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Broader context

Electrochemical energy storage is essential for electrified transportation, renewable energy integration, and sustainable power systems. Achieving improvements in performance, safety, and lifetime remains challenging due to complex, coupled interactions among electrodes, electrolytes, and dynamic interphases. Meanwhile, artificial intelligence (AI) and machine learning (ML) are increasingly applied in battery research, producing a rapidly growing literature that can be difficult to navigate for scientists focused on materials and electrochemistry rather than computational methods. This mini-review provides a materials-focused perspective on AI-enabled approaches, highlighting their use in electrolyte design, electrode discovery, and battery health modeling. By emphasizing practical applications, limitations, and opportunities, it aims to make AI concepts accessible to battery researchers and help bridge the gap between data-driven strategies and experimental practice.

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AI-Driven Approaches for Navigating Battery Complexity

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ABSTRACT

Artificial intelligence (AI) is emerging as a powerful approach for navigating the complexity of battery materials and electrochemical systems. This mini-review highlights recent advances in AI-enabled battery research from a materials and electrochemistry perspective, with emphasis on electrolyte and electrode design. Key modeling frameworks, including physics-based, data-driven, and hybrid approaches, are discussed alongside representative machine-learning methods used to predict electrochemical performance, degradation behavior, and interfacial phenomena. Persistent challenges, including limited data quality, restricted model generalizability, and limited interpretability, remain significant barriers to widespread adoption. By outlining both opportunities and limitations, this review emphasizes the importance of integrating AI with physical insight and experimental validation to accelerate the development of safer, longer-lasting, and higher-performance energy storage technologies.

KEYWORDS: artificial intelligence; machine learning; batteries; electrolyte discovery; electrode materials

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1. Introduction

Electrochemical energy storage plays a critical role in the electrification of transportation, large-scale integration of renewable energy, and the decarbonization of industrial systems. Lithium-ion batteries (LIBs) have become the dominant technology for electric vehicles, grid storage, and portable electronics due to their high energy density and long cycle life. However, further improvements in performance, safety, and durability are increasingly constrained by materials-related challenges.[1–3] These challenges arise from complex, multiscale interactions among electrodes, electrolytes, and dynamic electrochemical interfaces that govern ion transport, interfacial reactions, and degradation processes. As LIB deployment continues to expand across demanding applications, the ability to accurately monitor and manage battery health throughout the operational lifetime has become essential for ensuring safety, reliability, and efficient utilization of stored energy.[1, 2, 4–6]

Within this coupled materials landscape, the electrolyte plays a central yet often underappreciated role. Beyond serving as an ionic conductor, the electrolyte directly influences interfacial chemistry, the electrochemical stability window, and failure modes such as lithium plating, gas evolution, and parasitic side reactions.[4, 6] Achieving high ionic conductivity, oxidative stability, and long-term reversibility simultaneously remains difficult, as these properties are frequently antagonistic.[7, 8] Similar trade-offs persist at the electrode level, where composition, morphology, and surface chemistry dictate ion transport pathways, mechanical integrity, and degradation kinetics. The intertwined nature of these processes makes rational, component-by-component optimization insufficient for next-generation battery systems.

Historically, electrolyte and electrode development has relied on empiricism, guided intuition, and incremental screening. However, the combinatorial design space encompassing solvents, salts, additives, binders, and composite architectures is effectively intractable using conventional experimental approaches alone. As battery chemistries diversify toward lithium-metal, multivalent, and hybrid systems, this challenge is further amplified by increasingly stringent interfacial and stability requirements. Overcoming these barriers demands new strategies capable of navigating high-dimensional materials spaces while preserving physical relevance.

Artificial intelligence (AI) is emerging as a transformative tool for addressing these challenges. Rather than replacing physical understanding, AI enables a shift toward data-informed materials design, where structure–property–performance relationships can be learned, generalized, and

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exploited at scale.[3, 6, 10, 11] In electrolyte research, machine learning (ML) models have been used to predict transport properties, electrochemical stability, and interphase behavior from molecular descriptors, while generative approaches enable investigation of chemistries beyond existing databases. For electrodes, AI-driven analysis is increasingly applied to correlate synthesis parameters, microstructure, and composition with electrochemical performance and degradation pathways. Together, these approaches support a move from isolated optimization toward co-design of materials and interfaces.

At the system level, AI has also become central to battery health assessment and lifetime prediction. Battery degradation manifests through capacity loss and resistance growth driven by a network of electrochemical, mechanical, and thermal processes that evolve over time.[1, 3, 4] Accurately quantifying the state of health (SOH) is essential for safety, reliability, and lifecycle optimization, yet remains challenging due to the nonlinear and history-dependent nature of degradation.[1, 4] ML-based SOH models typically infer health metrics directly from operational data, offering chemistry-agnostic adaptability at the expense of mechanistic transparency. Bridging this gap between predictive accuracy and physical interpretability remains a key open challenge.

In this mini-review, we critically examine recent advances in AI-enabled energy storage research from a materials and electrochemistry perspective, with emphasis on how data-driven methods are being applied to fundamental materials challenges. We focus on two interconnected domains: electrolyte design and electrode materials modeling. Emphasis is placed on dominant modeling paradigms, commonly employed algorithms, and the extent to which current approaches capture or overlook underlying electrochemical physics. By identifying unifying trends, critical gaps, and persistent limitations, this review outlines clear opportunities for more tightly integrating AI with physical insight. Ultimately, we position AI not simply as a predictive tool, but as a framework for uncovering complex, nonlinear relationships in battery systems (e.g., voltage, current, and temperature) and guiding the rational design of materials that overcome key trade-offs in electrochemical stability, volumetric expansion, conductivity, capacity, and safety.

2. Fundamentals of battery materials and challenges

Batteries consist of several interconnected components, including electrodes, electrolytes, separators, and current collectors, each of which plays a critical role in determining overall device

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performance.[5] During operation, complex physicochemical interactions occur among these components as the system attempts to deliver high capacity, power density, and long cycle life. These interactions can give rise to a range of degradation phenomena, including current collector corrosion or cracking, electrode fracture, solid–electrolyte interphase (SEI) formation and evolution, electrolyte oxidation and reduction, and dendrite growth.[5, 6] Such processes are highly coupled and often evolve simultaneously, complicating efforts to optimize battery performance through isolated materials design. The complexity of these coupled processes motivates the use of AI-driven approaches to enable efficient screening and predictive understanding of battery behavior. **Figure 1** highlights key parameters and AI-driven workflows for the screening and design of electrodes, electrolytes, separators, and their integration into industrial pipelines.

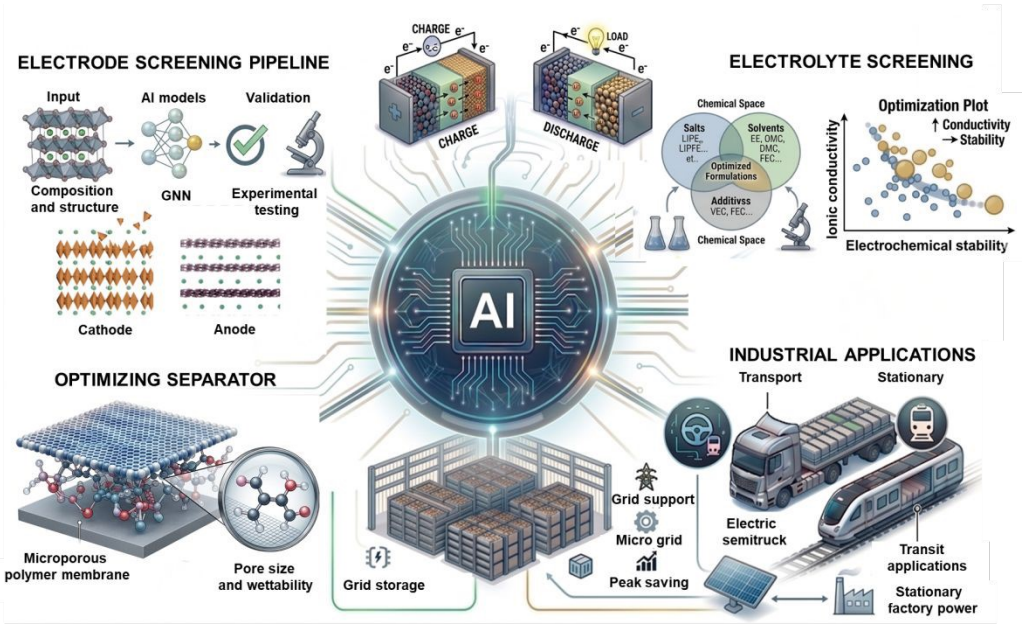

Figure 1. Schematic overview of the role of AI in addressing key battery challenges across electrodes, electrolytes, separators, and industrial applications. The figure illustrates AI-driven workflows for electrode screening, as well as predicted outputs for electrolyte and separator design, and highlights applications in stationary and transportation energy storage systems. The image was generated with the assistance of Google Gemini.

2.1 Electrolyte Design Trade-offs and Stability Challenges

The electrolyte is a pivotal component in battery systems, governing energy density, safety, and cycle life by enabling ion transport between electrodes. Carbonate-based solvents, such as ethylene

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carbonate (EC), provide high ionic conductivity but exhibit poor reductive stability against lithium metal anodes.[4, 12] In contrast, ether-based solvents are commonly used in lithium metal batteries (LMBs) due to their improved compatibility with the metal anode, although they often suffer from limited oxidative stability. Fluorinated ethers have been developed to enhance anodic stability; however, this modification frequently reduces reductive stability compared with their non-fluorinated counterparts. In this context, AI-enabled approaches can be leveraged for materials prediction, discovery of new solvent molecules, and analysis of solvation structures, enabling the systematic navigation of trade-offs to optimize ionic conductivity, electrochemical stability, and Coulombic efficiency (CE) in electrolyte design.[4, 7]

Such trade-offs become particularly pronounced in high-voltage battery systems. For example, the spinel cathode $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) operates at potentials of approximately 4.7 V vs. Li^+/Li, exceeding the electrochemical stability window of most conventional organic electrolytes.[6] Under these conditions, solvents such as EC undergo oxidative decomposition, producing reactive species including glycolic acid and difluorophosphoric acid that can accelerate transition-metal dissolution from the cathode. These degradation pathways also contribute to dendrite formation, voltage fade, and performance instability across varying temperatures and C-rates. Accurately predicting degradation behavior and profiles under high-voltage operation can enable strategies for dendrite suppression and mitigation of capacity fade, impedance growth, and progressive degradation of the electrode–electrolyte interface.[6,8,9]

Electrolyte additives represent one of the most effective and widely adopted approaches for improving interfacial stability. Additives such as vinylene carbonate (VC), lithium difluoro(oxalato)borate (LiDFOB), and trimethylsilyl phosphite (TMSPi) promote the formation of protective SEI on electrode surfaces. These interphases suppress parasitic reactions by forming a passivating barrier that limits electrolyte decomposition and transition-metal dissolution, thereby improving interfacial stability and battery reversibility.[6]

2.2 Electrode Materials and Performance Trade-offs

Cathodes and anodes serve as the positive and negative electrodes in a battery, respectively, and their composition and structure strongly influence overall electrochemical performance.[5, 10] Cathodes are typically composed of electrochemically active material combined with conductive additives and polymer binders to ensure efficient electron transport and mechanical integrity.

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Widely used cathode materials in LIBs include layered oxides such as lithium cobalt oxide ($LiCoO_2$, LCO), lithium nickel manganese cobalt oxides ($LiNi_xMn_yCo_zO_2$, NMC), and lithium nickel cobalt aluminum oxide ($LiNi_xCo_\gamma Al_zO_2$, NCA), as well as olivine-structured lithium iron phosphate ($LiFePO_4$, LFP) and spinel lithium manganese oxide ($LiMn_2O_4$, LMO).[11] These composite electrodes typically contain 80–95 wt% active material, 2–10 wt% conductive additive, and 2–10 wt% binder, depending on the electrode design and application.[11]

Commercial cathode materials generally exhibit specific capacities of ~140–240 mAh g^{-1} and operate within voltage windows of approximately 3.4–4.7 V vs. Li^+/Li.[12, 13] However, each chemistry presents inherent trade-offs. Layered oxides such as LCO, NMC, and NCA provide high energy density but can suffer from structural degradation and thermal instability during prolonged cycling.[10] In contrast, LFP exhibits excellent thermal stability and long cycle life but operates at lower voltages (~3.4 V) and has comparatively lower electronic conductivity.[10, 13] Spinel LMO offers lower cost and environmental compatibility but may experience capacity fading due to structural instability during repeated cycling.[10]

AI-driven approaches can address these trade-offs by enabling the discovery and screening of novel electrode materials with high specific capacity and wider voltage windows, while also predicting performance and degradation behavior. In particular, AI can be used to forecast battery aging, identify degradation pathways such as dendrite initiation and propagation, and guide materials design to mitigate these effects.[7, 14] Beyond screening, AI also enables the design of materials with tailored properties, including tunable conductivity, engineered layered structures, and targeted chemical functionalities (e.g., MXenes).[15-17]

Anode materials face similar design constraints. Carbon-based anodes, particularly graphite, dominate commercial batteries due to their low cost, stable lithium intercalation, and long cycle life, with theoretical capacities of ~372 mAh g^{-1} and high Coulombic efficiency.[18] Alloy-type anodes, including silicon and tin, offer significantly higher theoretical capacities (often >1000 mAh g^{-1}) but undergo large volume expansion during lithiation, leading to mechanical degradation and capacity fading.[13, 18] Conversion-type anodes, such as transition metal oxides and sulfides, also exhibit high capacities but are often limited by poor electronic conductivity and voltage hysteresis. Consequently, electrode design requires balancing capacity, structural stability, conductivity, and interfacial compatibility to achieve high-performance and durable battery systems.[18, 19]

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3. Artificial Intelligence for Battery Materials and Systems

AI and ML are increasingly used to analyze and predict battery behavior across materials and system levels. In battery research, AI is primarily implemented through computational modeling frameworks that aim to describe performance and degradation under varying operating conditions.[3, 4] These approaches can generally be grouped into three categories: physics-based models, purely data-driven (ML) models, and hybrid approaches that combine elements of both (**Figure 2**).[12,13]

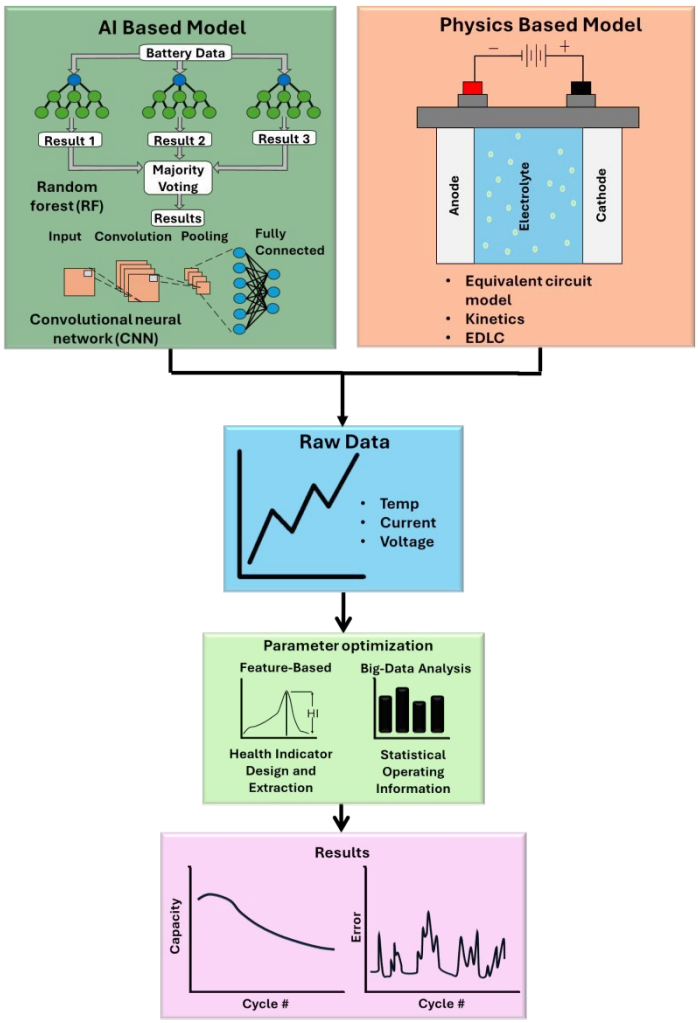

Figure 2. Flowchart illustrating common battery modeling approaches, including random forests (RF), convolutional neural networks (CNN), and physics-based models for parameter optimization and performance prediction. Partially adapted from ref.[20] with permission from John Wiley & Sons Ltd, copyright 2024.

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Physics-based models rely on electrochemical theory, transport equations, and thermodynamic principles to describe processes such as ion diffusion, charge transfer, and interphase growth.[1, 21, 22] These models offer strong interpretability and physical consistency, but they are often computationally intensive, sensitive to parameter uncertainty, and difficult to generalize across chemistries, cell formats, and operating conditions.[6, 12] Physics-based models excel for molecular-level electrolyte optimization and structure-based materials discovery, where mechanistic insight into ion transport, thermodynamics, and kinetics is essential for screening candidates and understanding degradation drivers.[1, 21, 22] As battery systems become more complex and data-rich, purely physics-based approaches alone often struggle to capture real-world variability and long-term degradation behavior.[2]

In contrast, ML models treat batteries as data-generating systems, learning relationships between measurable inputs, such as voltage, current, temperature, and cycling history, and target outputs including capacity fade, internal resistance, remaining useful life, or SOH, as illustrated in **Figure 2**.[3, 23] A wide range of algorithms has been applied to predict battery degradation behavior. Here, we highlight two commonly used approaches: Gaussian process regression (GPR) and random forests, two widely used classical ML methods, as well as convolutional neural networks (CNNs), a deep-learning architecture. Other deep-learning models frequently used in battery prediction include multilayer perceptrons (MLPs), recurrent neural networks (RNNs), and long short-term memory (LSTM) networks.

Classical ML methods such as Gaussian Process Regression (GPR) and random forests have been widely used for battery modeling and degradation prediction. Random forests are an ensemble machine-learning method that combines multiple decision trees to generate a prediction. Each tree is trained on a randomly selected subset of the data and evaluates different combinations of features, reducing overfitting and improving model generalization.[24, 25] In battery modeling, the final prediction is obtained by averaging the outputs of individual trees, enabling the model to capture relationships between operational variables such as temperature, current, internal resistance, and cycling conditions.

GPR models, in contrast, provide a probabilistic framework that learns nonlinear relationships between inputs and outputs while also estimating prediction uncertainty. This capability makes GPR particularly useful for optimization and materials discovery tasks where experimental data

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are limited.[26] Despite their effectiveness, a major limitation of many ML models, including random forests, is their strong dependence on the availability and diversity of training data.[24, 25] Currently, only a limited number of publicly available battery datasets exist, including the NASA Ames Prognostics Center of Excellence, Oxford battery degradation dataset, CALCE dataset (Center for advanced life cycle engineering, University of Maryland), and the Sandia National Laboratories battery repository, which constrains the ability of models to generalize across all operating conditions.[23]

Deep learning, a subset of machine learning based on artificial neural networks, has gained increasing attention in battery research due to its ability to capture complex, nonlinear degradation behavior.[27] Among these methods, CNNs, originally developed for image processing, are widely used for identifying patterns in sequential data.[28] In battery applications, charge–discharge data such as voltage, current, or capacity over time can be treated as structured signals that CNNs analyze by scanning the data in small segments to extract relevant features. This capability enables the models to identify indicators of battery aging and degradation without requiring handcrafted rules, making CNNs particularly effective for predicting remaining useful life and SOH.[19] However, deep-learning approaches typically require larger datasets and higher computational resources than classical ML methods such as random forests.[29]

Beyond CNNs, other deep-learning architectures, including MLPs, RNNs, and LSTM networks, have also been applied to battery prediction tasks. Additionally, autoencoders have been used for dimensionality reduction and anomaly detection, graph neural networks for learning structure–property relationships in electrode materials, and generative models for exploring battery degradation pathways and materials design spaces.[30, 31] Together, these approaches provide flexible data-driven tools for battery modeling, while highlighting ongoing challenges related to data availability, interpretability, and physical consistency. Pure ML models are well suited for operational-data-driven SOH prediction in grid applications, enabling rapid forecasting across diverse cycling conditions where scalability and predictive performance are prioritized over mechanistic interpretability.[3, 30]

To address these limitations, hybrid and physics-informed AI models have emerged as a promising middle ground. These approaches incorporate physical knowledge, such as monotonic degradation trends, conservation laws, or simplified electrochemical descriptors, into machine-learning frameworks through feature engineering, constrained loss functions, or tailored model

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architectures.[1, 2, 32] By integrating physical insight with data-driven learning, hybrid models can improve generalization, reduce data requirements, and enhance interpretability compared with purely data-driven approaches, while retaining the flexibility needed to capture nonlinear and multiscale battery behavior.[2, 21] In this way, hybrid frameworks help bridge laboratory-scale research and industrial deployment by embedding physical consistency into scalable predictive models.[33, 34] Although implementation complexity and computational cost remain important challenges, hybrid AI approaches are increasingly viewed as a promising route toward robust and scalable battery modeling.

3.1 AI-Enabled Electrolyte Discovery and Interfacial Design

Recent advances have integrated ML algorithms with automated experimentation to create closed-loop optimization platforms for electrolyte discovery. In one example, a Bayesian optimization algorithm (Dragonfly) was coupled with a robotic liquid-handling system (Clio) to optimize non-aqueous lithium-ion electrolyte compositions consisting of ethylene carbonate (EC), ethyl methyl carbonate (EMC), dimethyl carbonate (DMC), and $LiPF_6$ salt.[35] The AI system autonomously selected and tested candidate formulations, balancing investigation of uncertain mixtures with exploitation of promising compositions. Within 42 automated experiments, the platform identified a previously unreported high-conductivity electrolyte formulation (EC:DMC 40:60 by mass with 0.9 m $LiPF_6$) with an experimentally measured ionic conductivity of 13.7 mS cm^{-1}. Practical constraints include chances of contamination while testing different ratios/compositions of electrolytes, variations in peak conductivity at lower molality, and time required for electrolyte evaluation (30-40 mins for complete evaluation).[35]

When implemented in graphite‖$LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ pouch cells, the AI-optimized electrolyte enabled up to a 13% improvement in discharge capacity during 4C fast charging compared with baseline electrolytes.[35] As illustrated in **Figure 3**, ML workflows combine curated datasets with predictive models to screen candidate formulations efficiently, thereby accelerating the identification of electrolytes suitable for advanced battery chemistries.[36]

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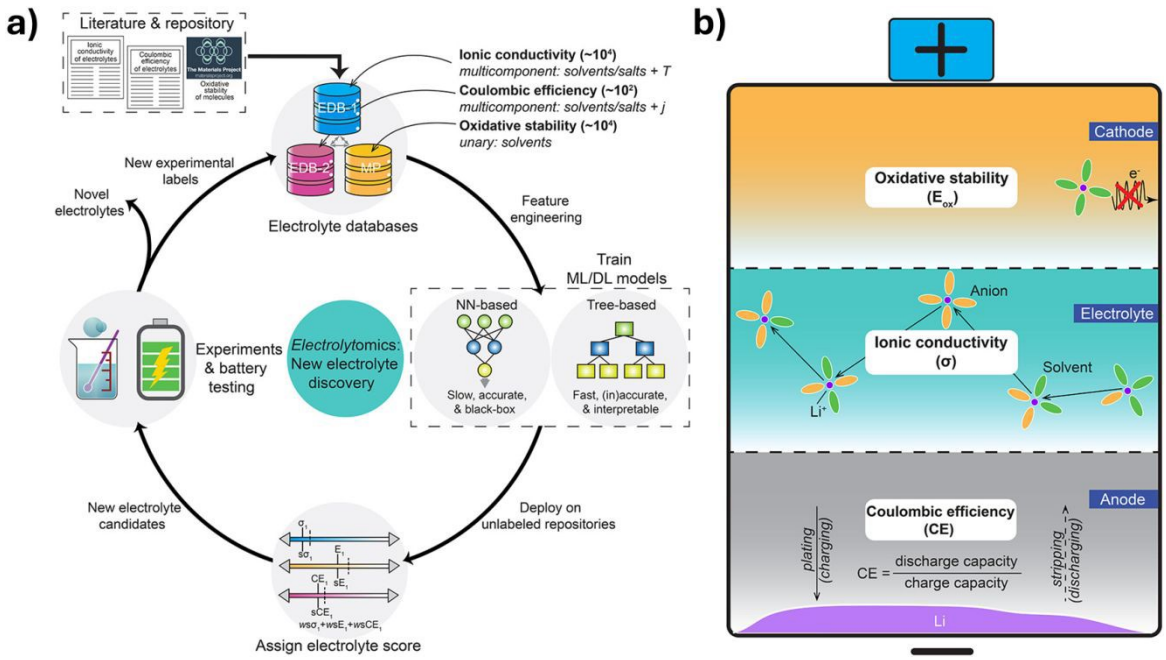

Figure 3. (a) Schematic illustrating the overall ML-based workflow utilized in the discovery of unexplored LMB electrolytes. (b) Illustration depicting three key figures of merits of a typical electrolyte: ionic conductivity, oxidative stability, and Coulombic efficiency. MP = Materials project, EDB-1 = ionic conductivity database, EDB-2 = Coulombic efficiency database. Reproduced from ref.[36] with permission from American Chemical Society, copyright 2025.

For properties supported by large historical datasets, such as ionic conductivity in solid-state electrolytes, graph-based deep learning models have demonstrated strong predictive capability. Graph neural networks (GNNs), which represent materials as graphs where atoms are treated as nodes and interatomic interactions as edges, have emerged as particularly powerful tools for learning structure–property relationships in crystalline materials. In solid-state lithium systems, large-scale GNN frameworks such as graph networks for material science (GNoME) have expanded the known stable materials dataset by ~381,000 new entries and demonstrated accurate ionic conductivity predictions for 623 novel compositions, indicating strong model generalizability. This approach also addressed the compositional limitations of databases such as the Materials Project (~69,000 entries) by generating diverse candidate structures and rigorously filtering training data, reducing prediction errors to approximately 40 meV atom^{-1}. A meta-generalized gradient approximation was further used to validate practical experimental feasibility, resulting in the identification of 528 promising solid-state lithium-ion conductors with ~84% agreement.[37]

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Finally, electrolyte performance is governed not only by bulk properties but also by interfacial stability, particularly the formation of the SEI. Predicting SEI behavior remains challenging due to the complex and multistep nature of electrolyte decomposition reactions, especially in high-voltage systems such as $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) operating near 4.7 V, where conventional carbonate solvents undergo oxidative degradation.[38, 39] To address this challenge, ML approaches have been integrated with laboratory battery testing to optimize electrolyte additives for improved interfacial stability. This study overcomes the limitations of small datasets by engineering custom, highly interpretable molecular descriptors that explicitly encode formal charge, atomic coordination, and ring inclusion, effectively capturing structural diversity while balancing machine-learning model complexity.

In another study, GPR models were trained on an initial experimental dataset of 28 single and dual additives, including vinylene carbonate (VC), lithium difluorooxalato borate (LiDFOB), and trimethylsilyl phosphite (TMSPi), to learn structure–property relationships governing electrolyte performance.[38] The trained model was then used to virtually screen 125 unexplored additive combinations by predicting key electrochemical metrics such as area-specific impedance (ASI), impedance growth, and final specific capacity. Based on these predictions, the most promising candidates were experimentally validated in 5 V graphite‖LNMO coin cells.[38] The predictions were later confirmed with experimental tests using coin cells and also confirmed mitigations including transition metal dissolution and lithium inventory loss. The optimized additive pair, 1 wt% lithium bis(oxalato)borate (LiBOB) and 1 wt% succinic anhydride (SA), delivered the highest final capacity (95.49 mAh g^{-1}) while significantly reducing impedance compared with the baseline electrolyte.[38]By directly linking ML-guided screening with experimental validation, such approaches extend AI-driven electrolyte design beyond computational prediction toward practical optimization of interfacial stability and battery performance.

3.2 AI-Enabled Electrode Discovery and Design

Across anode and cathode materials for monovalent and multivalent metal batteries, graph-based deep learning models have been particularly effective in predicting key electrochemical metrics, including operating voltage, specific capacity, formation energy, diffusion barriers, and structural stability. Crystal graph convolutional neural networks (CGCNNs) represent one of the most widely adopted architectures for electrode screening (**Figure 4**).[40] By representing crystalline

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structures as graphs, CGCNNs learn directly from atomic connectivity and local chemical environments, enabling accurate prediction of electrochemical properties across diverse materials classes.[40]

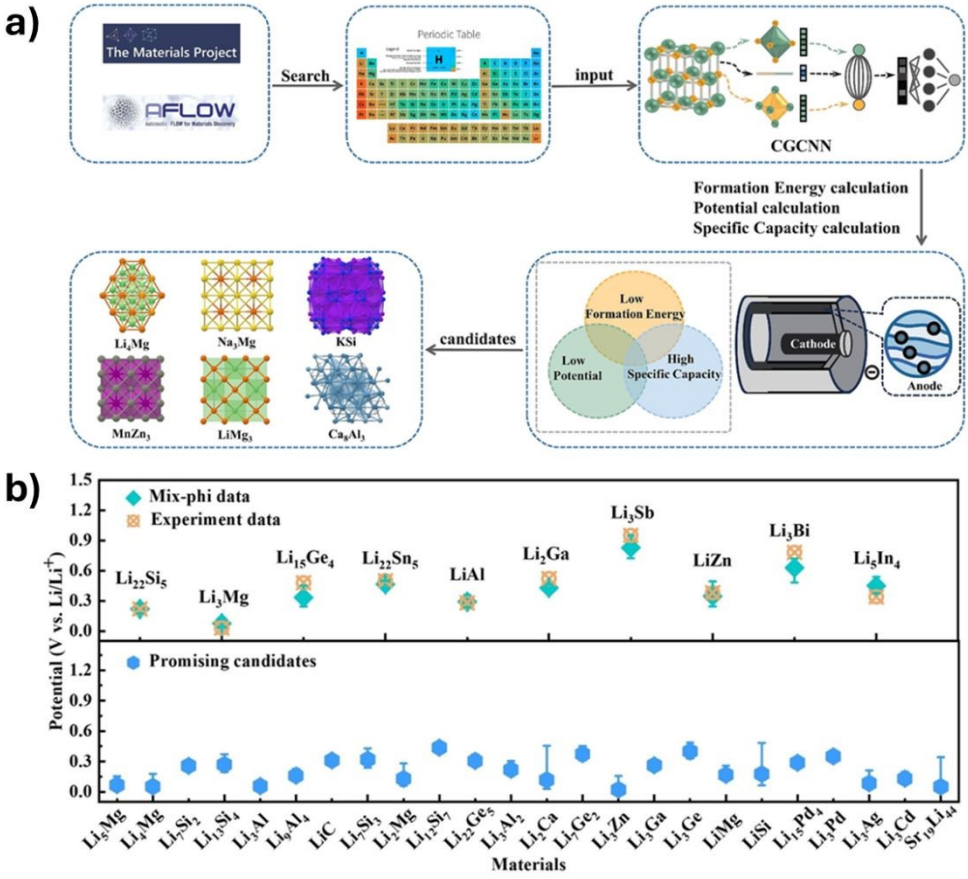

Figure 4. (a) Workflow for ML-assisted screening of alloy anode materials for lithium batteries. Data from the Materials Project (MP) and Automatic FLOW for materials discovery (AFLOW) databases were used to train a crystal graph CGCNN model to predict formation energy, electrochemical potential, and specific capacity. (b) Comparison between predicted and experimental potentials for selected Li alloy anodes, with error bars indicating uncertainty. Candidate materials are arranged from left to right in order to decrease theoretical specific capacity. Reproduced from ref.[40] with permission from Elsevier, copyright 2025.

Using databases such as the Materials Project and Automatic FLOW for materials discovery (AFLOW), CGCNN-based studies have identified low-voltage, high-capacity binary alloy anodes for lithium, sodium, potassium, magnesium, and aluminum batteries.[40] Screening based on formation energy, voltage, and capacity revealed numerous candidate materials, including Li–Mg,

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Li–Al, and Li–Si alloys, with several lithium-based systems exhibiting capacities exceeding 600 mAh g^{-1} at voltages below 0.3 V. The primary modeling targets included low operating potential and high specific capacity. Larger and more diverse datasets improved both predictive accuracy and model generalizability, with reported R^2 values approaching 1.[40]

Similar frameworks have also been applied to zinc-ion batteries, where CGCNN screening of oxides, fluorides, sulfides, and phosphates yielded approximately 80 cathode candidates with predicted voltages above 0.5 V and capacities exceeding 100 mAh g^{-1}. Notably, SrO_2 and CoO_2 were identified as high-capacity oxide cathodes with predicted capacities of 447 and 294 mAh g^{-1}, respectively, with model predictions showing good agreement with available experimental data. A DFT-based solver was trained to predict Gibbs energies for cathode materials using a dataset of approximately 190,000 materials from the AFLOW and Materials Project databases, achieving excellent predictive performance with R^2 values greater than 0.98.[41]

Beyond crystalline alloys and oxides, graph-based deep learning has also enabled the discovery of unconventional electrode materials. In one study, CGCNN screening of over 560,000 structures identified a boron-doped graphene anode (B_5C_{27}) as a promising candidate for alkali-metal-ion batteries.[42] This material exhibited predicted theoretical capacities of 2262, 2546, and 1131 mAh g^{-1} for Li, Na, and K systems, respectively, alongside low open-circuit voltages of approximately 0.09, 0.07, and 0.47 V.[42] The high capacity and favorable voltage profile were attributed to strong alkali-metal adsorption, low diffusion barriers, and a correlation between adsorption energy and substrate work function, illustrating how AI models can uncover structure–property relationships beyond conventional materials classes. CGCNN was also compared against other graph neural network architectures, including GCN, and exhibited the best predictive performance for correlating work function, adsorption behavior, and achievable capacity in boron-doped graphene systems.[42]

Complementary deep learning approaches have focused on paired charged–discharged electrode structures to capture volume changes and energy density simultaneously. Deep neural network (DNN) models trained on combined Materials Project and AFLOW datasets have identified electrode pairs with specific energies approaching 1000 Wh kg^{-1} and volume expansion below 20%.[43] For example, the $Li_7Fe(O_2F)_2$–$Fe(O_2F)_2$ redox pair exhibited a predicted capacity of 908 mAh g^{-1} with 18.5% volume expansion, while $LiSiNiO_4$–$SiNiO_4$ showed minimal volume change (0.1%) at higher voltage but lower capacity. These results highlight the ability of AI models

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to balance competing electrochemical and mechanical constraints that are difficult to optimize simultaneously. The DNN model reported predictive errors of approximately 11–13%, and the input features included active metal type, valence state, charged/discharged electrode energies, and crystal structure descriptors.[43]

More recently, large language model (LLM)-based frameworks have begun to bridge data-driven discovery with experimental decision-making. The ChatBattery platform represents an early demonstration of LLM-assisted electrode design, integrating hypothesis generation, computational screening, and experimental validation within a closed-loop workflow.[44] Using a GPT-3.5-based agent, the framework identified modified NMC cathodes, including NMC–SiMg, NMC–SiCa, and NMC–MgB, with experimentally validated capacities of 174, 169, and 160 mAh g^{-1}, corresponding to improvements of up to ~29% over conventional NMC811. These materials also exhibited stable cycling within a 2.6–4.3 V window and distinct microstructural features, underscoring the potential of LLMs to guide not only materials selection but also synthesis and characterization strategies.[44]

4. Challenges and Limitations of AI-Driven Battery Design

Despite rapid progress, the widespread deployment of AI-driven approaches in battery research remains constrained by several fundamental challenges, most notably data availability, dataset quality, and limited model generalizability (**Figure 5**). Unlike fields where large, standardized datasets exist, battery data are often sparse, high-dimensional, and fragmented across the literature. Experimental results frequently vary due to differences in measurement protocols, material purity, cell formats, and operating conditions, introducing inconsistencies that obscure reliable structure–property–performance relationships.[27, 36, 45] As a result, ML models may perform well within known regions of the design space but struggle to extrapolate to new materials or chemistries.

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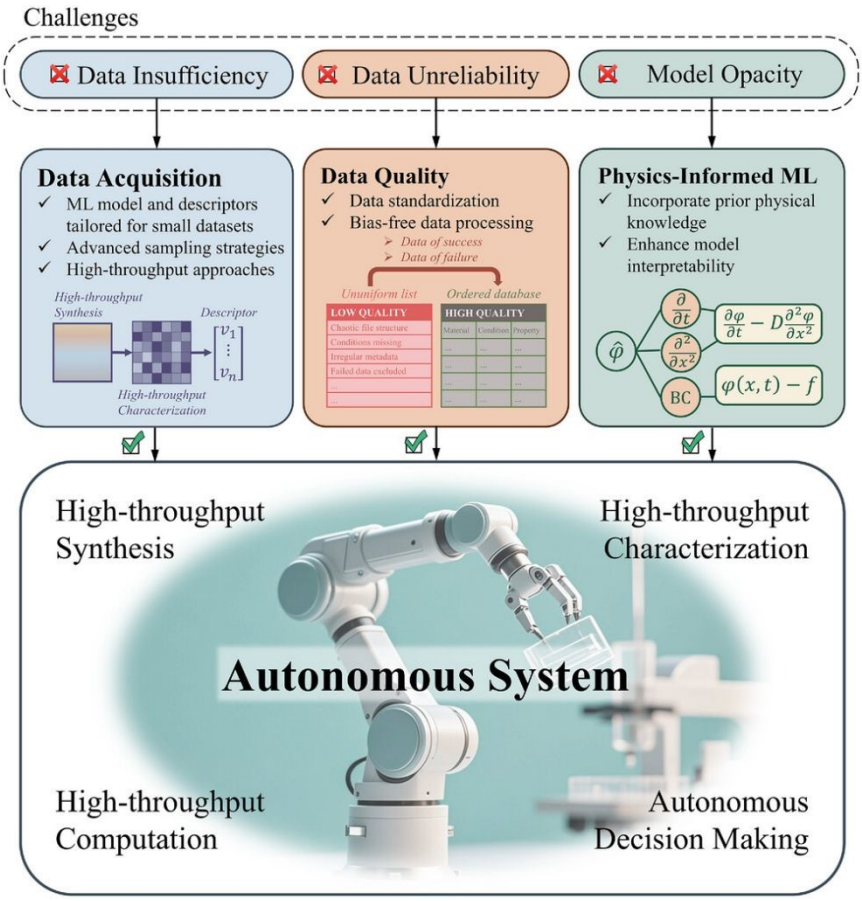

Figure 5. Primary challenges and opportunities in AI for materials design in rechargeable battery technology. Reproduced from ref.[46] with permission from Wiley-VCH GmbH, copyright 2025.

These challenges are further compounded by evaluation biases in model development. Many studies rely on random or stratified data splitting strategies, which can produce overly optimistic performance estimates.[2, 45] When models are tested using chemically or structurally distinct datasets, such as cluster- or scaffold-based splits, their predictive accuracy often decreases significantly.[23] This behavior indicates that many models primarily interpolate within familiar data distributions rather than learning transferable physical trends, limiting their reliability for discovering genuinely novel battery materials and chemistries.[27, 47]

Current AI models in battery research frequently suffer from generalization failures because they rely on controlled laboratory datasets that ignore the complex influences of real-world operating conditions.[48] Additionally, the high cost of experimental testing results in data scarcity and heterogeneous datasets, which often leads to algorithmic overfitting and systematic biases that

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limit predictive accuracy.[49] These technical limitations are exacerbated by commercial data privacy concerns, as industry confidentiality restricts the sharing of real-world operational metrics required to train robust frameworks.[2]

Model generalization beyond the training distribution represents a second, closely related challenge. AI models trained predominantly in specific materials classes, such as carbonate-based electrolytes, layered oxide cathodes, or commercial lithium-ion cycling data, often struggle to extrapolate to underrepresented systems, including fluorinated solvents, multivalent electrodes, or unconventional operating regimes.[25, 36] Prediction uncertainty tends to increase sharply as chemical or structural similarity to the training data decreases, highlighting the difficulty of applying data-driven models to emerging battery chemistries. Although large-scale foundation models pretrained on millions of molecules or crystal structures show improved robustness, reliable extrapolation to entirely new materials families and multicomponent formulations remain an open problem.[25, 36]

Practical deployability further constrains AI-driven battery design. Many current workflows prioritize optimization of isolated performance metrics, such as ionic conductivity, voltage, or capacity, without fully accounting for synthesis feasibility, material cost, environmental impact, safety, or scalability.[35, 50] For example, an AI-identified electrolyte or electrode material may exhibit exceptional predicted performance yet be impractical due to synthetic complexity, limited precursor availability, or poor stability under realistic operating conditions.[35, 50] Emerging frameworks that integrate retrosynthesis prediction, cost estimation, and manufacturability constraints represent important progress, but comprehensive multi-objective optimization across performance, feasibility, and sustainability remains computationally and methodologically challenging.[35, 50]

Similar limitations arise in AI-based battery health and degradation modeling. ML approaches for SOH estimation and lifetime prediction often perform well on curated laboratory datasets but generalize poorly across different cell designs, manufacturers, chemistries, and real-world usage profiles.[2, 45, 51] Battery degradation is influenced by multiple coupled factors, including charge–discharge rates, C-rates, temperature, and cycling history, which increases modeling complexity. Common AI/ML approaches such as LSTM networks and CNNs each offer distinct advantages but also present important limitations. For example, LSTM models can capture long-term temporal dependencies but typically require large training datasets, and CNN-based approaches often

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involve extensive preprocessing and high computational cost despite their strong performance in analyzing spatially resolved features.[52]

These challenges are further exacerbated by the difficulty of acquiring large, representative aging datasets, as battery degradation evolves over thousands of cycles and extended time periods, accelerated aging experiments require substantial infrastructure, and field data are often incomplete or noisy.[53] As a result, many ML models risk overfitting to specific datasets or experimental conditions rather than capturing universal degradation mechanisms. Moreover, the predominantly empirical nature of SOH labels and evaluation metrics complicates comparison across studies and limits mechanistic interpretability.[2, 54]

Finally, model transparency and physical consistency remain persistent concerns. Purely data-driven models can generate predictions that violate known physical constraints, particularly when operating outside the training domain or under atypical conditions. While hybrid and physics-informed approaches mitigate some of these issues, they introduce additional complexity, computational cost, and challenges in balancing physical priors with data-driven flexibility. Establishing community-wide standards for data reporting, adopting FAIR (Findable, Accessible, Interoperable, and Reusable) data practices, and systematically integrating physical knowledge into AI models will be essential for overcoming these barriers.[1, 21, 27, 55]

5. Applications and Future Directions

AI-assisted electrochemical discovery and battery management are already demonstrating tangible techno-economic benefits across the battery value chain by shortening development cycles, reducing experimental overhead, and enabling improved asset utilization.[49, 56] Data-driven workflows integrating large electrolyte databases with graph neural networks enable rapid in silico screening of extensive chemical spaces prior to synthesis, shifting effort away from labor- and material-intensive trial-and-error experimentation toward comparatively inexpensive computational evaluation.[36, 49] These approaches allow experimental efforts to focus on the most promising and manufacturable candidates while substantially reducing the cost and time associated with electrolyte optimization. For example, Bayesian optimization frameworks have identified non-intuitive high-conductivity carbonate electrolytes capable of delivering ~13% improvement in 4C fast-charging capacity in graphite–$LiNiMnCoO_2$ pouch cells using only 42 automated experiments. [35]

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At the cell and system level, ML-based lifetime prediction frameworks have improved extrapolation accuracy for lithium-ion battery aging by 13–77% compared with semi-empirical models, while reducing required aging-test durations from approximately 280 to 140 days.[57] These improvements enable more accurate battery pack sizing, thinner safety margins, and more aggressive yet controlled fast-charging strategies in techno-economic optimization studies. Furthermore, probabilistic battery health diagnostics that explicitly quantify predictive uncertainty enable warranty, replacement, and reserve-capacity decisions to be evaluated within a risk-aware economic framework, which is critical for incorporating AI models into levelized cost of storage and total cost of ownership analyses.[48] These capabilities are increasingly being integrated into techno-economic assessment frameworks for grid-scale and second-life battery systems, where accurate degradation forecasts strongly influence economic viability. For example, recent analyses of second-life batteries coupled with photovoltaics indicate that refurbished battery packs become financially attractive only when their purchase cost is approximately 40% or less than that of new batteries, a threshold that depends sensitively on projected lifetime and utilization profiles that AI-enhanced prognostics can help constrain.[58]

In parallel, the future of AI-enabled battery research will increasingly rely on the convergence of autonomous experimentation, multi-modal data integration, and physically informed learning frameworks. As battery systems continue to diversify in chemistry, architecture, and operating conditions, traditional workflows that separate computation, experimentation, and modeling are becoming increasingly inefficient.[37] In response, autonomous or "self-driving" laboratories (SDLs) are emerging as a powerful paradigm for accelerating materials discovery and optimization (**Figure 6**). By integrating AI-driven decision-making with robotic synthesis, characterization, and data analysis, SDLs enable closed-loop workflows that iteratively propose, test, and refine materials or operating conditions with minimal human intervention.[59] Early demonstrations have shown that such platforms can investigate hundreds of candidate formulations or processing conditions in days rather than months, significantly reducing development timelines.

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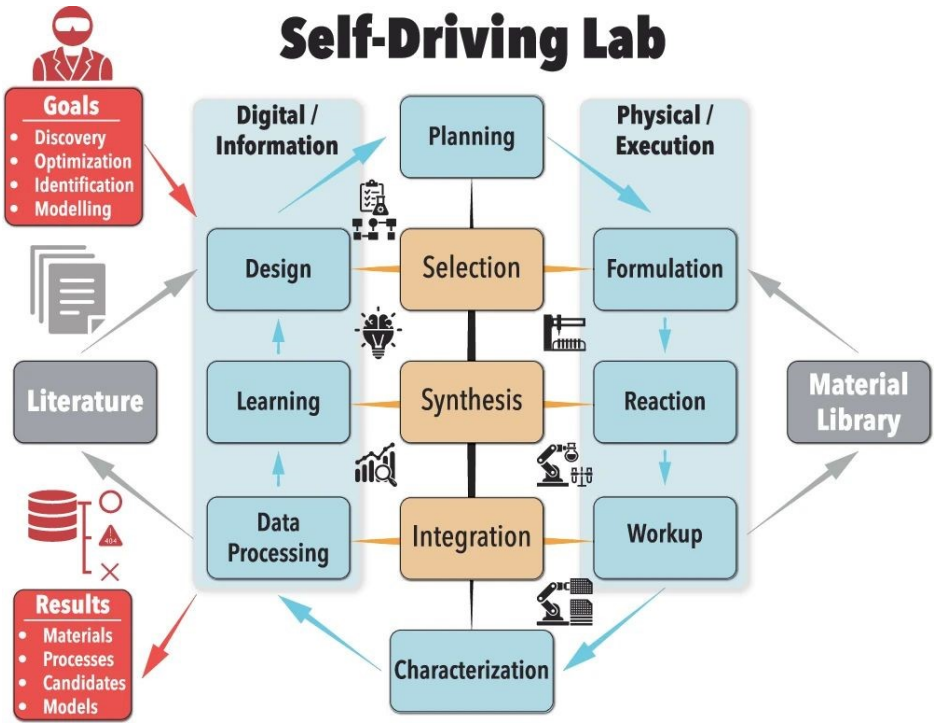

Figure 6. Schematic of a self-driving laboratory (SDL) operation. Reproduced from ref.[60] with permission from Springer Nature, copyright 2025.

Looking forward, the success of autonomous discovery platforms will depend on multi-modal AI frameworks capable of integrating heterogeneous datasets. Future battery "digital twins" are expected to combine experimental measurements with atomistic simulations, continuum-scale models, and operational data to capture coupled phenomena across multiple spatial and temporal scales.[55] Such integration will be particularly important for extending AI methodologies beyond well-established liquid electrolyte systems to more complex materials platforms, including solid-state electrolytes, polymer-based electrolytes, and composite electrodes, where transport, interfacial stability, and mechanical behavior are strongly intertwined. Similar opportunities exist at the system level, where combining electrochemical, thermal, mechanical, and operational data could enable more accurate lifetime prediction and adaptive energy storage management strategies.[61, 62]

As AI models continue to evolve, interpretability and physical consistency will remain critical for their long-term impact in battery science. Although purely data-driven models have demonstrated impressive predictive capabilities, their limited transparency can hinder trust and

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scientific insight. Increasing attention is therefore being directed toward explainable AI (XAI) and physics-informed learning frameworks that incorporate domain knowledge directly into model architectures.[27, 63] These approaches offer a pathway toward AI models that are not only predictive but also mechanistically interpretable, ultimately enabling more reliable and deployable AI-driven battery design.

Overall, while the direct computational cost of AI models is negligible compared with battery manufacturing capital expenditure (CapEx), their demonstrated ability to accelerate discovery timelines, de-risk deployment decisions, and extend usable battery lifetime positions AI as an increasingly important tool for reducing levelized cost and improving the reliability and commercial viability of next-generation electrochemical energy storage systems. Fully realizing this potential, however, will require continued progress in data quality, model generalization, interpretability, and standardization through the development of open datasets, physics-informed frameworks, and community-wide reporting protocols.[49]

6. Conclusion

AI is rapidly evolving from a computational accelerator into a foundational component of battery research and development. Its greatest potential lies not in replacing physical understanding, but in augmenting it, enabling rational navigation of high-dimensional design spaces that span materials, interfaces, and operating conditions. Continued progress will require coordinated advances in data curation, model development, experimental automation, and community-wide standards. When coupled with rigorous physical insight and experimental validation, AI-driven approaches are poised to play a defining role in the design of safer, longer-lasting, and higher-performance energy storage technologies.[27, 59, 64, 65]

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Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

Notes

There are no conflicts to declare.

Data availability

No new data were generated or analyzed in this study. All information discussed in this review is available in the cited literature.

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Data availability

No new data were generated or analyzed in this study. All information discussed in this review is available in the cited literature.