Next-generation EVs, aerospace, compact grid storage.	[22,23]
Flow Batteries (e.g., VRFBs)	Energy stored in liquid electrolytes in external tanks; decoupled power and energy capacity.	Scalable; Long operational life; High safety; Flexible system design.	Low energy density; Bulky system; Complex balance-of-plant.	Grid-scale renewable integration, load leveling, backup storage.	[24]

3.1.5 Emerging Chemistries

Specialized chemistries like lithium-sulfur (Li-S) and metal-air batteries are being developed beyond the mainstream. Due to the multi-electron redox ability of sulfur, Li-S batteries offer a very high theoretical energy density. Metal-air systems (e.g., zinc-air, lithium-air) rely on abundant oxygen from the air as one cathodic reactant and can drastically reduce weight.

These systems show rapid capacity fading lithium-sulfur (Li-S) due to polysulfide dissolution, and air cathodes (metal-air batteries) are unstable, according to [25]. To overcome them, a breakthrough in electrode design, electrolyte, and material engineering is needed.

Different electrochemical systems available today have several trade-offs in energy density, safety, cost, and scalability. Ongoing energy storage demands across sectors highlight the need for innovation in systems to meet more complex energy needs.

3.2 Chemical and Physical Processes

The underlying physical and chemical processes govern the operation and performance of all electrochemical storage systems.

3.2.1 Ion Transport

The primary battery operation mechanism is the migration of ions between the electrodes through the electrolyte. In LIBs, lithium ions move from one terminal to another when charge and discharge occur between two terminals. This transport depends on the ionic conductivity of the electrolyte, the porosity of the electrode, and diffusion pathways.

3.2.2 Electrode-Electrolyte Interfaces

The interface between the electrode and electrolyte is crucial to the stability and performance of the battery; it is stable by design, but it is dynamic in nature. The formation of a solid-electrolyte interphase on the anode of LIBs acts as a protective layer and can slow down electrolyte decomposition through its ion transport control mechanism that is effective in further suppressing side reactions. The formation of SEI, however, consumes active lithium, reducing the capacity of the battery at the beginning. Simultaneously, a corresponding cathode−electrolyte interphase (CEI) constructs on the cathode surface, which prevents oxidative degradation and stabilizes the high-voltage interface [26]. Long-term interfacial stability requires both SEI and CEI layers. According to a recent study, dendrite penetration and poor interface contact remain serious challenges to commercialization in SSBs.

3.2.3 Degradation Mechanisms

Battery cycling over a long period causes numerous degradation processes that decrease the life and efficiency of batteries. Phase transformations and structural collapse can cause deterioration of cathode, plating and dendrite growth of lithium are dangerous as well, such as internal short-circuit. Decomposition of electrolytes could produce gas which enhances internal resistance and poor performance. Also, thermal instability, in particular, with conditions of fast-charging, further enhances the process of battery damage. In order to comprehend and address these concerns better, sophisticated diagnostic methods, along with spectroscopy methods with the ability to monitor in real-time and in situ, are being utilized more and more [27].

3.2.4 Thermal Effects

Thermal management is another critical issue. Heat generation during operation leads to chemical degradation and increases the risk of thermal runaway. In high-power applications [28], battery design must incorporate effective thermal regulation strategies for safety and high performance.

3.3 Limitations of Conventional Modeling Approaches

Even though we have progressed extensively in battery science, conventional modeling approaches are still inadequate to tackle electrochemical systems.

3.3.1 Simplified Assumptions

Conventional models often assume dominantly idealized ion transport, electrode kinetics, and thermodynamic equilibria. These simplifications do not capture multiscale interactions, from the atomic level to the system level [29].

3.3.2 Predictive Gaps

Standard models show limitations in their ability to predict capacity fade, safety risks, and cycle life for different conditions. For example, mechanisms of degradation, such as SEI growth, dendrite penetration, and cathode phase transitions, are challenging to model deterministically due to their stochastic nature [30].

3.3.3 Computational Costs

Simulations that are based on physics, like DFT and MD, are helpful but require many calculations. Scaling these techniques to cover the vast material space of potential electrode and electrolyte candidates is not feasible in a reasonable timeframe.

3.3.4 Transition Toward Data-Driven Models

In light of these limitations, data-centric and AI-based models leveraging either extensive experimental datasets or large computational datasets will be helpful to uncover hidden correlations, predict optimal material combinations for better performance, and optimize battery operation in real-time. Methods powered by AI can create a solution to the theory and practice gap. This could help in discovering new chemistries while saving efforts on costly trial-and-error methods.

Battery chemistry is all about how the different materials and chemicals work together, as well as how the battery is put together as a whole. At present, LIBs are the dominant technology competing for the commercial market. However, other systems such as SIBs, SSBs, and flow batteries are also on the rise. More importantly, new chemistries like Li-S and metal-air are emerging as possibilities, as the global community continues to seek more sustainable sources that can potentially scale up. The issues with ions moving, stability of substances, and wear hereby prove the need for advanced methods beyond standard modeling techniques. All these challenges provide an exciting opportunity for AI applications to fast-track the material discovery, performance optimization, and real-time monitoring in electrochemical energy storage systems.

Now that we have established a strong understanding of the fundamental processes at work in battery systems, it becomes evident how computational methods are essential in advancing the design and functionality of these systems.

Table 3 summarizes the major limitations inherent in traditional modeling frameworks used in electrochemical systems--including LIBs, emerging Na-ion and solid-state systems, and other next-generation chemistries. The table categorizes common challenges such as oversimplified assumptions, predictive shortcomings in capturing non-linear degradation phenomena, computational constraints associated with first-principles methods, and the growing need for adaptive, data-driven modeling techniques. Understanding these limitations is critical for evaluating why AI- and ML-based approaches are increasingly adopted to enhance multiscale prediction accuracy, accelerate materials discovery, and support the modeling of complex electrochemical environments.

Table 3. Limitations of conventional modeling approaches in electrochemical systems.

Limitation	Concise Description	Impact on Modeling Accuracy	Ref.
Simplified Assumptions	Idealized ion transport and homogeneous kinetics assumptions Overlook atomistic and interfacial effects crucial for realistic behavior	Poor multiscale accuracy Limited capture of transient and interfacial dynamics	[29]
Predictive Gaps	Cannot model non-linear processes (e.g., SEI growth, dendrite formation, phase transitions) Struggle with stochastic, multi-physics behavior	Weak long-term forecasting of cycle life, capacity fade, and safety	[30]
High Computational Cost	DFT and MD restricted by small system size and timescale Expensive for large-scale material screening	Limits exploration of new chemistries Slows material innovation and optimization	[31]
Transition Toward Data-Driven Models	AI and ML integrate simulation and experimental data Capture complex non-linear correlations	Improve predictive power and degradation modeling Accelerate discovery and design cycles	[32]
Emerging Systems Beyond LIBs	Na-ion, solid-state, Li-S, and metal-air systems introduce new modeling challenges Require adaptable frameworks	Increase modeling complexity Demand transferable, multiscale approaches	[33]

4. Computational Approaches to Battery Systems

To effectively create enhanced battery systems, electrochemical processes must be well understood at many different levels at once. This includes those at the level of atoms to processes taking place at the cell level [34]. Computational modeling plays an increasingly important role in battery research by providing predictive frameworks that can inform material design, performance optimization, and degradation mitigation. In this part, we consider the primary computational methods used in battery science. These include quantum chemical methods, MD simulations, continuum, and multiscale techniques. Next, we discuss their strengths and weaknesses. Finally, we discuss their future integration into data-driven methods.

4.1 Quantum Chemical Methods (DFT and Ab Initio Studies)

At their most basic level, quantum chemical calculations shed light on the electronic structure, bonding, and charge distribution of the materials making up battery electrodes and electrolytes. DFT has become the most used quantum mechanical method because of the right balance between accuracy and computability [31].

DFT provides scientists with an opportunity to examine the most important atomic-level phenomena that determine battery performance. It is used to measure the energy needed to add or remove lithium or sodium ions in electrode lattices, measure band structures and the electrical conductivity of electrode materials, and determine the ranges of electrochemical stability of several battery systems. DFT can also offer information on the reaction pathways of electrodeelectrolyte interfaces as well as help in comprehending the creation and development of the solid-electrolyte interphase. These lessons are important in uncovering the degeneration or breakdown of batteries and in informing ways to avoid such breakdowns [35].

Ab initio methodologies can be more accurate than DFT, Examples are coupled cluster or many-body perturbation theory, where electron correlation is treated explicitly. Nonetheless, their computing demand limits their adoption to tiny clusters or model systems. Consequently, they serve a more useful purpose as benchmarks of DFT approximations [32]. Quantum chemical methods can provide resolution of structure-property relationships at the atomic level, thus guiding experiment and validating new materials.

4.2 Molecular Dynamics Simulations

MD simulations enable the examination of the time-dependent motion of atoms and ions within a material, thus going beyond the DFT static picture. MD simulations can be categorized into two main classes.

Ab Initio Molecular Dynamics (AIMD) is based on DFT, which provides highly accurate dynamical trajectories that can capture bond breaking, charge transfer, and solvation structures in electrolytes. Though the picosecond timescales and nanoscale system sizes limit AIMD as much as DFT, making it impractical for large-scale studies.

Using reactive or empirical force fields, classical MD greatly increases the accessible time scales (nanoseconds to microseconds) and system sizes (thousands to millions of atoms). This makes it possible to study ion diffusion pathways, the mechanical stability of solid electrolytes, and the evolution of electrode interface morphology [31].

Reactive force field methods like Reactive Force Field (ReaxFF) try to mimic bond-breaking and forming actions. This increases the use of MD in SEI growth and electrode degradation. Spin-dependent interactions in transition metal oxides, which are important in cathode chemistries [36], are often beyond the capability of these force fields.

Simulations help understand how ions move in specific and general conditions and binding site interactions in liquid electrolytes. Nevertheless, the accuracy of MD is heavily determined by the force field quality, which usually needs parameterization from higher-level quantum calculations, demonstrating a need for integrated multiscale workflows [32].

4.3 Continuum and Multiscale Models

Battery behavior at larger scales may be captured by continuum models. The continuity, governed by partial differential equations, consists of ion and electron transport, electrochemical kinetics, and thermal effects.

Continuum-scale models are used to model macroscopic behavior of batteries, including charge and mass transport in electrodes and electrolytes, reaction kinetics of electrochemical reactions based on ButlerVolmer equations, and other cell-scale influences, including power losses, polarization of concentrations, and thermal runaway. These aspects combined can be used to predict the overall battery performance and optimally design more efficient and stable energy-storage systems.

Engineers use continuum models to maximize the shaping of cellular geometry, the cycling protocol, and the temperature control. The predictive accuracy of these models is contingent, among others, upon the diffusion coefficients and (reaction) rates input in the model, which are usually obtained via atomistic (e.g., DFT, MD) studies and/or experiments [34].

We need multiscale modeling frameworks to get from atomic to macroscopic scales. For example, DFT, and MD insights at the atomic level can provide continuum parameters such as diffusion constants or reaction rate coefficients. In a similar manner, continuum models can guide targeted atomistic simulations by pinpointing bottlenecks in ion transport or heat dissipation.

This kind of hierarchical approach is beneficial for understanding dendrite growth, mechanical fracture of solid electrolytes, gas evolution in liquid electrolytes, etc., some of the instances of degrading interfaces.

4.4 Challenges in Traditional Computational Models

Even though they have made great strides, conventional computational approaches still face challenges when applied to complex electrochemical systems.

4.4.1 Computational Cost and Scale Limitations

Since DFT and AIMD methods have small system sizes and short timescales, they cannot capture mesoscale processes like SEI evolution or dendrite growth [32]. Simulation studies initiated explain bulk behavior and also show that MD

simulations can increase system size with limited accuracy, depending on force fields. In other words, often force fields are not enough for the complex joining of multi-components to materials [36].

4.4.2 Integration Across Scales

The major problem is linking atomic-level insights to large-scale models systematically. For instance, the processes impacting capacity fade are longer than the processes impacting ion migration, which occur on picosecond timescales. The uncertainties are not appropriately propagated, and the emergent behaviors are not captured [35].

4.4.3 Complex Chemistry

The operation of batteries is complex; it involves electrolyte breakdown, harmful gases, and metal dissolution. Recent developments in excised-cell photodissociation studies from the Karpowicz lab are also promising in generating hydrogen and oxygen from water photolysis. The Sinha and Teo labs have developed single-atom catalysts to generate hydrogen from water using photothermal catalytic processes efficiently.

4.4.4 Toward Data-Driven Integration

To get around these issues, there is an increasing reliance on ML and AI-based potentials that can yield quantum accuracy at a low computational cost. Methods like neural network potentials and Gaussian approximation potentials allow for atomistic simulations of larger systems for longer timescales [37,38]. By being linked to handcrafted and existing methodologies, these approaches will bridge scale gaps and enhance material discovery and predictive power.

We can start with quantum chemical calculations of atomic interactions and end with continuum descriptions of device-scale phenomena. The insights it provides into battery chemistry and performance are crucial. Quantum and MD simulations provide high fidelity at the atomic scale. Concepts of continuum models allow for engineering-level optimization. However, the natural multiscale complexity of electrochemical systems creates difficulties that traditional computational methods cannot solve alone. Blending these approaches with ML- and AI-based frameworks promises new avenues for developing scalable, accurate, and predictive simulations to enable the design and deployment of next-generation electrochemical energy storage systems.

While computational approaches have paved the way for understanding the fundamental behavior of battery systems, their integration with AI is where significant advancements are taking place. There is a need to know how AI, by leveraging vast datasets and advanced algorithms, is transforming battery chemistry, improving material discovery, accelerating optimization processes, and enhancing the accuracy of performance predictions.

5. AI in Battery Chemistry

As battery systems become more complex, with widely varied mixtures of electrodes and electrolytes and nonlinear dynamics of electrochemical reactions, modeling and experimental approaches are becoming increasingly insufficient and, at best, are useful approximations of reality. The application of AI, especially ML and deep learning, offers different computational paradigms that can lower the complexity of data, reveal new patterns, and shorten the discovery cycles [39]. AI methods are changing the way scientists conduct battery material design, reaction analysis, performance prediction, and degradation modelling by supplementing or replacing traditional trial-and-error experimentation.

5.1 Machine Learning for Material Property Prediction

Utilizing ML will enable one to predict material properties without relying too heavily on expensive methods like DFT. Random forests, support vector machines, and gradient-boosted trees are being deployed to associate chemical composition and structural descriptors with electrochemical performance. These methods enable researchers to test new materials quickly and to predict the ionic conductivity, stability windows, and redox potential of their electrodes [8].

The ability to predict and tailor new materials for performance is needed for the enormous design space of electrode and electrolyte materials. This design space is too ample to be thoroughly investigated in the lab. For instance, ML-based models are capable of quickly rejecting candidates that were predicted to have poor electrochemical stability or low ion mobility, thus down-selecting a promising pool of candidates for experiments [9]. What this means is that these approaches are able to predict things more than conventional DFT. Moreover, this allows the evaluation of new things, compositions, and architectures that would otherwise be impossible to do.

5.2 Deep Learning for Reaction Mechanism Discovery

Even though ML can predict properties well, deep learning can isolate nonlinearity and hidden linkages well in high-dimensional data or image analysis. Battery operation processes such as reaction kinetics, electron transfer, and structural rearrangements have increasingly been modelled using deep neural networks, convolutional models, and recurrent architectures.

One key area where it is valid is the analysis of in situ and operando data streams, such as X-ray diffraction, Raman spectroscopy, or electrochemical impedance spectroscopy. Usually, such datasets are large, noisy, and complex. Therefore, they are ideal candidates for deep learning models that extract reaction signatures and mechanistic trends [39]. Can identify temporal or spatial correlations in the data to provide insight into intermediate phases, reaction pathways, and rate-limiting steps in charge-discharge cycles. It is essential to understand such complicated processes, e.g., SEI formation, dendrite growth, or cathode degradation mechanisms, that are hard to model theoretically [40].

5.3 AI-Enabled Electrode and Electrolyte Design

Another way that AI can transform the field is by making the design of electrodes and electrolytes faster. Conventional design relies on empirical tests and iterative changes, which are very expensive and time-consuming. On the other hand, models of AI can quickly explore multi-dimensional design spaces of their own and identify the best combinations of composition, structure, and operational conditions.

AI may help navigate trade-offs between capacity, stability, and cost concerning electrode materials involving transition metal oxides, polyanionic compounds, and composite architectures. The transport, viscosity, dielectric constants, and electrochemical stability windows of electrolytes can be predicted by AI, ultimately leading to faster discovery of safer and better formulations [41].

By including economic and other constraints, they can also help satisfy performance constraints with sustainability. With cost factors, recyclability, and abundance metrics incorporated into the design process, optimization of performance is ensured, not just electrochemical performance alone [9].

5.4 Data-Driven Models for Lifetime and Degradation Prediction

One of the biggest hurdles in battery science right now is long-term performance and degradation prediction for commercial viability. In traditional testing, you need years of cycling data. AI allows us to predict capacity fade, impedance growth, and failure modes from a shorter-term data stream.

Using inputs like operating conditions and in situ measurements, data-driven models expose patterns of degradation using thermal data and cycling history. Methods such as time-series forecasting, ensemble learning, and hybrid physical-ML models can predict remaining useful life (RUL) with high accuracy from partial datasets [42].

It is essential that electric vehicles and grid-scale storage have the ability to predict failure and their accelerated degradation to avoid added cost and safety risks. Additionally, these models can be adapted in real-time for intelligent battery management systems (BMS) that can monitor the health of the device and adjust ways of operation to extend battery life [43].

However, these methods rely heavily on the availability of significant, high-quality, and interpretable data. It is still a challenge to combine data from different sources, reproduce results, and use small sample sizes, which may overfit models [39].

Blending AI with battery chemistry is a significant paradigm shift in studying, optimizing, and deploying energy storage technologies. AI has the power to predict material properties of interest, reveal hidden reaction pathways, design electrodes and electrolytes, and predict long-term degradation, thus complementing traditional computational and experimental approaches. Innovations taking place in battery research will obtain a significant boost from the application of AI. However, challenges still exist relating to data quality, interpretability, and transferability [39,42].

AI has shown its potential in some battery chemistries, but its true value emerges when AI is being used in conjunction with traditional computational approaches. Bringing AI's data-driven capabilities together with model physics-based delivers more accurate, efficient, and adaptable systems.

6. Integration of AI with Computational Frameworks

AI is changing the way we do computational science. It is delivering modes of efficiency and modes of insight far beyond simulation. The increased availability of data, better algorithms, and High-performance computing (HPC) infrastructure has converged to a level where AI not only complements a number of existing workflows, but it also modifies these workflows. New ways to speed up battery research and development that include predictive models, adaptive simulations, and real-time electrochemical process monitoring are enabled by this integration. In this area, hybrid AI-computational approaches are becoming leading enablers of next-generation battery technologies. These techniques combine quantum-level understanding and multiscale modelling with digital twin architectures.

6.1 Hybrid AI + Quantum Chemistry Workflows

Quantum chemistry methods, such as DFT and ab initio simulations, remain indispensable for capturing fundamental interactions in electrode materials, electrolytes, and interfacial regions. However, the computational cost of these methods often restricts their applicability to small systems and short timescales. AI integration helps overcome these bottlenecks by creating surrogate models trained on high-fidelity quantum chemistry datasets, capable of predicting

electronic properties, charge transfer, and reaction energetics with near- DFT accuracy but at a fraction of the computational expense [44].

In this hybrid paradigm, AI does not replace physics-based approaches entirely but enhances them. For example, neural network potentials or Gaussian process regressors can extend the predictive capability of ab initio data into larger, more complex systems that would otherwise be intractable. This enables researchers to efficiently screen new electrode compositions, probe solvation effects in electrolytes, or evaluate structural stability under various conditions. The synergy between AI acceleration and quantum rigor thus provides a scalable pathway for materials discovery, positioning hybrid workflows as a cornerstone of computational battery research [45].

6.2 AI-Assisted Multiscale Modeling

Battery systems span a wide range of scales: from electronic interactions at the quantum level to ion transport at the molecular level and finally to macroscopic behavior such as capacity fade and thermal management. Multiscale models attempt to bridge these levels, but their accuracy and efficiency are often constrained by the difficulty of integrating disparate scales consistently. AI-assisted frameworks can act as the “glue” that binds these levels together, enabling predictive connections across scales.

For example, AI models can learn effective parameters from atomistic simulations, such as diffusion coefficients or interfacial reaction rates, and feed them into continuum-scale models describing electrode kinetics and electrolyte transport. Conversely, system-level data from cycling experiments or thermal monitoring can be used to refine parameters at the lower scales through inverse modeling techniques. This bi-directional coupling allows for a feedback loop between simulations and experiments, reducing uncertainty and improving predictive reliability [46].

Such AI-assisted multiscale integration is particularly relevant for capturing complex degradation processes like SEI formation, lithium dendrite growth, or cathode phase transitions, which manifest across multiple scales. By embedding ML potentials within multiscale models, researchers can capture these nonlinear phenomena more accurately, thereby accelerating the development of safer and longer-lasting batteries [31].

6.3 Digital Twins for Real-Time Battery Monitoring

The concept of a digital twin, a virtual replica of a nuclear power plant's functioning, updated continuously based on data from the real world, is rapidly gaining traction in nuclear energy technologies. Digital twins for batteries can combine experience.

The concept of a digital twin, a virtual replica of a nuclear power plant's functioning, updated continuously based on data from the real world, is rapidly gaining traction in nuclear energy technologies. Digital twins for batteries can combine experimental data, modeling, and AI analytics to provide real-time insights into system health and performance, as well as degradation pathways.

AI helps these twins overcome the limits of a one-off yoga session. AI adds adaptive learning algorithms to digital twins. These algorithms react to new input streams from sensors. Examples of sensors are voltage, current, temperature, and impedance measurements. The technology can predict problems, such as capacity fade and safety threats. It can also offer suggestions on how to solve them. Essentially, digital twins enable the creation of practical, deployable systems for electric vehicles, grid storage, and portable electronics by scaling down laboratory insights to a high-resolution representation [47].

Integrating AI into digital twin structures enables efficient edge processing, meaning the AI can process data at the location where it is collected. Real-time monitoring is possible for distributed energy systems, microgrids, and large-scale energy infrastructures, where rapid decision-making is important [48].

6.4 Case Studies of AI-Augmented Computational Simulations

The integration of AI and computing is already yielding tangible improvements in battery technology in the real world. AI is used in one type of application as a surrogate model for costly first-principles simulations. For example, ML, particularly the application of convolutional neural networks to spectroscopic data, can quickly classify electrode degradation modes without the need for lengthy experimental characterization.

AI enhances existing workflows on various scales. AI will learn the parameters that link atomistic processes to system-level performance.

For instance, researchers have been utilizing reinforcement learning algorithms to develop in silico charging strategies. They will balance the fast charging with capacity fade. We can integrate AI into the simulations, which will then be validated experimentally, and the models will be further refined.

The implementation of digital twins in pilot projects begins to yield tangible results, whereby AI model feedback is utilized in decision-making for large-scale storage installations. The systems on display show the ability to combine AI-

in-HPC, AI-out-HPC, and AI-about-HPC into integrated workflows that manage simulation accuracy and infrastructure efficiency [44,49].

The way scientists and engineers use batteries is changing quickly because of how AI works with code. Scientists will hasten discovery and improve prediction, enabling real-time decision-making by creating hybrid workflows that combine AI with quantum chemistry for multi-scale modeling and developing digital twin architectures. These innovations are part of a broader trend of using AI to enhance high-performance computing, thereby alleviating computational hindrances and enabling new scientific discoveries at unprecedented speed [48,50].

There is a need to examine the current and emerging applications of AI-driven methods in battery research, from improving performance and longevity to facilitating the design of more sustainable and efficient energy storage solutions. Additionally, we highlight key trends that are paving the way for the next wave of breakthroughs in battery technology.

7. Applications and Emerging Trends

AI now quickly aids the evolution of battery technology. This is thanks to the revolutionary tools that ease challenges in the entire lifecycle of electrochemicalsystems. AI is proving to be a vital enabler of sustainability and efficiency, from the discovery of new electrode and electrolyte materials to the optimization of large-scale manufacturing, recycling strategies, and integration with renewables. Through connecting materials science with process engineering and systems integration, AI-driven approaches are opening the door toward resilient and sustainable energy infrastructures [39,41]. In this section, we will delve into significant applications and interesting areas of AI impact, particularly related to materials discovery, smart manufacturing, recycling, circularity, and integration in renewable energy.

7.1 AI-Guided Discovery of Electrode and Electrolyte Materials

A growing field in battery research is finding new electrode materials and electrolyte materials that are safer, have a higher energy density, and have better cycling stability. The classic trials do not work in school because they take time and are limited by high space requirements. AI approaches help in screening material candidates quickly. They can also predict essential electrochemical properties and learn complex relationships within material datasets that typical models cannot [39].

ML algorithms can analyze materials' structural, thermodynamic, and electronic descriptors to discover promising electrode candidates like high-capacity anodes or stable cathode chemistries. The optimization of electrolytes for batteries is very critical. Though the optimization process involves a lot of deep learning tools, it also requires a delicate balance of ionic conductivity, stability, and interfacial compatibility to accelerate the process. AI-driven discoveries thus reduce the time to market for new chemical introductions, offering a systematic framework for sustainable materials innovation in next-generation batteries.

7.2 Smart Optimization of Battery Manufacturing

AI is smartening up battery manufacturing processes, besides helping in the discovery of a material, tungsten carbide. Modern manufacturing lines are dependent on multiple stages, such as electrode coating, electrolyte filling, cell assembly, etc. The difference in conditions at each stage can impact performance and yield. Conventional process controller methods have a hard time adjusting to changing circumstances, leading to wasted production costs.

Real-time monitoring and control of manufacturing processes is possible using AI with edge computing technologies [47]. ML models placed at the network edge can identify anomalies, predict equipment failures, and recommend corrective actions without cloud-latency issues. Because with this system, we can predict breakdowns and improve the quality of products. Companies are using reinforcement learning techniques to automatically tune process parameters, achieving optimal trade-offs between throughput, cost, and performance. AI supports scalable and viable battery manufacturing required to keep up with global demand by making production lines more agile.

7.3 AI-Driven Insights into Recycling and the Circular Economy

Sustainable Solutions to Its Challenges. End-of-life batteries' sustainability issues underline the need for effective recycling strategies and circular economy frameworks. Current recycling technologies suffer from recovery of material gullies, being energy costly, and being complex in terms of safety. By enhancing recycling processes, bolstering material recovery, and prolonging the useful life of batteries, AI offers innovative solutions.

ML models can predict the remaining capacity and health of used batteries and sort them efficiently based either on second-life applications (like stationary energy storage) or recycling. AI algorithms can create strategies to disassemble things, making the process easier and safer. AI identifies the most sustainable recycling pathways to recover critical materials like lithium, cobalt, and nickel through chemical and operational data assessment. The improvements commence the closed loop for using and reusing valuable materials [41]. Thus, the carbon footprint of battery production is less.

7.4 Comparative Sustainability Metrics and Environmental Impact Assessment

Although sustainability considerations have thus far been mentioned throughout our review, a rigorous quantitative analysis of various electrochemical storage chemistries could deliver a much clearer insight into environmental trade-offs. Life cycle assessment (LCA) studies have shown that common LIBs usually produce 60-80 kg CO_2 equivalent per kWh of capacity, while SIBs have a significantly lesser impact of about 40-50 kg CO_2 equivalent per kWh because of the lower energy requirement for mining and refining [51].

Different systems show different recyclability performance. According to Peters et al.[52], LIBs technologies recover 40 to 50% of materials. Meanwhile, flow and aqueous systems can recover more than 70%. The latter is mainly due to the easy reclamation of electrolytes for less energy-intensive separation processes.

The material criticality index points out that cobalt and nickel limited availability brings battery sustainability issues for LIBs, but the high abundance and geographical distribution of sodium makes metallic sodium scarcity issues not prevalent in SIBs [52]. The inherent benefit and lesser energy requirement to manufacture SIBs make them environmentally friendly options to LIBs, especially from a complete life cycle view [53].

New studies of sodium-ion battery cells have come out in 2023. These cells all include a Prussian white cathode and a hard carbon anode. So far, the cradle-to-gate CO_2 equivalent impact per kWh is about 40-50 kg. For comparison, Wickerts et al. claim that various LIB configurations have constructed a cradle-to-gate carbon footprint ranging from 64 to 120 kg CO_2 equivalent per kWh. This decrease is most likely due to the increased incorporation of renewable energy sources in grid electricity mixes and ongoing decarbonization of industrial sectors such as steel.

SIBs that particularly utilize the cathode of Prussian white show a marked lower potential abiotic depletion potential (ADP) for abiotic resource depletion than LIBs. Even adding the fluorine-based electrolyte components to the analysis, the outcome does not alter. The overall ADP figures of SIBs are noted to be 71-83% lower compared to that of LIBs [52]. In reality, the abiotic depletion of SIBs having Prussian white and hard carbon electrodes lies in the range of 0.38-0.49 kg Sb-equivalent/kWh, which is much lower than that of LIBs [54], which is in the range of 1.95-2.22 kg Sb-equivalent/kWh.

The use of these measures of sustainability shows the importance of material and supply chain selection in reducing environmental impacts. SIBs have been identified as a promising solution for large-scale energy storage. Their advantages in terms of resource availability, lower life cycle carbon footprint, and overall environmental impact make them a sustainable energy storage solution [54].

Table 4 provides a comparative assessment of key sustainability indicators for three major electrochemical energy-storage systems: LIBs, SIBs, and VRFBs. Metrics evaluated include carbon footprint, recyclability potential, critical raw-material dependence, ADP, and lifecycle energy demand. Values represent typical ranges reported in contemporary literature. The table highlights how SIBs generally offer lower GHG emissions, utilize more abundant materials, and exhibit reduced resource depletion impacts relative to LIBs.

Table 4. Comparative sustainability metrics of major electrochemical storage systems.

Metric	LIBs	SIBs	Flow Battery (e.g., VRFB)	Sustainability Implication	Ref.
CO_2 Footprint (kg CO_2-eq/kWh)	60-80 (up to 120)	40-50	45-55	SIBs show lower GHG emissions due to reduced mining and processing energy.	[51,54]
Material Recovery / Recyclability (%)	40-50	60-70	70-80	Higher recyclability of SIBs and flow systems supports circular economy goals.	[52,53]
Critical Raw Materials	Cobalt, Nickel, Lithium	Sodium, Iron, Manganese	Vanadium	SIBs use abundant, widely distributed, and non-critical materials.	[52]
ADP (kg Sb-eq/kWh)	1.95-2.22	0.38-0.49	0.55-0.68	SIBs reduce mineral scarcity impact by up to 83% compared to LIBs.	[52,54]
Lifecycle Energy Demand (MJ/kWh)	600-800	450-550	500-650	Lower manufacturing energy requirement makes SIBs environmentally competitive.	[33,53]
Overall Environmental Ranking	Moderate to High Impact	Low to Moderate Impact	Moderate Impact	SIBs provide the most balanced performance-sustainability trade-off.	[53]

7.5 Ethical and Geopolitical Dimensions of Material Sourcing

In this part, we will see the ethical and geopolitical issues relating to the procurement of basic raw materials required for electrochemical energy storage. It further screens the ESG impact of global supply chains. Energy storage plays an important role in meeting the escalating demand for improved energy efficiency. Assessment of such factors at an early stage of technological development can avoid expensive corrective measures and support a secure, just transition to a decarbonized economy [55]. Analyzing supply chain flaws with a focus on geographical concentration and governance, along with social justice issues and local environmental harm due to a higher material demand [55,56].

Many materials are regarded as critical and are strategically significant. Therefore, their extraction and refining activity often takes place in a limited number of regions. Moreover, this creates vulnerabilities that can be leveraged to create market disruption or geopolitical tension [55]. For instance, cobalt and nickel are mined essentially in just a few countries, where governance issues and social unrest heighten supply risks. Also, lithium extraction in South America's "lithium triangle" has raised concerns about water scarcity and environmental harm. So, it is important to adopt a proactive framework during the early stages that assesses supply chain implications (of doing battery technologies) and environmental and social justice implications to mitigate future impacts [55].

A framework like this can ease geopolitical uncertainties that arise from the concentration of supply chains; these supply chains often transform the global energy transition into a race between nations on technology and economy [57]. In addition, spotting a variety of other materials early on that are of little or no harm to the environment and society can make the development of technologies with better supply chains and sustainability [55]. The limited availability of essential raw materials combined with geopolitical control by limited countries affecting availability negatively impacts the global transition to renewables and the equitable deployment of energy storage technologies [58].

The energy sector can move towards a more resilient, responsible, and just energy transition by incorporating ethical sourcing principles, governance transparency, and equitable access to resources into the design of electrochemical storage systems for use in modern devices.

7.6 Integration with Renewable Energy and Smart Grids

Using solar and wind energy presents new challenges for power generation in terms of grid stability and reliability. More and more AI-enhanced batteries are being acknowledged as essential for damping power fluctuations and enabling effective integration of renewables [47].

AI helps predict demand patterns and renewables generation levels, and it optimizes the real-time charging and discharging cycles of energy storage systems using predictive algorithms. This smart coordination makes sure that energy is saved during high surplus energy generation and is discharged when there is a peak load demand. Moreover, smart grids leverage AI to balance energy flows across distributed storage units, EVs, and stationary systems - effectively functioning as decentralized energy ecosystems.

The addition of edge AI makes grids more resilient by enabling local decision-making in microgrids. In turn, this reduces latency and dependence on central infrastructure [48]. By making grids more adaptable to renewable fluctuations, natural disasters, or cyber disruptions, this localized intelligence ensures long-term energy sustainability.

While the integration of AI into battery research holds great promise, the path to realizing its full potential is not without challenges. As we look to the future, it is essential to recognize the barriers that still need to be overcome.

7.7 Role of Large Language Models in Literature Mining, Materials Design, and Autonomous Laboratory Control

Recent advances in large language models (LLMs) have introduced new capabilities that significantly accelerate battery research. LLMs can rapidly mine and synthesize insights from vast scientific literature, extracting trends in electrolyte chemistry, electrode degradation mechanisms, and sustainability metrics that would be impractical to review manually. Beyond information extraction, LLMs can support materials design by generating candidate formulations, predicting structure-property relationships, and translating textual chemical knowledge into machine-actionable data for downstream ML models. When integrated with autonomous laboratories, LLMs enable high-level orchestration of experiments--formulating hypotheses, planning reaction sequences, and adapting protocols based on real-time analytical feedback. This emerging human-AI-robot collaboration streamlines discovery cycles, reduces experimental redundancy, and offers a scalable framework for accelerating innovation in next-generation electrochemical storage systems.

8. Challenges and Limitations

Though integrating AI-based control (decision making, learning, and optimization) into electrochemical energy storage systems is promising, challenges and limitations exist. Technical limitations are not the only challenges problem-solving designers face. There are also social, ethical, and environmental challenges. It is important to carefully think this through if we want to ensure a responsible path forward for AI-powered battery R&D and deployment.

8.1 Data Scarcity and Quality Concerns

The effectiveness of AI systems depends on having good-quality datasets that represent the use case. Battery research continues to face an obstacle of limited data. Electrochemical performance data are often privileged, dispersed across institutions, and produced under inconsistent lab conditions. When data is spread out, it stops us from making strong ML models. They need extensive, well-organized data sets to work well.

Since there is much variety in battery chemistries, aggregating information is also difficult. There are lithium-ion and solid-state batteries, along with sodium-ion and multivalent ones. The datasets that were collected for lithium-ion cells

cannot simply be used for SIBs because of differences in reaction mechanisms, compatibility with electrolytes, and degradation pathways. New approaches for goal-oriented user research and development are continuously emerging as organizations strive to outperform one another.

To overcome these barriers, global collaboration will be needed to establish uniform protocols and open-access repositories. However, data sharing is often disincentivized by issues of IP, data ownership, and competition. If the persistent lack of competitive research and industrial infrastructure is not addressed, the application of AI in battery technologies will remain confined to niche demonstrations rather than achieving large-scale implementation.

8.2 Model Interpretability and Transparency

Many AI models, particularly deep learning architectures, are often referred to as "black boxes" because their decisions cannot be easily interpreted. In battery research, where science and mechanics matter, a lack of interpretability means less trust and adoption. For example, suppose an AI model predicts how long a certain battery will last. In that case, researchers may be reluctant to draw on the model to build electric vehicles or grid-scale energy storage due to the lack of an explanation of which parameters drive degradation.

In addition, regulatory authorities and industry stakeholders need transparent models to validate safety-critical decisions. The importance of interpretability features increases when models are employed to predict failure modes, where unknown errors can cause dangerous effects like thermal runaway.

To improve interpretability of models, physics-informed machine learning (PIML) integrates well-known electrochemistry into AI models. Even though these methods bring great potential, they are still being developed, and optimizing them often involves a trade-off between predictive accuracy and interpretability. To safely and reliably deploy AI-driven systems, we need to balance these attributes so they are both predictive and scientifically interpretable.

PIML's role in electrochemical energy research has expanded significantly in recent times. According to [59], embedding physical laws into AI models helps improve the reliability, interpretability, and data efficiency of battery degradation models, PIML helping us out here. A comparison of different architectures, including physics-constrained neural networks and hybrid electrochemical-data models, shows how they are better than purely data-driven methods when datasets are limited. Future research can incorporate frameworks that close the gap between predictive accuracy and physical transparency, promoting sustainable and interpretable AI solutions for energy storage systems.

8.3 High Computational Cost and Reproducibility

Teaching advanced AI models takes a lot of computer power. HPC clusters or specialized hardware like Graphics processing unit (GPU) and Tensor processing unit (TPU) are often necessary. The energy and environmental impact, along with the associated costs, are significant. Training a single large-scale deep learning model can consume as much electricity in a year as several households do. This raises concerns about the carbon footprint of 'green' technologies.

Reproducibility is another concern. Different hardware and software frameworks, along with choices of hyperparameters and randomness in initialization, can lead to differences in model outcomes. This presents a significant obstacle for battery science, where reproducibility is necessary for scientific validity. Failure to model the pipeline in the energy domain and benchmark the model rigorously may spill over from other AI-heavy disciplines into the energy sector.

To resolve these issues, improved algorithms, energy-aware computing strategies, and standardized reporting will aid us in achieving reproducibility and sustainability of AI in battery research.

8.4 Ethical and Environmental Implications

The integration of AI into battery technologies raises ethical and environmental concerns, as well as technical issues. The environment does not just suffer from the computation needed to train large models. These systems also risk ramping up demand for raw materials. For example, relying on AI to find new electrode chemistries could lead to batteries using more cobalt or nickel, which are scarce and harmful materials.

Ethical concerns also involve data governance. Bias, privacy, and global inequality in access to AI resources reflect higher-level debates on issues in the digital economy. If only a few well-resourced institutions possess the most advanced AI-battery models, we may see asymmetries in scientific advance and an increasing technology gap among countries.

Moreover, the social justice dimension must not be ignored. People living near mines often pay the price with their lives, livelihood, and environment. Unless sustainability and equity are integrated into research priorities, the AI-impelled acceleration of battery deployment could deepen these injustices.

Despite the hurdles that remain, the potential for AI to revolutionize battery technology remains immense. With ongoing advancements in ML, data analytics, and computational modeling, overcoming current challenges will unlock new possibilities for more efficient, sustainable, and scalable energy storage systems.

9. Future Directions

Nevertheless, in spite of the challenges involved, there are still major opportunities that AI can be used to revolutionize electrochemical energy storage. New technologies like quantum computing, federated learning (FL), and autonomous laboratories are the technologies that will transform the process of discovering, producing, and implementing batteries. These urgency and complex systems will continue to be studied in future studies to understand the critical role of practical use cases in driving innovation, sustainability and progress. In a bid to explain technology readiness, the two subsections below show the current trends as well as old ones in the field. Some of the solutions, such as FL frameworks and AI-driven materials discovery, are already being tested in industrial and academic consortia, but other solutions, especially quantum machine learning and autonomous laboratories, are in their early stages of development. This differentiation is stressed to make readers realize that there are different levels of maturity of AI applications in electrochemical energy storage.

9.1 Opportunities in Quantum Machine Learning

Quantum computing presents a strong new way to solve complex materials science and energy systems problems. Models of classical AI are inadequate for the many possible battery materials and reactions. Quantum machine learning (QML) can mimic quantum interactions in their native form, which could enable unprecedented accuracy in material simulation.

There could be a significant boost in the design of solid-state electrolytes using QML , which can accurately model ion transport dynamics at the atomic level. The classical models only approximate that with crude quality. In addition, combining classical ML with quantum algorithms would result in a hybrid approach that enables tractable simulations of large systems while maintaining precision.

QML is a young discipline, but it will take a crucial place in the next-generation batteries, taking the theoretical knowledge of the field and applying it in real-life situations. In its current form, QML is mostly theoretical and much of the research is currently focused on theoretical modeling and small-scale proof-of-concept simulations. Experimental validation cannot be done without the constraints of current quantum hardware but initial hybrid QML-classical models are starting to be experimented with through a series of common research efforts.

9.2 Federated Learning and Global Data Sharing Platforms

FL is an approach to model training that is capable of addressing the issue of data sparsity. FL allows different organizations to collaborate in training AI systems without using the same data. By expanding datasets and addressing issues related to privacy and intellectual property, this solves multiple problems at once.

Federated platforms could bring together stakeholders from industry, academia, and government labs in the domain of batteries while keeping proprietary data under wraps and allowing global participation. For instance, a company working on new lithium-sulfur cells could participate and benefit from a shared model without sharing confidential experimental details.

FL initiatives have the potential to standardize protocols, enhance reproducibility, and expand access to high-quality models, thereby accelerating innovation across the entire energy ecosystem. Currently, FL is actively being piloted in materials informatics and battery research and development, especially through collaborations between industry and academia focused on secure model sharing. Early-stage federated platforms have been implemented for applications such as performance prediction and electrode design, demonstrating practical feasibility, although deployment at a global scale is still in progress.

9.3 Role of AI in Sustainable Next-Gen Energy Materials

AI's role in enhancing sustainability is going to increase, as batteries move from conventional lithium-ion systems to sodium-ion, zinc-air, and multivalent chemistries. Future materials have a low impact on the environment and low use of rare materials. However, they also create new uncertainties and suffer from stability issues and complex electrochemistry.

AI can help researchers determine combinations of materials that will be stable. Similarly, it will assist with predicting where items will fail and how to make them. Apart from discovering new materials, optimisation across the lifecycle could enable both the design of high-performance chemistries and the assurance of their ecological and social sustainability.

When sustainability is prioritized within AI research, the development of next-generation batteries can be guided by frameworks that emphasize both circular economy principles and climate resilience. Currently, AI-enabled sustainability screening is partially implemented, particularly in areas such as material selection, lifecycle modeling, and process optimization. However, fully integrated AI systems that simultaneously balance performance and

sustainability metrics are still in the developmental and conceptual stages, with large-scale industrial adoption yet to be realized.

9.4 Toward Autonomous Labs and Self-Driving Battery Research

One of the most exciting future directions is the emergence of autonomous laboratories, sometimes described as "self-driving labs." These systems integrate robotics, high-throughput experimentation, and AI algorithms to conduct experiments, analyze results, and design follow-ups without human intervention.

Robot labs equipped with AI that rediscover simple batteries will develop batteries or supercapacitors in hours through thousands of increasingly complex tests. The period for discovering new battery chemistries may be cut down from decades to a few years with this approach.

Battery for Autonomous Vehicles research envisages a closed-loop of computational simulation and experimental validation. For instance, an AI model can predict a good cathode material, a robot can synthesize and test it, and data from the tests will be fed to the AI model immediately. This loop can make battery science significantly quicker, more efficient, and less intensive by orders of magnitude.

As we look to the future of battery technology, AI's potential to revolutionize energy storage becomes increasingly clear. The integration of computational models and machine learning techniques is driving new breakthroughs aimed at overcoming current industry challenges. Currently, the concept of autonomous or self-driving laboratories is in its early pilot phase. While several research institutions have successfully demonstrated AI-robotics integration for high-throughput experimentation, widespread deployment remains confined to prototype settings. The broader vision of fully automated, closed-loop discovery systems is still a future aspiration rather than an operational reality.

10. Conclusion

Merging AI and electrochemical energy storage brings about a change in the world of sustainable energy technology. AI's potential is being demonstrated in accelerating the discovery of materials, optimizing stations' production processes, enhancing recycling efficiency, and integrating renewable energies. Together, these abilities make AI a key aspect in making the energy transition of our globe possible. Despite this potential, there are many problems to overcome. The inadequacy of high-quality and standardized datasets, lack of interpretability of complex AI models, their high computational cost, and the ethical issues concerning data governance and environmental fairness continue to represent major obstacles. We can help you with a background information thesis statement. That is, a simple sentence providing some background information regarding the subject of your essay.

New technologies like QML, FL, and autonomous laboratories can enhance the resolution of existing features. If these two technologies were integrated, it could lead to the development of secure, decentralized, and efficient AI frameworks that meet sustainability objectives. In the future, designing and using AI in energy storage should focus on sustainability, equity, and the circular economy. By doing so, AI will not only enhance existing technology but also change the way energy systems are designed, thus advancing a resilient, just, and sustainable global energy future through human and machine intelligence.Ultimately, the continued co-evolution of human expertise and machine intelligence holds the potential to drive industry innovation, inform future research priorities, and accelerate the transition toward a more just, reliable, and sustainable global energy future.

11. Limitations

Due to the available literature and the immature nature of research on different AI approaches, this review is limited in scope. Because of different performance metrics, proprietary datasets, and different experimental conditions, we could not make quantitative comparisons between studies. Also, measures like recyclability or lifecycle impact aren't standardized, limiting any comparisons that might be made. Future reviews should use meta-analytic techniques and structured sustainability indicators, which will allow for more rigorous benchmarking based on data of AI applications in electrochemical energy storage.

Conflict of Interest

The authors declare they have no conflicts of interest.

Generative AI statement

The authors declare that no Gen AI was used in the creation of this manuscript.

References

[1] Vidas L, Castro R. Recent developments on hydrogen production technologies: state-of-the-art review with a focus on green-electrolysis. Applied Sciences, 2021, 11(23), 11363. DOI: 10.3390/APP112311363

[2] Qin Z, Ma J, Zhu M, Khan TA. Advancements in energy storage technologies: Implications for sustainable energy strategy and electricity supply towards sustainable development goals. Energy Strategy Reviews, 2025, 59, 101710. DOI: 10.1016/j.esr.2025.101710

[3] Razmjoo A, Ghazanfari A, Østergaard PA, Jahangiri M, Sumper A, Ahmadzadeh S, et al. Moving toward the expansion of energy storage systems in renewable energy systems A techno-institutional investigation with artificial intelligence consideration. Sustainability, 2024, 16(22), 9926. DOI: 10.3390/su16229926

[4] Xin H, Mou T, Pillai HS, Wang S, Huang Y. Interpretable machine learning for catalytic materials design toward sustainability. Accounts of Materials Research, 2023, 5(1), 22-34. DOI: 10.1021/accountsmr.3c00131

[5] Lombardo T, Duquesnoy M, El-Bouysidy H, Årén F, Gallo-Bueno A, Jørgensen PB, et al. Artificial intelligence applied to battery research: hype or reality? Chemical reviews, 2021, 122(12), 10899. DOI: 10.1021/acs.chemrev.1c00108

[6] Yao Z, Lum Y, Johnston A, Mejía-Mendoza LM, Zhou X, Wen Y, et al. Machine learning for a sustainable energy future. Nature Reviews Materials, 2022, 8(3), 202. DOI: 10.1038/s41578-022-00490-5

[7] Brindha R, Rao RP, Chellappan V, Ramakrishna S. Towards sustainable fuel cells and batteries with an AI perspective. Sustainability, 2022, 14(23), 16001. DOI: 10.3390/su142316001

[8] Barrett DH, Haruna AB. Artificial intelligence and machine learning for targeted energy storage solutions. Current Opinion in Electrochemistry, 2020, 21, 160. DOI: 10.1016/j.coelec.2020.02.002

[9] Sanghvi AH, Manjoo A, Rajput P, Mahajan N, Rajamohan N, Abrar I. Advancements in biohydrogen production–a comprehensive review of technologies, lifecycle analysis, and future scope. RSC Advances, 2024, 14(49), 36868-36885. DOI: 10.1039/D4RA06214K

[10] Martins VL, Neves HR, Monje IE, Leite M, Oliveira PFM de, Antoniassi RM, et al. An overview on the development of electrochemical capacitors and batteries–part II. Anais da Academia Brasileira de Ciências, 2020, 92(2), e20200800. DOI: 10.1590/0001-3765202020200800

[11] Liao C. Electrolytes and additives for batteries Part I: fundamentals and insights on cathode degradation mechanisms. eTransportation, 2020, 5, 100068. DOI: 10.1016/j.etran.2020.100068

[12] Richardson G, Korotkin I, Ranom R, Castle M, Foster JM. Generalised single particle models for high-rate operation of graded lithium-ion electrodes: Systematic derivation and validation. Electrochim Acta, 2020, 339, 135862. DOI: 10.1016/j.electacta.2020.135862

[13] Adebanjo IA, Eko J, Agbeyegbe AG, Yuk SF, Cowart SV, Nagelli EA, et al. A comprehensive review of lithium-ion battery components degradation and operational considerations: A safety perspective. Energy Advances, 2025, 4(7), 820-877. DOI: 10.1039/d5ya00065c

[14] Guo Y, Zhang Q, Chen J, Wan L. Preface: Special topic on rechargeable battery technology. Science China Chemistry, 2023, 67(1), 1. DOI: 10.1007/s11426-023-1907-y

[15] Saldarini A, Longo M, Brenna M, Zaninelli D. Battery electric storage systems: advances, challenges, and market trends. Energies, 2023, 16(22), 7566. DOI: 10.3390/en16227566

[16] Pokhriyal A, Rueda-García D, Gómez-Romero P. To flow or not to flow. A perspective on large-scale stationary electrochemical energy storage. Sustainable Energy Fuels, 2023, 7(23), 5473-5482. DOI: 10.1039/d3se00955f

[17] Grey CP. Prospects for lithium-ion batteries and beyond–A 2030 vision. Nature Communications, 2020, 11(1), 6279. DOI: 10.1038/s41467-020-19991-4

[18] Kaliaperumal M, Dharanendrakumar MS, Prasanna S, Abhishek KV, Chidambaram RK, Adams S, et al. Cause and mitigation of lithium-ion battery failure–A review. Materials, 2021, 14(19), 5676. DOI: 10.3390/ma14195676

[19] Rahman MA, Chowdhury MA, Hasan MM. Exploring lithium-ion battery degradation: A concise review. Batteries, 2024 10(7), 220. DOI: 10.3390/batteries10070220

[20] Xie XH, Guan SJ, Murayama M, Zhao X. A review on research progress in electrolytes for sodium-ion batteries. Scientia Sinica Technologica, 2019, 50, 247-260. DOI: 10.1360/sst-2019-0218

[21] Karahan Toprakci H A, Toprakci O. Recent advances in new-generation electrolytes for sodium-ion batteries. Energies, 2023, 16(7), 3169. DOI: 10.3390/en16073169

[22] Radjendirane AC, Maurya DK, Ren J, Hou H, Algadi H, Xu BB, et al. Overview of inorganic electrolytes for all-solid-state sodium batteries. Langmuir, 2024, 40(32), 16690-16712. DOI: 10.1021/acs.langmuir.4c01845

[23] Massaro A, Squillantini L, De Giorgio F, Scaramuzzo FA, Pasquali M, Brutti S. Advancements in solid-state sodium-based batteries: A comprehensive review. arXiv preprint arXiv, 2025, 04391. DOI: 10.48550/arXiv.2505.04391

[24] Yu J, Duquesnoy M, Liu C, Franco AA. Optimization of the microstructure of carbon felt electrodes by applying the lattice Boltzmann method and Bayesian optimizer. Journal of Power Sources, 2023, 575, 233182. DOI: 10.1016/j.jpowsour.2023.233182

[25] Owen RE, Du W, Millichamp J, Shearing PR, Brett DJL, Robinson JB. Visualising the effect of areal current density on the performance and degradation of lithium sulfur batteries using operando optical microscopy. Journal of The Electrochemical Society, 2024, 171(12), 120523. DOI: 10.1149/1945-7111/ad9cc6

[26] Parvizi P, Jalilian M, Amidi AM, Zangeneh MR, Riba J. From present innovations to future potential: The promising journey of Lithium-Ion batteries. Micromachines, 2025 ,16(2), 194. DOI: 10.3390/mi16020194

[27] Vasta E, Scimone T, Nobile G, Eberhardt O, Dugo D, Benedetti MMD, et al. Models for battery health assessment: A comparative evaluation. Energies, 2023, 16(2), 632. DOI: 10.3390/en16020632

[28] Miao Y, Liu L, Xu K, Li J. High Concentration Heightens Risk for Power Lithium-ion Battery Supply Chains Globally. DOI: 10.21203/rs.3.rs-2083016/v1

[29] Bhowmik A, Berecibar M, Casas-Cabanas M, Csányi G, Dominko R, Hermansson K, et al. Implications of the BATTERY 2030+ AI-assisted toolkit on future low-TRL battery discoveries and chemistries. Advanced Energy Materials, 2021, 12(17), 2102698. DOI: 10.1002/aenm.202102698

[30] Stenina I, Yaroslavtsev A. Modern technologies of hydrogen production. Processes, 2022, 11(1), 56. DOI: 10.3390/PR11010056
[31] van Hees A, Zhang ZY, Sudhama A, Zhang C. Molecular modelling of aqueous batteries. arXiv preprint arXiv, 2024, 2406.00468. DOI: 10.48550/arxiv.2406.00468
[32] Atkins D, Ayerbe E, Benayad A, Capone FG, Capria E, Castelli IE, et al. Understanding battery interfaces by combined characterization and simulation approaches: challenges and perspectives. Advanced Energy Materials, 2021, 12(17), 2102687. DOI: 10.1002/aenm.202102687
[33] Zhang S, Steubing B, Potter HK, Hansson PA, Nordberg Å. Future climate impacts of sodium-ion batteries. Resources, Conservation and Recycling, 2023, 202, 107362. DOI: 10.1016/j.resconrec.2023.107362
[34] Li G, Monroe CW. Multiscale lithium-battery modeling from materials to cells. Annual Review of Chemical and Biomolecular Engineering, 2020, 11(1), 277. DOI: 10.1146/annurev-chembioeng-012120-083016
[35] Morgan LM, Islam MM, Yang H, O'Regan K, Patel AN, Ghosh A, et al. From atoms to cells: Multiscale modeling of LiNixMnyCozO2 cathodes for Li-Ion batteries. ACS Energy Letters, 2021, 7(1), 108-122. DOI: 10.1021/acsenergylett.1c02028
[36] Leung K. DFT modelling of explicit solid–solid interfaces in batteries: methods and challenges. Physical Chemistry Chemical Physics, 2020, 22(19), 10412-10425. DOI: 10.1039/c9cp06485k
[37] Dai FZ, Sun Y, Wen B, Xiang H, Zhou Y. Temperature dependent thermal and elastic properties of high entropy (Ti0.2Zr0.2Hf0.2Nb0.2Ta0.2) B2: molecular dynamics simulation by deep learning potential. Journal of Materials Science & Technology, 2021, 72, 8-15. DOI: 10.1016/j.jmst.2020.07.014
[38] Nekahi A, Dorri M, Rezaei M, Bouguern MD, Madikere Raghunatha Reddy AK, Li X, et al. Comparative issues of metal-ion batteries toward sustainable energy storage: lithium vs. sodium. Batteries. 2024, 10(8), 279. DOI: 10.3390/batteries10080279
[39] Liu S, Xu H, Ai Y, Li H, Bengio Y, Guo H. Expert-Guided LLM Reasoning for Battery Discovery: From AI-Driven Hypothesis to Synthesis and Characterization. arXiv preprint arXiv:2507.16110. 2025 Jul 21. DOI: 10.48550/arxiv.2507.16110
[40] Jha S, Yen M, Salinas YS, Palmer EM, Villafuerte JA, Liang H. Machine learning-assisted materials development and device management in batteries and supercapacitors: performance comparison and challenges. Journal of Materials Chemistry A, 2023, 11(8), 3904. DOI:10.1039/d2ta07148g
[41] Valizadeh A, Amirhosseini MH. Machine learning in lithium-ion battery: applications, challenges, and future trends. SN Computer Science, 2024, 5(6), 717. DOI:10.1007/s42979-024-03046-2
[42] Wang Y. Application-oriented design of machine learning paradigms for battery science. NPJ Computational Materials, 2025, 11(1), 89 DOI:10.1038/s41524-025-01575-9
[43] Xue P, Qiu R, Peng C, Peng Z, Ding K, Long R, et al. Solutions for lithium battery materials data issues in machine learning: overview and future outlook. Advanced Science, 2024, 11(48), 2410065. DOI: 10.1002/advs.202410065
[44] Brewer W, Gainaru A, Suter F, Wang F, Emani M, Jha S. AI-coupled HPC workflow applications, middleware and performance. arXiv preprint arXiv:2406.14315, 2024. DOI: 10.48550/arxiv.2406.14315
[45] Zhu S, Yu T, Xu T, Chen H, Dustdar S, Gigan S, et al. Intelligent computing: The latest advances, challenges and future. Intelligent Computing, 2023, 2, 0006. DOI: 10.34133/icomputing.0006
[46] Navaux POA, Lorenzon AF, Serpa MS. Challenges in high-performance computing. Journal of the Brazilian Computer Society, 2023, 29(1), 51-62. DOI:10.5753/jbcs.2023.2219
[47] Gill SS, Golec M, Hu J, Xu M, Du J, Wu H, et al. Edge AI: A taxonomy, systematic review and future directions. Cluster Comput, 2025, 28(1), 18. DOI: 10.1007/s10586-024-04686-y
[48] Ficili I, Giacobbe M, Tricomi G, Puliafito A. From sensors to data intelligence: Leveraging IoT, cloud, and edge computing with AI. Sensors, 2025, 25(6), 1763. DOI: 10.3390/s25061763
[49] Chappidi SR. Agricultural Intelligence: AI-driven performance frameworks for modern farming. International Journal of Science and Research Archive, 2025, 14(1), 1078-1084. DOI: 10.30574/ijsra.2025.14.1.0160
[50] Weber P, Carl KV, Hinz O. Applications of explainable artificial intelligence in Finance a systematic review of finance, information systems, and computer science literature.Management Review Quarterly, 2024, 74(2), 867-907. DOI: 10.1007/s11301-023-00320-0
[51] Phogat P, Dey S, Wan M. Powering the sustainable future: A review of emerging battery technologies and their environmental impact. RSC Sustainability, 2025, 3, 3266-3306. DOI: 10.1039/d5su00127g
[52] Peters JF, Baumann M, Binder JR, Weil M. On the environmental competitiveness of sodium-ion batteries under a full life cycle perspective–a cell-chemistry specific modelling approach. Sustainable Energy Fuels, 2021, 5(24), 6414. DOI: 10.1039/d1se01292d
[53] Molaiyan P, Bhattacharyya S, dos Reis GS, Sliz R, Paolella A, Lassi U. Towards greener batteries: Sustainable components and materials for next-generation batteries. Green Chemistry, 2024, 26(13), 7508-7531. DOI: 10.1039/d3gc05027k
[54] Wickerts S, Arvidsson R, Nordelöf A, Svanström M, Johansson P. Prospective life cycle assessment of sodium-ion batteries made from abundant elements. Journal of Industrial Ecology, 2023, 28(1), 116-129. DOI:10.1111/jiec.13452
[55] Putsche VL, Pattany J, Ghosh T, Atnoorkar S, Zuboy J, Carpenter A, et al. A framework for integrating supply chain, environmental, and social justice factors during early stationary battery research. Frontiers in Sustainability, 2023, 4, 1287423. DOI: 10.3389/frsus.2023.1287423
[56] Martin N, Madrid-López C, Villalba G, Talens-Peiró L. New techniques for assessing critical raw material aspects in energy and other technologies. Environmental science & technology, 2022, 56(23), 17236-17245. DOI: 10.1021/acs.est.2c05308
[57] Tao H, Zhuang S, Xue R, Cao W, Tian J, Shan Y. Environmental Finance: An Interdisciplinary Review. Technological Forecasting and Social Change, 2022, 179, 121639. DOI:10.1016/j.techfore.2022.121639
[58] Mahnoor M, Chandio R, Inam A, Ahad IU. Critical and strategic raw materials for energy storage devices. Batteries, 2025, 11(4), 163. DOI:10.3390/batteries11040163
[59] Navidi S, Thelen A, Li T, Hu C. Physics-informed machine learning for battery degradation diagnostics: A comparison of state-of-the-art methods. Energy Storage Materials, 2024, 68, 103343.