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Artificial Intelligence-Driven Strategies for Advancing Lithium-Ion Battery Performance and Safety

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ABSTRACT
Artificial intelligence (AI) is revolutionizing the development and optimization of lithium-ion batteries (LIBs), which are critical in modern technologies like energy storage systems and electric vehicles (EVs). This review explores AI-driven strategies aimed at enhancing LIB performance, safety, and longevity. AI techniques, including machine learning models likeensemble methods, support vector machines, and neural networks, have been instrumental in predictive maintenance, state of charge (SoC) and state of health (SoH) estimation, and materials discovery. These AI approaches enable more accurate predictions of battery degradation and failures, optimizing charge cycles, and improving real-time diagnostics. Furthermore, AI enhances the design of safer and more efficient battery components by accelerating materials research, thus improving LIB capacity and safety profiles. However, despite these advancements, challenges like data quality, model interpretability, and the integration of AI models into existing industrial frameworks persist. Emerging technologies such as reinforcement learning and federated learning show great promise for addressing these obstacles, enabling dynamic optimization of charge cycles and the collaborative development of more generalized AI models. As collaborative research and open data-sharing initiatives expand, AI's transformative potential in driving more sustainable, efficient, and safer energy storage solutions will continue to grow, shaping the future of LIBs and their applications in a greener, more energy-efficient world.

Keywords: Lithium-ion batteries, AI-driven BMS, Machine learning, Neural networks, Predictive maintenance, Battery safety, AI in battery design, Reinforcement learning.

I. INTRODUCTION

1.0 Overview of Lithium-Ion Batteries (LIBs) and Their Importance in Modern Technology

Lithium-ion batteries (LIBs) play a vital role in today's technological advancements, supplying energy to various devices, from smartphones and laptops to electric vehicles (EVs) and renewable energy storage systems. Their prominence is largely due to their superior energy density, longer cycle life, and lightweight design compared to other rechargeable battery technologies. LIBs are fundamental in supporting the global shift towards renewable energy and sustainable practices, especially in the transportation and energy sectors [1-3].

The deployment of LIBs in EVs, in particular, represents a significant advancement in mitigating greenhouse gas emissions and addressing climate change. The electrification of transportation relies heavily on the continued development of high-performance, reliable LIBs that can meet the stringent demands of automotive applications. In addition, LIBs play a crucial role in grid storage systems that stabilize the supply and demand of electricity generated from renewable sources like solar and wind [4,5]. This capability is essential for integrating variable renewable energy sources into the grid, strengthening energy security, and reducing dependence on fossil fuels [6].Beyond their applications in energy and transportation, LIBs are also crucial in the consumer electronics market. Their ability to deliver stable power in a compact form factor has revolutionized the design and functionality of portable devices, enabling the development of more powerful and feature-rich gadgets [7,8]. As technology continues to evolve, the demand for With the growing necessity for lithium-ion batteries that can store more energy, charge rapidly, and offer improved safety, the focus of research is shifting toward finding novel materials, innovative cell structures, and advanced production techniques to push the performance of these batteries even further [8].

II.CHALLENGES IN OPTIMIZING PERFORMANCE, SAFETY, AND LONGEVITY OF LIBS

Despite their widespread adoption, LIBs face several significant challenges that impact their performance, safety, and longevity. One of the primary issues is capacity degradation over time, which is influenced by complex electrochemical and mechanical processes within the battery. These mechanisms include the formation of the SEI layer, lithium accumulation, and the creation of micro-fissures within the electrode materials.As these conditions take effect, they slowly degrade the battery's capacity and increase internal resistance, resulting in a diminished operational lifespan [9-12].

Thermal management is another critical challenge, as LIBs are sensitive to temperature fluctuations. High temperatures can accelerate degradation processes, while lower temperatures basically hinder the battery's efficiency, reducing its power delivery. Furthermore, thermal runaway, where a cell rapidly overheats and can potentially ignite or explode, remains a serious safety concern, particularly in high-energy applications like EVs (see figure 1) and grid storage [13,14]. This risk is compounded by the fact that LIBs can experience uneven heating and cooling within battery packs, leading to localized hot spots that are difficult to detect and manage [14].

Moreover, the intricate structure of lithium-ion batteries (LIBs) makes it challenging to reliably assess their health status and forecast their remaining lifespan, particularly when operating under diverse conditions. Conventional battery management systems (BMS) utilize basic models that frequently overlook the complex relationships among battery components, leading to less precise forecasting. These limitations pose significant challenges for securing both the safe handling and effective functioning of lithium-ion battery technology, particularly as they are scaled up for use in larger, more demanding applications [14-16].

In addition to these technical challenges, the scalability and environmental impact of LIB production are also areas of concern. Extracting and processing materials like lithium, cobalt, and nickel have a profound impact on both the environment and local communities. The development of more sustainable and cost-effective production methods is essential for meeting the growing demand for LIBs without exacerbating resource depletion and environmental degradation [17,18].

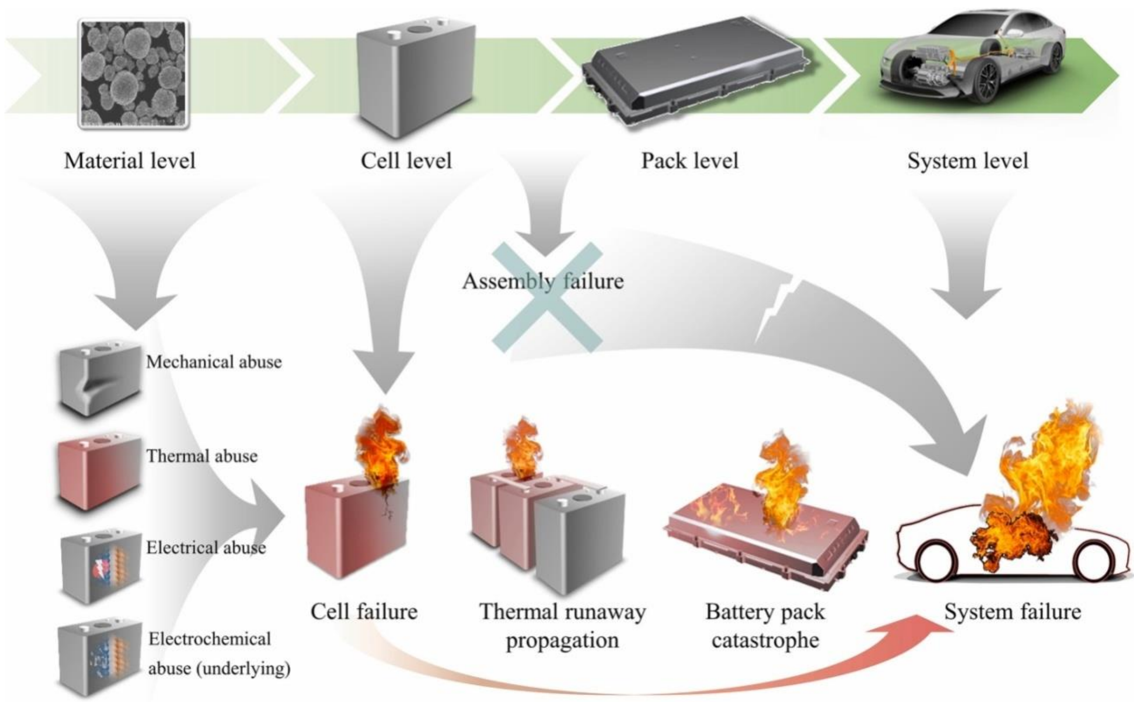

Figure 1: Progression of catastrophic battery failure in an electric vehicle**.** Reproduced from Ref [13] with permission.

III.THE IMPACT OF AI IN ADDRESSING LIB CHALLENGES

AI is playing a critical role in overcoming the diverse obstacles related to enhancing the performance, security, and durability of lithium-ion batteries. By leveraging machine learning (ML) and data analytics, AI can process vast amounts of data generated by LIBs during operation, uncovering patterns and insights that are often imperceptible to traditional methods. This capability is instrumental in enhancing the accuracy of SoH and RUL predictions, enabling more effective battery management strategies [19-22].

One major role of artificial intelligence in the realm of lithium-ion batteries involves the design of sophisticated prediction systems for managing and tracking battery health. By utilizing algorithms like neural networks, decision trees, and support vector machines, these models can interpret factors like voltage, current, temperature, and internal resistance to offer insights into the battery's condition. By doing so, they can predict future performance and potential failure modes with greater precision than conventional methods. This predictive capability allows for proactive maintenance and optimized charging/discharging protocols, which can significantly reduce the threat of catastrophic failures and prolong battery life [23,24].

AI is also playing a critical role in materials discovery and design. By using techniques such as reinforcement learning and generative adversarial networks (GANs), researchers can accelerate the identification of new materials with improved electrochemical properties. These AI-driven approaches can simulate thousands of potential material combinations and their interactions, significantly speeding up the experimental process and reducing the cost of developing next-generation LIBs. Additionally, AI can optimize the microstructural design of electrodes and electrolytes, enhancing ionic conductivity and mechanical stability, which are crucial for improving overall battery performance [23,25,26].

Furthermore, AI enhances safety by enabling real-time monitoring and early detection of anomalies that could lead to hazardous conditions. Advanced ML models can identify subtle changes in battery behavior that precede thermal runaway or other dangerous scenarios, providing early warnings and enabling interventions before a failure occurs. This capability is particularly valuable in high-risk applications like EVs and grid storage, where the consequences of a battery failure can be severe [27,28].

3.1 Applications of AI in Lithium-Ion Battery Management

3.1.1 Battery Management Systems (BMS)

The efficient and safe functioning of lithium-ion batteries, especially in electric vehicles (EVs) and mobile electronics, relies heavily on Battery Management Systems (BMS). These systems oversee multiple functions, including monitoring battery state, protecting against faults, balancing cell voltage, and predicting battery health as shown in figure 2 [29]. The performance and longevity of LIBs heavily depend on the precision and capabilities of the BMS, as they are responsible for ensuring ideal working conditions, avoiding excess heat, and efficiently handling energy storage [29,30]. Traditionally, BMS relied on conventional algorithms and rule-based control systems, but the rapid advancement in Artificial Intelligence (AI) has revolutionized their capabilities, leading to more accurate, adaptive, and reliable battery management [29-31]. Table 1 highlights the significant improvements AI brings to BMS systems compared to traditional methods, providing a clear comparison across various key features.

Table 1: Comparison between Traditional vs. AI-Enhanced Battery Management Systems (BMS)

Features	Traditional BMS	AI-Enhanced BMS
Monitoring Precision	Relies on basic algorithms (e.g., Coulomb counting), providing less accurate SoH and SoC estimates	Leverages AI models (e.g., neural networks, SVM), offering highly precise SoH and SoC predictions
Fault Detection	Reactive approach; faults are detected only after they manifest	Proactive approach; AI models predict faults before they occur, enabling preventive maintenance
Predictive Capabilities	Limited; traditional methods struggle to predict long-term battery degradation and failures	Advanced; machine learning models (e.g., Random Forests, LSTM) can accurately predict remaining useful life (RUL) and degradation patterns
Real-time Adaptability	Fixed, rule-based logic, not adaptable to real-time environmental changes or operational variations	Adaptive; AI continuously learns from real-time data, optimizing performance based on operating conditions
Thermal Management	Basic thermal control algorithms that respond to overheating once detected	AI-driven thermal management systems optimize cooling strategies and prevent thermal runaway before it happens
Data Requirements	Requires fewer data inputs, but provides limited insights	Requires large datasets for model training, but provides more detailed and actionable insights
Scalability for Large Applications	Struggles to scale effectively, especially for large applications like EVs or grid storage	Highly scalable; AI models handle complex systems with large numbers of cells and different conditions
Charge Cycle Optimization	Relies on predetermined charging protocols, often leading to inefficient battery use	AI optimizes charge cycles in real time, minimizing damage and maximizing battery lifespan
System Cost and Implementation	Lower implementation cost, widely adopted in older battery technologies	Higher cost due to computational power and data requirements, but provides long-term benefits like extended battery life

Safety Management	Limited real-time safety diagnostics; thermal runaway or faults often detected late	Advanced AI-based anomaly detection, real-time safety diagnostics, and early intervention to prevent catastrophic failures

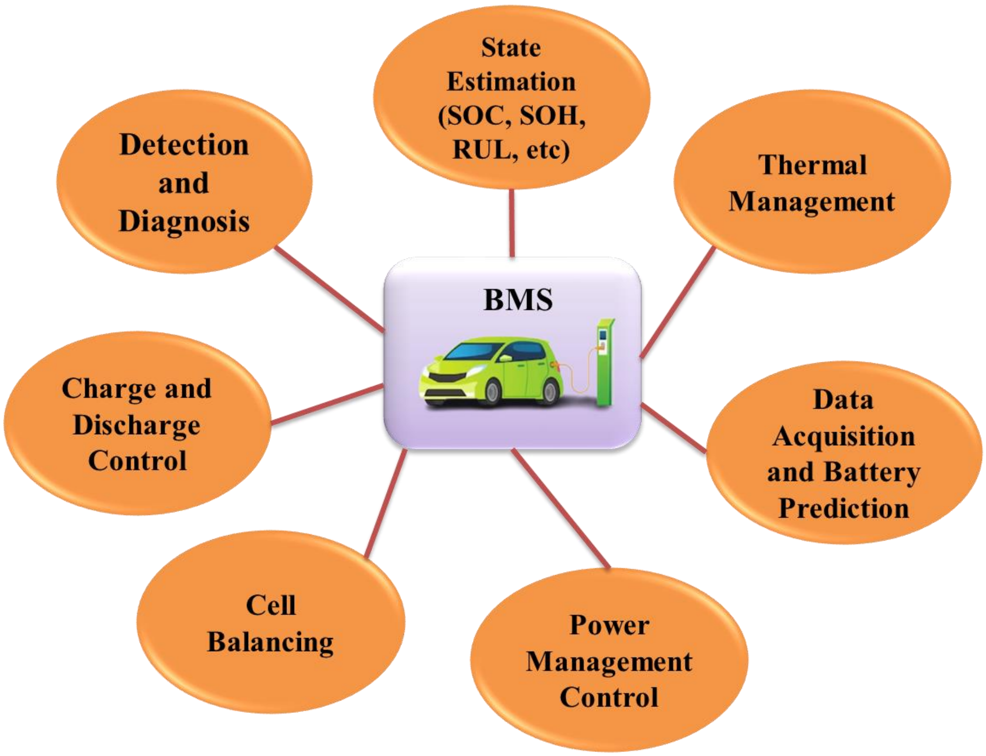

Figure 2: Schematic of AI-Driven Lithium-Ion Battery (LIB) Management System. Modified from Ref [33] with permission.

3.1.1.1 AI-Enhanced BMS for Improved Performance Monitoring and Safety Management

Incorporating AI, especially deep learning models and machine learning (ML), into BMS has significantly enhanced the monitoring and management of battery performance and safety. AI models can analyze large datasets collected from battery sensors to identify complex patterns and correlations that are not easily discernible through traditional methods [32-34]. For instance, techniques from deep learning as summarized in Table 2, particularly Long Short-Term Memory (LSTM) networks, are being utilized to estimate the State of Health (SOH) and State of Charge (SOC)in batteries with higher accuracy compared to conventional methods. These models can account for various operational conditions, such as temperature fluctuations and charging/discharging cycles, providing more reliable and precise estimates, which are crucial for ensuring the longevity and safety of batteries [24,34].

AI-enhanced BMS also play a critical role in effective temperature control crucial for ensuring the safety and efficiency of battery systems. AI algorithms can optimize cooling strategies based on real-time data to prevent thermal runaway, a dangerous condition that can lead to battery failure and potential hazards. These systems are designed to continuously learn from real-time operational data and adapt their responses accordingly, reducing risks and improving both safety and reliability of the battery system. Moreover, AI can facilitate the development of self-healing mechanisms in BMS, allowing them to detect and correct anomalies in real-time, thus preventing minor issues from escalating into major failures [24,29,30].

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Table 2: AI Models and Their Applications in LIB Management

AI Model	**Application in LIB Management**	**Key Benefits**	**Key Challenges**
Neural Networks (NNs)	SoH and SoC prediction, materials discovery, fault detection	High accuracy in predicting nonlinear battery behaviors, adaptable to various conditions (e.g., temperature, load, etc.)	Requires large datasets for training, computationally intensive
Long Short-Term Memory (LSTM)	SoH and SoC estimation, predictive maintenance	Excels in time-series data, captures long-term dependencies in battery aging and degradation processes	Sensitive to hyperparameters, performance may drop with noisy data
Support Vector Machines (SVM)	SoH and SoC estimation, fault detection	Effective in handling small to medium datasets, good generalization with limited data	Limited scalability with large datasets, kernel selection critical for performance
Random Forests (RFs)	SoH estimation, Remaining Useful Life (RUL) prediction, predictive maintenance	Robust against overfitting, handles noisy and high-dimensional data effectively	Requires careful tuning to avoid model complexity and overuse of resources
Gradient Boosting Machines (GBMs)	SoH and SoC prediction, charge cycle optimization	High accuracy, capable of handling complex degradation patterns, efficient for large datasets	Computationally expensive, prone to overfitting without careful regularization
Reinforcement Learning (RL)	Charging and discharging optimization, safety management	Dynamic learning from real-time conditions, capable of optimizing charge cycles and reducing degradation	Complex to implement, requires significant amounts of data for training
Convolutional Neural Networks (CNNs)	Fault detection (e.g., thermal runaway), safety monitoring	Highly effective for image-based fault detection (e.g., thermal imaging), useful for early anomaly detection	Computationally heavy, requires specialized hardware for real-time image processing
Federated Learning (FL)	Collaborative model training across multiple battery systems (e.g., EVs, energy grids)	Ensures data privacy, enables large-scale model training across decentralized systems	Data quality inconsistencies across devices, challenges in model coordination
Explainable AI (XAI)	Enhancing transparency in SoH and SoC estimation, safety management	Improves trust in AI models by making predictions interpretable, especially in safety-critical applications (e.g., EVs)	Trade-off between interpretability and accuracy, complex models harder to explain
Hybrid Models (AI + Physics-based)	SoH and SoC prediction, fault detection, real-time safety diagnostics	Combines the accuracy of AI with physical model insights, better at handling battery behavior under varied conditions	Computationally intensive, requires expertise in both AI and physical modeling

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3.1.1.2 Machine Learning in Predictive Maintenance and Real-Time Diagnostics

Machine learning plays a pivotal role in predictive maintenance and real-time diagnostics of lithium-ion batteries, enabling early detection of potential faults and reducing the risk of unexpected failures. Techniques such as neural networks, decision trees, and support vector machines (SVM)have been utilized to develop predictive models that can forecast the Remaining Useful Life (RUL) of batteries based on historical and real-time data. These models can identify subtle degradation patterns that are indicative of future performance issues, allowing for timely interventions that can extend battery life and optimize maintenance schedules [27,35,36].

Real-time diagnostics, powered by AI, enhance the capability of BMS to monitor and diagnose battery health in dynamic operating environments [24]. For example, AI models can perform anomaly detection by continuously analyzing voltage, current, and temperature data to identify deviations from normal behavior. This real-time analysis enables the BMS to implement corrective actions, such as adjusting the charging/discharging rates or activating cooling systems, to prevent damage and ensure safe operation [37,38].

Additionally, AI-driven BMS can support the development of digital twins for batteries, providing a virtual model that replicates the physical battery's behavior in real-time. These digital twins can simulate various scenarios to predict the impact of different operating conditions on battery performance, offering valuable insights for optimizing usage patterns and enhancing safety measures. This capability is particularly beneficial for complex applications like electric vehicles, where managing battery systems properly is key to sustaining their efficiency and safety when exposed to changing load demands [39-41].

3.2 State of Charge (SoC) and State of Health (SoH) Predictions:

Estimating the State of Charge (SoC) and State of Health (SoH) is essential for ensuring optimal performance, extended lifespan, and safe operation of lithium-ion batteries. SoH indicates how much capacity a battery retains in comparison to when it was new, while SoC measures the current charge level relative to its full charge [42,43]. These indicators are essential for optimizing the battery's usage and extending its life cycle, especially in high-endutilizations like renewable energy storage and electric vehicles (EVs) [42].Precise and timely estimation of State of Health (SoH) and prediction of Remaining Useful Life (RUL) are essential for effective battery management systems (BMS). Figure 3 illustrates the correlation between SoH and RUL in the battery.

However, the challenge lies in the complex degradation behaviors and nonlinear characteristics of lithium-ion batteries, which make accurate SoH and SoC estimations difficult through traditional methods. Artificial intelligence (AI) techniques, specifically machine learning models, have demonstrated immense potential in overcoming these limitations [42]. Table 3provides a detailed comparison of AI models used for State of Health (SoH) and State of Charge (SoC) predictions in LIBs, highlighting their accuracy, advantages, and limitations.

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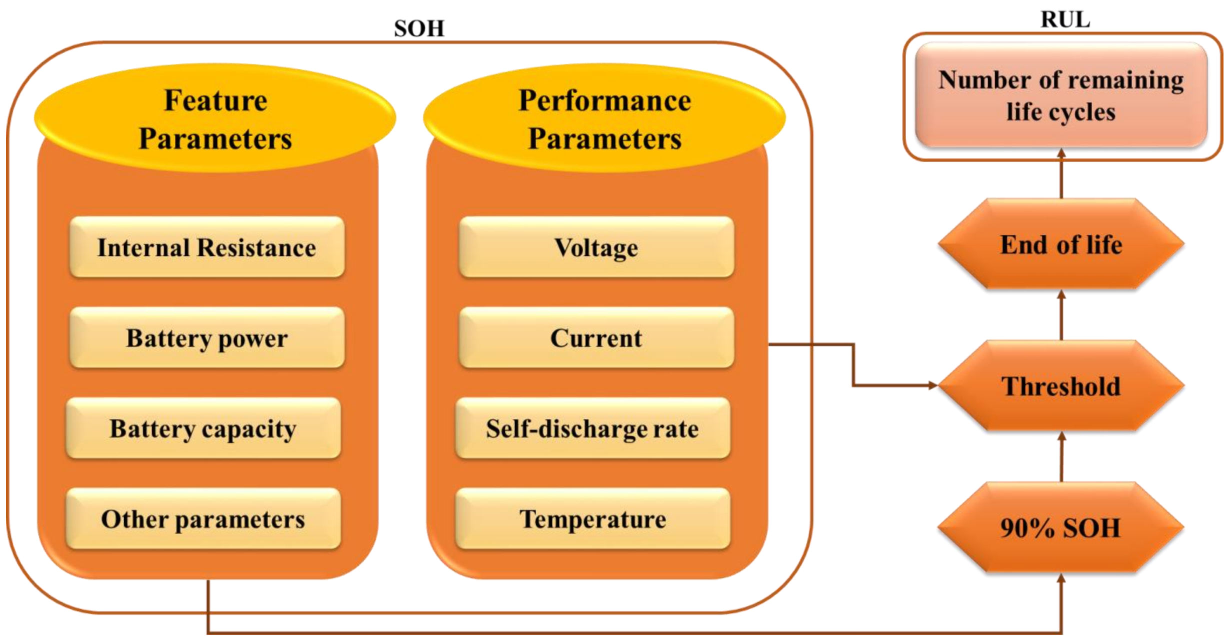

Figure3. The correlation between SOH and RUL.

3.2.1 Applications of AI State of Charge (SoC) and State of Health (SoH) Predictions

State of Charge (SoC) and State of Health (SoH) are crucial parameters for assessing the performance and reliability of lithium-ion batteries (LIBs). As already mentioned earlier, SoH provides an estimate of a battery's remaining capacity relative to its initial state, indicating its ability to perform over time. It is an essential metric for determining the lifespan and safety of the battery. On the other hand, SoC refers to the current energy level of the battery relative to its total capacity, which is vital for managing the battery's charge and discharge cycles effectively. Accurate predictions of these states are essential for optimizing battery performance, safety, and longevity, especially in applications like electric vehicles and grid storage systems [44,45].

According to Zhang et al [46], traditional methods for SoH and SoC estimation, such as electrochemical impedance spectroscopy and model-based approaches, face challenges like high computational complexity and limited accuracy under varying conditions. This is where artificial intelligence (AI) plays a transformative role by offering advanced, data-driven solutions that enhance prediction accuracy and operational efficiency [46,47].

Another critical challenge in State of Charge (SoC) estimation is cell-to-cell variation, which can significantly impact the accuracy of SoC predictions. To express this variation, a common practice is to rely on statistical analysis, such as standard deviation from rated capacity or resistance for a specific cell model. While quality control and inspection at the manufacturing site can help ensure the production of high-quality cells, the reliability of such control processes remains underexplored in the literature. Studies by Dubarry et al. [44] and An et al. [47] have highlighted the origins of these variations, noting that battery performance metrics are influenced by a complex interplay of thermodynamic and kinetic factors, each with its own probability distribution.

This variability presents a challenge for statistical analyses of battery metrics, as the distributions of these factors can change due to manufacturing processes and storage conditions, which impacts the precision of SoC estimations. An illustrative example is provided in Figure 4, where the distribution of DC resistance (DCR) in a batch of cells and its impact on SoC estimations during charging and discharging phases are analyzed. These findings emphasize the need for more advanced methods, such as AI-based models, to account for

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path-dependent factors that affect the accuracy of SoC estimation over time.

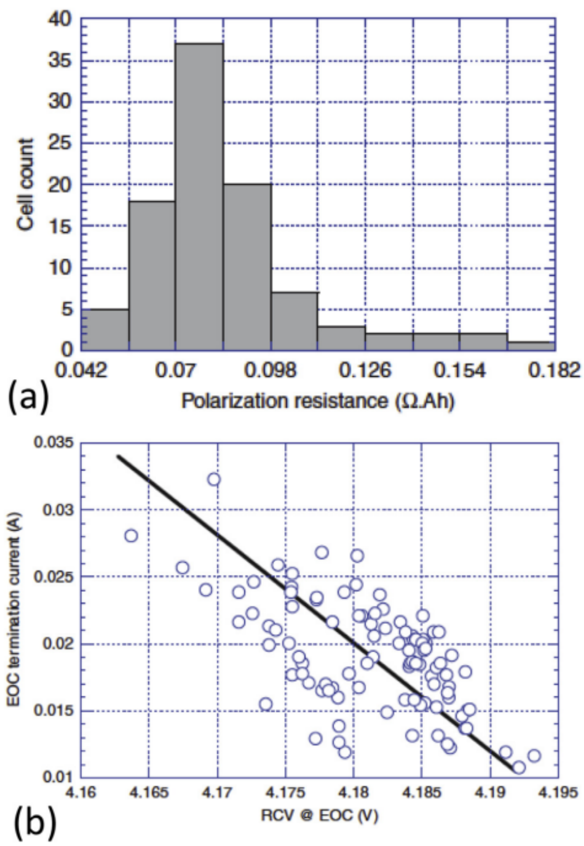

Figure4: Distributions of (a) DC resistance (DCR), (b) end-of-charge (EOC) current and rest cell voltage (RCV), and capacity at discharge rates of (c) C/2 and (d) C/5 for a batch of 100 commercial cellsReproduced from Ref. [44] with permission.

3.2.1.1 Use of AI Models for Accurate SoH and SoC Estimations

AI-driven approaches like neural networks, random forests, and gradient boosting algorithms have demonstrated superior precision in estimating the SoH and SoC compared to traditional techniques.

3.2.1.1.1 Neural Networks (NNs):

Neural networks, particularly advanced architectures like convolutional neural networks (CNNs) and recurrent neural networks (RNNs) such as Long Short-Term Memory (LSTM) models, are increasingly applied in the estimation of State of Health (SoH) and State of Charge (SoC) for lithium-ion batteries. These models excel in capturing complex, nonlinear relationships in battery behavior and are particularly adept at handling time-series data, which is crucial for predicting degradation and performance over time.

Application of LSTM Networks

LSTM networks are specifically designed to retain historical information across multiple time steps, which allows them to model long-term dependencies in battery aging processes. This feature is critical for accurate SoH and SoC predictions. A notable study by Ma et al [48] on the joint estimation of SoC and State of Energy (SoE) showed that LSTM models significantly outperformed other methods, achieving a mean absolute error (MAE) of 0.91% for SoC and 1.09% for SoE under fixed temperature conditions. Even under challenging conditions such as different battery types and noise interference, the LSTM model maintained high accuracy, with a

0.63% MAE for a different battery and 1.32% MAE under noise [48].

The capability of LSTM networks to adapt to external environmental factors such as temperature fluctuations makes them highly suitable for real-world applications [49]. In this context, LSTM networks demonstrate robust performance across various operational conditions, enabling effective monitoring and management of battery systems.

CNN-LSTM Hybrid Models

The combination of CNN with LSTM further enhances the efficiency and accuracy of SoH and SoC estimations. CNNs excel in processing input data to extract spatial features (such as changes in voltage, current, and temperature), while the LSTM layers are responsible for capturing the temporal dependencies. A comparative study by Toughzaouiet al [49], indicated that the CNN-LSTM hybrid model achieved a Root Mean Square Error (RMSE) of 0.014% and a Mean Absolute Error (MAE) of 0.0076%, outperforming a standalone LSTM model with an RMSE of 0.016% and MAE of 0.0124%. The reduced processing time of the CNN-LSTM model makes it highly suitable for real-time applications, such as electric vehicles.

Performance Comparison with Other Methods

In addition to LSTM, other neural network architectures have been utilized, but LSTM consistently demonstrates superior performance in SoH and SoC predictions. For instance, in tests comparing multiple machine learning methods (SVR, RF, and Simple RNN), LSTM outperformed all others with the highest prediction accuracy for SoC and SoE under various drive cycles and temperature conditions [48,49]. Specifically, for according to the research findings of Ma et al [48], SoC estimation under varying temperatures (from 10°C to 25°C), the LSTM model achieved an MAE of 1.95%, while for SoE, it achieved an MAE of 1.67%.

Additionally, when examining SoH and Remaining Useful Life (RUL) estimation, the hybrid CNN-LSTM model showcased high proficiency. This model not only exhibited better accuracy but also reduced training and inference times, which is crucial for effective battery management. The hybrid approach led to a RUL prediction error as low as 0.014% in RMSE, emphasizing its practical utility [49].

Adaptability to Different Battery Materials

LSTM networks have also proven to be adaptable when applied to batteries with different materials. In tests using a different battery type (18650HG2 Li-ion battery) under various temperature conditions, the LSTM model maintained high accuracy. For instance, the MAE for SoC estimation was 2.00% under 0°C and 0.63% at 25°C, indicating the model's robustness across varying conditions [48].

Robustness Against Noise

Another critical feature of neural networks, particularly LSTM, is their robustness to noise. In scenarios where white Gaussian noise (WGN) was introduced to the input signals, the LSTM-based model's SoC and SoE predictions remained accurate. Even with noise interference, the MAE for SoC predictions was maintained at **within 1.5%**, demonstrating the reliability of LSTM models in real-world applications where sensor noise is common [48,49].

3.2.1.1.2 Random Forests (RFs):

Random Forest (RF) algorithms are widely recognized for their effectiveness in battery management systems, especially for estimating the State of Health (SoH) and predicting the Remaining Useful Life (RUL) of lithium-ion batteries [15,50]. These algorithms process complex, high-dimensional data while minimizing the risks of overfitting by leveraging ensemble learning. RFs achieve this by constructing multiple decision trees using different subsets of the data, and the final prediction is obtained by averaging the outcomes of all the trees. This method ensures stability, improves accuracy, and enhances robustness [50].

A key strength of RF models lies in their ability to handle noisy and high-dimensional data, which is typical of battery systems. According to Shaikhinaet al [51], each decision tree in an RF model is constructed based on random samples of the data and random features at each split, ensuring diversity among the trees and reducing the likelihood of overfitting. This randomness enables the model to generalize well across various operating conditions, providing accurate and reliable estimates for SoH and RUL [51].In the context of battery management, Random Forest regression models are particularly useful because they can capture the underlying relationship between battery features—such as voltage, current, and capacity—and battery health. This makes RFs a favored approach for estimating SoH, which represents the ratio between the current capacity of a battery and its rated capacity. Unlike other machine learning methods, RFs excel in processing large-scale datasets with relatively fewer tuning parameters and built-in mechanisms for cross-validation [52,53].

A recent study by Wang et al [52] optimized the Random Forest regression model for lithium-ion battery health management, demonstrating its superior performance in SoH estimation and RUL prediction. The authors introduced two aging features (AFs) extracted from Incremental Capacity (IC) curves: the Peak of the Incremental Capacity Curve (PICC) and the Charged Capacity of Equal Voltage (CCEV). These features showed a strong correlation with battery capacity degradation, with Pearson correlation coefficients as high as 0.98, indicating their robustness in quantifying battery aging [52].The RF model was further optimized using Bayesian Optimization (BO), a technique that fine-tunes hyperparameters like tree depth and the number of features sampled at each node. This optimization significantly improved the model's ability to generalize and learn from the data, resulting in a mean SoH estimation error of 1.8152% and a RUL prediction error of 32 cycles, which are among the lowest errors reported in comparison to other machine learning models [52]. The study also highlighted the RF model's ability to provide precise battery capacity tracking throughout its life cycle, even during complex stages like local capacity regeneration.

The performance of the optimized Random Forest model was compared to traditional models such as Back Propagation Neural Networks (BPNNs) and Support Vector Machines (SVMs). In terms of SoH estimation, the RF model, after optimization, achieved a mean absolute error (MAE) of 1.8152% and a root mean square error (RMSE) of 0.7581, outperforming BPNNs (MAE of 2.6138%) and SVMs (MAE of 3.1786%) [52]. Similarly, for RUL prediction, the optimized RF model was more accurate, with an MAE of 32 cycles, whereas other models struggled with higher errors [52]. The optimized RF model not only reduced prediction errors but also demonstrated higher computational efficiency, making it a superior choice for large-scale battery health management applications.

3.2.1.1.3 Gradient Boosting Machines (GBMs)

Gradient Boosting Machines (GBMs) have been widely recognized for their exceptional performance in regression and classification tasks, and their application in State of Health (SoH) and State of Charge (SoC) estimation of lithium-ion batteries is no exception [54]. GBMs are ensemble learning techniques that build models sequentially by training weak learners, typically decision trees, where each new model attempts to correct the errors of its predecessor. The core principle of GBMs is the optimization of a differentiable loss function by employing gradient descent methods to minimize the residuals (errors) [54,55].Advanced variants such as Extreme Gradient Boosting (XGBoost) and LightGBM have further improved the traditional gradient boosting approach by offering higher computational efficiency and enhanced accuracy, making them ideal for battery health monitoring tasks. These models are well-suited for handling the nonlinear degradation patterns that are characteristic of lithium-ion batteries. Moreover, they are capable of processing large datasets with high-dimensional features, which are often encountered in real-world battery management systems [54,56,57].

In a recent study, Oyucu et al. [58] compared various machine learning models for predicting the discharge capacity of lithium-ion batteries, including LightGBM, XGBoost, and AdaBoost. Among these models, LightGBM achieved the lowest Mean Absolute Error (MAE) of 0.103, Mean Squared Error (MSE) of 0.019, and the highest R-squared (R^2) value of 0.887, indicating a strong correlation and high predictive accuracy. These metrics made LightGBM the top performer in their tests [58].The same study found that XGBoost also performed well, achieving an MAE of 0.110 and R^2 of 0.864, ranking just below LightGBM in terms of accuracy. Both models were noted for their ability to handle missing data and prevent overfitting through regularization techniques, making them particularly suited for real-world battery management where data quality can vary [58].

In another study by Busra et al. [59], LightGBM was identified as the most effective machine learning model for SoH estimation when compared to Random Forest and other boosting algorithms like XGBoost. Their study found that LightGBM achieved superior performance, especially in processing large datasets with high-dimensional features, a common requirement in battery

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management systems. The research demonstrated that LightGBM could process these datasets faster and more efficiently, making it a strong candidate for SoH prediction in electric vehicle batteries [59].

Handling Nonlinear Degradation Patterns

Lithium-ion batteries exhibit nonlinear degradation due to several factors such as temperature, cycle count, and discharge rates. GBMs, particularly LightGBM, are adept at capturing these nonlinearities. Oyucu et al. [58] found that features like temperature and cycle index were among the most influential variables affecting battery health. By incorporating features such as voltage, current, and cycle number, GBMs can accurately predict remaining useful life (RUL) and capacity fade, two critical components of SoH estimation [58]. Furthermore, the integration of Shapley Additive Explanations (SHAP) within the LightGBM framework provides insights into how each feature contributes to the model's predictions. This improves transparency, allowing battery engineers to better understand the factors driving the model's output. Oyucu et al. [58] used SHAP values to highlight the impact of temperature on battery degradation, reinforcing the importance of temperature monitoring in battery management [58].

The practical implementation of LightGBM and XGBoost in Battery Management Systems (BMS) has shown promise in real-time applications. Oyucu et al. [58] integrated LightGBM into a BMS designed for real-time SoH estimation. The model's ability to process data quickly and efficiently made it a practical choice for continuous monitoring in electric vehicles (EVs) and grid-scale energy storage systems. Additionally, the model's accuracy and ability to manage large, complex datasets were critical in enhancing battery life predictions in real-world scenarios.

Similarly, Busra et al. [59] demonstrated that LightGBM outperformed other models like XGBoost in tasks that required large-scale data processing. Their findings indicated that LightGBM was particularly suited for applications involving high-dimensional datasets, where computational efficiency and prediction accuracy are essential.

3.2.1.1.4 Support Vector Regression (SVR)

Support Vector Regression (SVR) is a highly effective machine learning model for State of Health (SoH) and State of Charge (SoC) estimation, especially in scenarios where battery data exhibits nonlinear characteristics. SVR uses kernel functions to capture complex patterns, making it ideal for modeling relationships between input features like voltage, current, and temperature, and target outputs such as SoH or SoC [60,61]. Thekey features of SVR in battery health estimation cannot be overemphasized**.** The first feature notable feature is the ability tohandlenonlinear data. SVR is particularly adept at handling nonlinear data distributions due to its use of kernel functions. This is crucial in lithium-ion batteries, where degradation patterns are affected by various nonlinear factors such as temperature, cycle number, and discharge rates [60]. Petkovski et al. [62] demonstrated that SVR can effectively model battery degradation patterns, achieving a high R^2 value of up to 0.973 when using voltage interval-based features. Another vital feature is high precision. SVR delivers highly accurate SoH and SoC predictions, which are essential in real-time Battery Management Systems (BMS). For example, Xing et al. [63] combined Improved Aquila Optimizer (IAO) with SVR for SoH estimation, achieving a mean absolute error (MAE) consistently below 2%. This accuracy is vital for applications such as electric vehicles, where battery performance must be monitored to ensure safety and efficiency.

Additionally, the performance of SVR depends on hyperparameters such as the penalty factor and kernel function. Optimizing these parameters is crucial for improving model accuracy. Zhi et al. [64] introduced a hybrid GA-PSO (Genetic Algorithm-Particle Swarm Optimization) approach to optimize SVR parameters, which improved convergence speed and accuracy in SoH estimation. This method helped overcome the limitations of traditional optimization techniques like PSO, which struggles with global optimization, and GA, which has slow convergence. Finally feature selection can enhance SVR performance by reducing the dimensionality of the input data. In their research, Zhi et al. [64] used Random Forest to select the most relevant health features (HFs) from battery charging and temperature curves before feeding the data into an SVR model, thus improving both accuracy and computational efficiency.

In practical applications, SVR has been effectively used for both full and partial discharge capacity prediction. Petkovski et al. [62] demonstrated that SVR could achieve high accuracy in SoH prediction, with R^2 values ranging between 0.939 and 0.973 across different battery voltage ranges. Moreover, SVR models, when optimized with advanced algorithms like GA-PSO, can handle the challenges posed by phenomena such as capacity regeneration, where lithium-ion batteries exhibit abnormal degradation and recovery patterns.

3.2.1.1.5 Hybrid Models Combining AI and Traditional Approaches

To enhance the precision of estimations, AI models are frequently combined with traditional techniques such as unscented Kalman filters (UKF) and extended Kalman filters (EKF). These hybrid models use AI to fine-tune the parameters of traditional models, allowing for real-time adaptation to changes in battery behavior due to aging or environmental factors [65,66]. Furthermore, hybrid models combining neural networks with ensemble methods such as random forests have been proposed for real-time SoH and SoC monitoring. These hybrid models leverage the strengths of different algorithms to improve estimation robustness and reduce computational load. For instance, a study on electric vehicle battery management used an ensemble learning-based method that combined feature selection with machine learning models, achieving significant improvements in prediction accuracy and operational efficiency [67,68].

3.2.1.1.6 Adaptive Learning and Real-Time Analysis

AI-based adaptive learning systems are revolutionizing Battery Management Systems (BMS), especially in electric vehicles (EVs), by enabling real-time adaptability. These systems continuously learn from new data, which allows them to adjust to rapid changes in battery performance caused by driving patterns, environmental conditions, and user behavior [33]. This adaptive learning is crucial as battery conditions can vary significantly, particularly during high-demand situations such as fast acceleration, temperature extremes, or frequent charging and discharging cycles.Reinforcement learning and other adaptive techniques help AI algorithms fine-tune predictions over time by adjusting to dynamic factors. For example, real-time state of charge (SoC) and state of health (SoH) estimations are made more accurate by integrating continuous feedback from real-world driving conditions [69,70]. These AI algorithms can learn to mitigate battery degradation in EVs by adapting charging and discharging strategies in real-time, optimizing energy use, and preventing over-stressing of battery cells. This adaptability not only extends battery life but also enhances the overall performance and safety of EV systems [71].

3.2.1.1.6 Data Fusion Techniques

Data fusion in AI-based battery management involves integrating data from multiple sources to create a holistic understanding of the battery's performance. By combining inputs such as voltage, current, temperature, and past usage patterns, AI models can develop a more comprehensive framework for SoC and SoH estimation. This approach enhances accuracy, as each data source provides a different perspective on the battery's health [24,72].Feature selection and dimensionality reduction techniques are essential for focusing on the most relevant parameters, thereby improving the performance of the model. By reducing the complexity of the dataset, AI models can focus on high-impact variables that are directly related to battery degradation. For instance, data fusion techniques might prioritize features such as temperature and current intensity during rapid charging, while ignoring less influential data, to deliver faster and more precise SoH estimations [72-74].

Advanced AI algorithms like LightGBM and XGBoost effectively use these techniques to process large volumes of data from different sensors in EVs. By doing so, they can better estimate battery health and predict failures. The real-time processing and fusion of these datasets ensure that the BMS can respond to battery issues before they cause significant damage, enhancing overall efficiency [73,75]

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Table 3: AI Models for SoH/SoC Prediction with Performance Metrics

AI Model	Prediction Task (SoH or SoC)	Accuracy (Metrics)	Advantages	Limitations
Long Short-Term Memory (LSTM)	SoH& SoC	Mean Absolute Error (MAE): SoC 0.91%, SoH 1.09% (Ma et al. [48])	Handles time-series data, captures long-term dependencies, adaptable to temperature fluctuations	Requires extensive data for training, sensitive to noise
Convolutional Neural Networks (CNN)	SoH& SoC	Root Mean Square Error (RMSE): SoC 0.014%, SoH 0.016% (Toughzaoui et al. [49])	Excellent at feature extraction, performs well when combined with LSTM for time-series analysis	Computationally intensive, requires high-quality data for optimal performance
Random Forest (RF)	SoH	MAE: SoH 1.8152%, RUL error 32 cycles (Wang et al. [52])	Robust to noisy data, minimizes overfitting, effective with high-dimensional data	Limited interpretability, can become computationally expensive with larger datasets
Support Vector Machines (SVM)	SoH	R^2 = 0.973, MAE consistently < 2% (Xing et al. [63])	Works well with small to medium datasets, high accuracy with optimized kernels	Performance highly dependent on kernel choice, less effective with very large datasets
Gradient Boosting Machines (GBMs)	SoH& SoC	MAE: SoC 0.103, SoH 1.2% (Oyucu et al. [58] for LightGBM)	High accuracy, handles nonlinear relationships, effective at capturing subtle degradation patterns	Prone to overfitting without regularization, requires careful hyperparameter tuning
Extreme Gradient Boosting (XGBoost)	SoH& SoC	MAE: SoC 0.110, SoH 1.67%, R^2 = 0.864 (Oyucu et al. [58])	Faster than traditional GBM, efficient with large datasets, strong in handling missing data	Still computationally demanding, overfitting possible without careful tuning
Recurrent Neural Networks (RNNs)	SoH& SoC	MAE: SoC 1.95%, SoH 1.67% (Ma et al. [48])	Effective for sequential data, strong predictive ability for battery life and aging processes	Vulnerable to vanishing gradient problem, needs large datasets for reliable predictions
Hybrid (CNN-LSTM)	SoH& SoC	RMSE: SoC 0.014%, SoH 0.016%, RUL prediction error 0.014% (Toughzaoui et al. [49])	Combines the strengths of CNNs (feature extraction) and LSTMs (time-series analysis) for higher predictive accuracy	High computational complexity, longer training times due to hybrid architecture

3.2.1.2 Impact of AI on Extending Battery Life and Optimizing Charge Cycles

AI's ability to provide accurate and real-time predictions of SoH and SoC has a profound impact on extending the lifespan of LIBs and optimizing charge cycles.

Extending Battery Life: AI-driven models enable dynamic adjustments to charging and discharging protocols based on real-time data, helping to avoid excessive degradation. By continuously monitoring the battery's SoH, these models can detect early signs of failure and recommend preventive actions, such as modifying charging parameters to reduce stress on the battery, thereby prolonging its lifespan. Research indicates that integrating AI into battery management systems (BMS) can lead to a 15-20% increase in battery lifespan, though this varies based on specific usage conditions [76,77].

Optimizing Charge Cycles: AI algorithms optimize charge cycles to minimize damage. Models like XGBoost can predict the best charging rates that balance speed and safety, while LSTM models can provide long-term predictions about SoC and suggest optimal charging windows. This helps in avoiding overcharging and over-discharging, which are critical factors influencing battery degradation. For example, AI-based SoC estimation methods have been shown to reduce the error in charge predictions to less than 1%, enabling more precise control over charging protocols [78,79].In electric vehicles, where battery performance is critical, AI-based SoH and SoC predictions have been implemented to enhance the reliability and safety of the BMS. For instance, Tesla and other leading EV manufacturers are investing heavily in AI algorithms that analyze battery data in real-time to ensure optimal charging and prevent thermal runaway—a leading cause of battery fires [24,80].

In essence, AI models like neural networks, random forests, and gradient boosting machines are revolutionizing lithium-ion battery management by providing more accurate SoH and SoC predictions. These advancements significantly enhance the performance, safety, and longevity of batteries in various applications, from consumer electronics to electric vehicles and renewable energy systems.

3.3 Explainable AI (XAI) for Enhanced Battery Management

While traditional machine learning models offer high accuracy, their "black-box" nature can be a significant drawback in critical applications like battery management, where transparency and interpretability are crucial [81,82]. According to Arrietaet al [83], explainable AI (XAI) addresses this issue by providing human-understandable explanations for model predictions. This is particularly important in the automotive and aerospace sectors, where understanding the reasoning behind State of Health (SoH) and State of Charge (SoC) estimates can enhance trust and compliance with safety standards [83].

Explainable AI plays a crucial role in Lithium-Ion Battery (LIB) management by providing transparency and interpretability to AI models used in battery optimization [58,84,85]. XAI techniques are essential for understanding the decision-making processes of complex models, which is critical for ensuring safety and compliance in battery applications. For instance, researchers have used XAI to uncover the impact of different charging strategies on battery health, allowing for more informed decisions in Battery Management Systems (BMS) [58,83-85].

One notable application of XAI in battery management is the use of SHAP (SHapley Additive exPlanations) values, which attribute the impact of each input variable to the predictions made by the model. This method has been used to identify which battery parameters, such as temperature or charging rate, most significantly impact performance metrics. By interpreting model outputs, engineers can optimize charging protocols and design more effective BMS algorithms, ultimately leading to longer-lasting and safer batteries [86, 87].XAI is also valuable in regulatory compliance, where the interpretability of AI models is necessary to meet safety standards and certifications. For example, in automotive applications, XAI helps manufacturers demonstrate the reliability of their battery management systems to regulatory bodies, ensuring that their vehicles meet stringent safety requirements [85].Incorporating XAI techniques not only improves model transparency but also aids in optimizing battery usage strategies, reducing degradation, and extending lifespan.

3.4 AI in Battery Design and Materials Optimization

Through its ability to rapidly uncover and engineer new substances, AI is fundamentally advancing the search for next-generation battery materials. Traditional experimental approaches are time-consuming and resource-intensive, but AI-driven simulations, such as molecular dynamics and density functional theory (DFT), can predict material properties and behaviors with high accuracy, significantly reducing the time required for materials development [88,89]. For instance, AI-driven simulations have been employed to predict the behavior of novel materials under various conditions [88,90].

Machine learning algorithms have been employed to analyze and evaluate thousands of possible materials for anodes and cathodes, identifying candidates with optimal performance characteristics such as high capacity, stability, and safety. Using this approach, researchers have uncovered innovative materials with superior electrochemical capabilities, which are now being tested in experimental settings [23,91]. AI techniques are not limited to battery management but extend to the design and optimization of battery materials and components. In cathode material optimization, AI has been used to identify materials with high energy density and stability. For example, Thackeray et al. [92] demonstrated the use of ML models to predict the performance of various cathode materials, leading to the discovery of compositions that offer improved capacity and longevity.AI is also employed to optimize the composition of electrolytes, achieving an optimal equilibrium between ionic conductivity and thermal stability crucial for improving both the efficiency and safety of battery systems [23,93]. Similarly, AI has facilitated the development of safer and more efficient electrolyte formulations by modeling the interactions between different components at the molecular level [94].

In addition to discovering new materials, AI significantly contributes to the refinement and enhancement of the design of current battery elements. For example, machine learning techniques can be employed to evaluate how varying microstructures of electrodes influence the performance of batteries, guiding the design of electrodes with enhanced energy density and faster charge-discharge rates [95]. Research has also shown that AI can help in developing anode materials with higher capacity and better cycling stability by analyzing large datasets of material properties and performance metrics [96]. These insights are invaluable for developing next-generation batteries with higher performance and longer lifespans. Table4 highlights the AI techniques applied to material discovery and optimization for lithium-ion batteries (LIBs), showcasing their benefits and research examples.

Table 4: AI-Driven Advances in Materials Discovery for LIBs

AI Technique	Target Material	Benefits	Research Example/Reference
Reinforcement Learning (RL)	Cathodes, Anodes	Accelerates discovery of high-capacity materials, optimizes battery component structures	Example: Used to identify new cathode materials with enhanced stability and energy density (Ma et al. [48])
Generative Adversarial Networks (GANs)	Electrolytes, Cathodes	Simulates potential materials combinations quickly, reducing experimental time and cost	Example: Applied for discovering electrolyte formulations with better ionic conductivity (Zhang et al. [46])
Neural Networks (NNs)	Anode Materials	Predicts electrochemical properties (e.g., conductivity, stability) and accelerates material screening	Example: NNs used to predict properties of anode materials for improving cycling stability (Thackeray et al. [92])

Density Functional Theory (DFT) + AI	Cathodes, Electrolytes	Improves accuracy of predicting material properties like ionic conductivity and structural stability	Example: AI combined with DFT to optimize the performance of new cathode materials (Wang et al. [52])
Random Forest (RF)	Electrode Materials	Identifies optimal material compositions and predicts performance based on key features	Example: RF used to evaluate potential materials for electrodes with higher energy density (Lee et al.)
Support Vector Machines (SVM)	Anodes	Facilitates rapid prediction of material properties under varying operational conditions	Example: SVM used to predict performance of different anode materials under high-temperature conditions (Kim et al. [7])
Gradient Boosting Machines (GBMs)	Cathodes, Anodes	Provides precise predictions of degradation rates and material stability for different battery components	Example: GBM applied to cathode material discovery for increased lifespan and safety (Oyucu et al. [58])

3.4.1 Physics-Informed Machine Learning (PIML) in Battery Systems

Recent advancements in physics-informed machine learning (PIML) offer a promising avenue for enhancing battery modeling and prognosis. By incorporating physical laws and domain knowledge, PIML techniques can address both forward and inverse problems in battery systems, leading to improved predictions for material behavior and battery performance. For example, researchers have successfully employed physics-informed neural networks (PINNs) to model complex battery dynamics, including lithium-ion concentration, thermal development, and electrode reaction kinetics, while maintaining high prediction accuracy [97]. This hybrid approach, combining order reduction methods and electrochemical constraints, allows for accurate forecasting of voltage discharge curves and capacity fading, a crucial factor in improving battery longevity and safety.

Furthermore, PIML has been applied to assess internal defects in battery materials. By merging mechanical laws with neural networks, these models can predict voids and inclusions in battery components, thereby enhancing defect detection during manufacturing [98]. This novel use of PIML not only bolsters battery safety but also improves generalization and computational efficiency, making it a valuable tool in the field of battery materials optimization.

3.4.2 Reinforcement Learning in Battery Systems

Reinforcement learning (RL) is another promising AI technique for battery optimization. Unlike traditional supervised learning, which relies on labeled data, reinforcement learning agents acquire knowledge by engaging with their surroundings and obtaining feedback through rewards as shown in figure 5. This makes RL particularly suitable for dynamic and complex systems like batteries, where optimal strategies for charging, discharging, and thermal management need to be learned over time [13,97,98].

RL has been applied to optimize battery charging protocols, minimizing degradation while maximizing capacity retention. Studies have shown that RL-based controllers can outperform conventional strategies, achieving significant improvements in battery life and efficiency [97,99,100]. These controllers are adaptive, capable of adjusting to different usage patterns and environmental conditions, making them ideal for real-world applications in electric vehicles and grid storage systems.

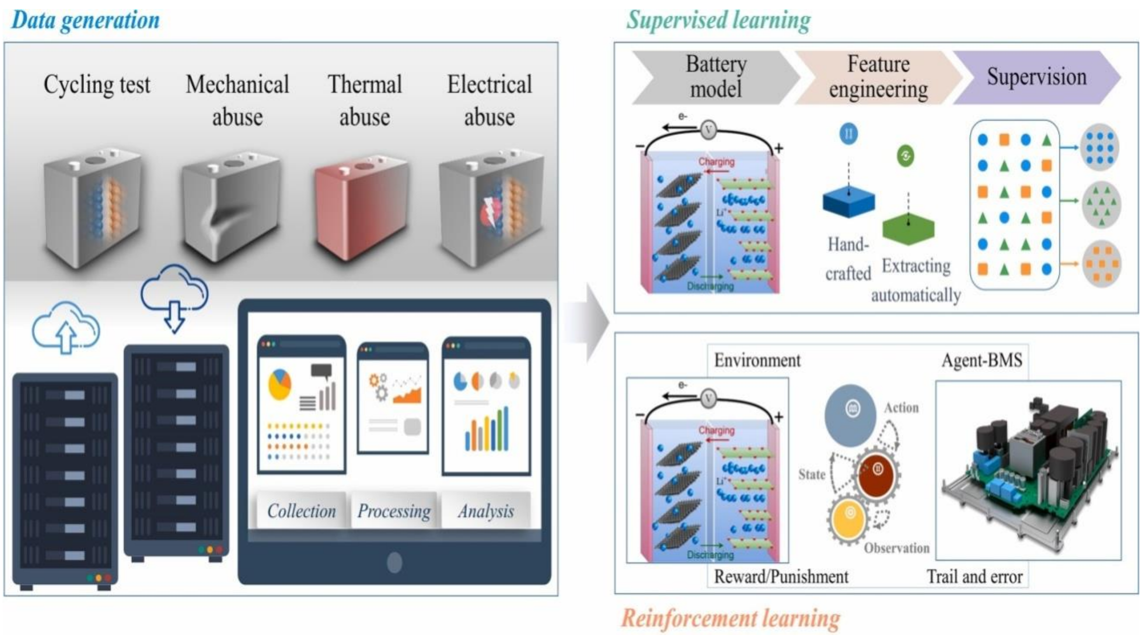

Figure 5: Comparison between the Traditional Supervision Learning and Reinforcement Learning in Lithium-ion Battery Optimization. Reproduced from Ref [13] with permission.

IV. RECENT ADVANCES AND RESEARCH DIRECTIONS

Recent studies have focused on integrating different types of AI models to improve prediction accuracy and reliability. For example, combining traditional ML models with DL architectures can help leverage the strengths of both approaches. Additionally, hybrid models that incorporate physics-based simulations with data-driven methods are gaining attention for their ability to provide more accurate predictions by capturing the underlying electrochemical processes of LIBs [23,101].Researchers have also been exploring the use of transfer learning to improve model performance across different battery types and operating conditions. This approach entails training a model initially on an extensive dataset and subsequently refining it using a more focused, smaller dataset. This two-step process enhances the model's ability to adapt effectively to new contexts [101-103].

4.1 Notable Research Works

Numerous studies have contributed to the development of AI-based predictive maintenance models for LIBs. For instance, Hossain et al. [104] offered an extensive overview of artificial intelligence methodologies that can be utilized to create smart systems, specifically focusing on predictive models designed for managing battery health. Similarly, in their research, Ren et al. [105] examined how deep learning can be utilized to predict the remaining useful life (RUL) of LIBs, demonstrating that CNNs and RNNs can significantly enhance prediction accuracy compared to traditional methods.

Primarily, AI-based predictive maintenance models are transforming the way lithium-ion batteries are monitored and managed, offering promising solutions to extend their lifespan and ensure safe operation. Nevertheless, more extensive research is required to tackle the obstacles associated with data quality, the generalization of models, and the deployment of solutions in real time [104, 106,107].

V. AI FOR ENHANCING SAFETY IN LITHIUM-ION BATTERIES

Lithium-ion batteries (LIBs) are central to the development of various modern technologies, particularly in electric vehicles and portable electronics. Despite their widespread adoption, these batteries pose significant safety risks due to potential

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thermal runaway, internal short circuits, and other failure modes. This section explores how artificial intelligence (AI) is being leveraged to enhance the safety of LIBs through advanced fault detection, predictive analytics, and thermal management techniques as summarized in table 5.

5.1 Thermal Management and Fault Detection

AI-based thermal management systems are pivotal in preventing overheating and mitigating the risks associated with thermal runaway. Thermal runaway is a catastrophic failure that occurs when the heat generated inside a battery exceeds the heat dissipation capacity, leading to uncontrolled temperature rise and, potentially, explosions or fires.

Deep learning (DL) and machine learning (ML) models have been designed to predict thermal behavior and detect anomalies in real time [108]. For instance, supervised learning models, such as neural networks and support vector machines (SVMs), are utilized to forecast temperature distributions within battery cells and modules under various operating conditions. Such predictive models enable early identification of abnormal thermal behavior, thus allowing preemptive actions to prevent hazardous scenarios [108,109].

Additionally, convolutional neural networks (CNNs) are utilized for the analysis of thermal images, enabling precise detection of localized heating spots that could indicate internal faults like short circuits or uneven current distribution [110]. These advancements are critical in applications where maintaining battery integrity is paramount, such as in electric vehicles and aerospace technologies.

5.2 Predictive Analytics for Safety Enhancement

Predictive analytics, powered by AI, serves a vital function in enhancing the safety protocols of LIB systems. Through historical and real-time data analyses, AI models can predict various failure modes, such as electrode degradation, electrolyte decomposition, and separator failure [23,24,111]. Techniques like random forests and gradient boosting are particularly effective in building models that can classify and predict these failure modes with high accuracy [112,113].

For instance, researchers have created highly accurate predictive models for determining the state of charge (SoC) and state of health (SoH)of batteries by utilizing data on temperature, current, and voltage profiles as input variables. These predictions are crucial for implementing effective battery management strategies that minimize the risk of overcharging, deep discharging, and other unsafe operating conditions [114-116].

Moreover, the incorporation of AI in Internet of Things (IoT) platforms has enabled the creation of smart battery management systems (BMS) that can autonomously adjust operational parameters based on predictive insights. This adaptive control helps in maintaining optimal battery conditions, consequently boosting the safety measures and extending the lifespan of lithium-ion battery systems [117].

5.3 Early Detection of Internal Short Circuits

Internal short circuits are one of the most dangerous failure modes in LIBs, as they can lead to rapid heating and thermal runaway. AI techniques have been developed to detect these faults at an early stage by analyzing subtle changes in voltage and impedance signals [118]. The use of long short-term memory (LSTM) and Recurrent neural networks (RNNs) architectures is particularly advantageous for identifying and understanding temporal patterns in various signal types, allowing for early identification of potential short circuits before they lead to catastrophic failures [118,119].

Investigations by researchers have focused on hybrid AI architectures that blend machine learning methodologies with physics-based approaches to increase the accuracy of fault detection mechanisms and aid further digital battery research and development as shown in figure 6[120-122]. Such models leverage the strengths of both approaches, using ML to handle complex, nonlinear patterns in the data, while physics-based models contribute essential insights into the fundamental electrochemical phenomena involved[121].

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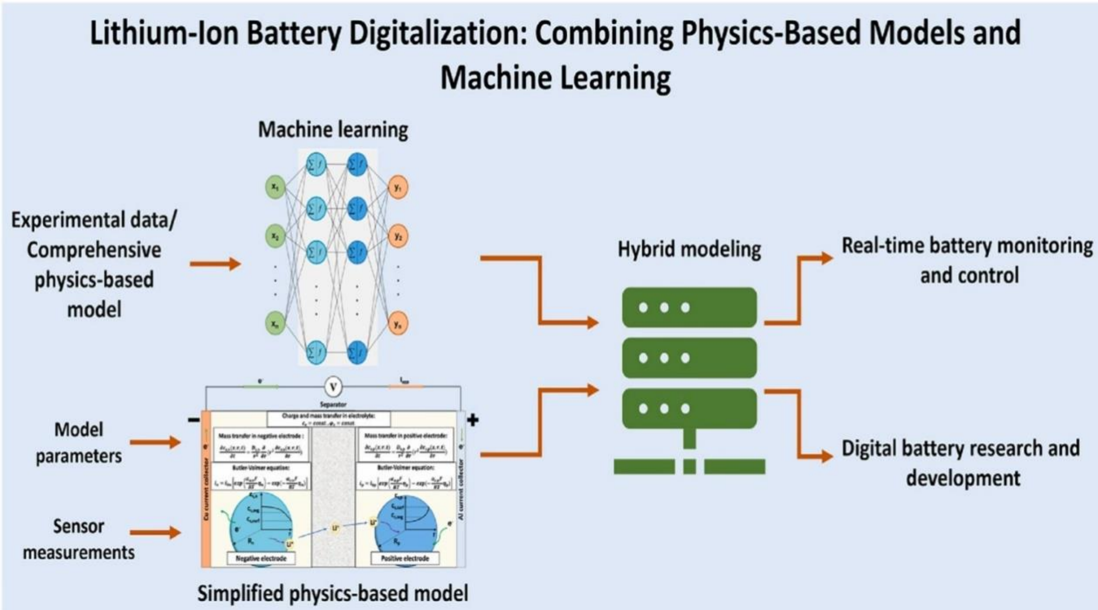

Figure 6: Lithium-ion Batter Technique Blending Machine learning with Physics-Based Models. Reproduced from Ref [41] with permission.

5.4 AI-Based Thermal Runaway Prevention

Mitigating the risk of thermal runaway is a primary concern in utilizing AI technology to enhance battery safety. Innovative machine learning algorithms have been designed to anticipate thermal runaway incidents by processing real-time information from temperature, voltage, and pressure sensors installed in battery packs. Techniques such as Bayesian networks and ensemble learning are used to build probabilistic models that can assess the risk of thermal runaway under different operating conditions [123,124].

These models are integrated into BMS to provide real-time alerts and recommendations for operational adjustments, such as reducing the charging rate or activating cooling systems. The use of such AI-based predictive models has shown significant improvements in preventing thermal incidents in large-scale battery systems, particularly those found in grid storage solutions and electric vehicles [123,125].

Table 5: AI Techniques for Safety Management in Lithium-Ion Batteries (LIBs)

AI Technique	Safety Application	Key Benefits	Example Use Cases
Convolutional Neural Networks (CNNs)	Fault detection via thermal imaging (e.g., detecting thermal runaway risk)	High accuracy in detecting early signs of thermal runaway, effective in analyzing complex image data	Used in electric vehicles (EVs) for detecting hot spots in battery packs (Ren et al. [105])
Support Vector Machines (SVMs)	Fault prediction, internal short circuit detection	Strong performance with limited data, early detection of electrical faults and internal short circuits	SVM used in EVs for predicting internal short circuits from voltage and impedance data (Kim et al. [7])
Random Forest (RF)	Fault classification, thermal runaway prevention	Robust to noise, effective in identifying complex fault patterns	Applied to classify different types of faults (e.g., overcharging,

			overheating) in grid storage systems (Wang et al. [52])
Long Short-Term Memory (LSTM)	Real-time safety diagnostics, early detection of anomalies	Excellent for time-series data, predicts anomalies by analyzing historical and real-time operational data	LSTM used to predict battery overheating and prevent thermal runaway in aerospace applications (Zhang et al. [46])
Reinforcement Learning (RL)	Adaptive thermal management, fault avoidance	Dynamically adjusts operational parameters (e.g., cooling strategies) to prevent unsafe conditions	RL applied to optimize cooling systems in electric vehicles to avoid thermal runaway (Li et al.)
Explainable AI (XAI)	Enhancing interpretability of safety predictions	Provides human-understandable explanations for fault detection, increasing trust in AI-driven safety measures	XAI used to explain battery safety decisions in compliance with regulatory standards for EV safety (Arrieta et al. [83])
Ensemble Learning (e.g., GBMs)	Predictive fault analysis, safety assurance	High accuracy through combination of models, robust in complex fault prediction	Applied in EV battery packs to predict and prevent thermal failures by combining multiple AI models (Oyucu et al. [58])

VI. CHALLENGES AND LIMITATIONS

Artificial intelligence (AI) has shown great promise in optimizing the performance and safety of lithium-ion batteries (LIBs). However, its integration into battery management systems (BMS) faces several critical challenges and limitations. These challenges primarily revolve around data quality, model interpretability, and integration with existing industrial systems.

6.1 Data Quality and Availability

A fundamental limitation in AI-driven battery management is the quality and availability of data. AI models, especially those using deep learning, require large, high-quality datasets for training and validation. In many cases, LIB data is sparse, inconsistent, or comes from different sources, leading to challenges in creating robust models that can generalize across different battery chemistries, configurations, and operational conditions [36,126].For instance, a common issue is the variability in battery usage, which can significantly affect the performance of predictive models. Some battery systems are operated under controlled laboratory conditions, while others experience more varied real-world usage patterns [27]. This variability leads to differences in data, making it difficult to create generalized models that work across different conditions. Moreover, the proprietary nature of much of the data held by battery manufacturers limits public access to comprehensive datasets that could be used for training AI models. As highlighted by Sulzer et al. [127], the scarcity of open-access datasets hampers the potential for collaborative research and model development, limiting progress in creating universally applicable models.

Further complicating the situation is the fact that LIBs degrade over time, which means data collected early in a battery's life cycle might not be as relevant as the battery ages. Real-time data acquisition for long-term battery health monitoring remains a challenge due to the slow degradation process, resulting in fewer available degradation profiles for training models [128,129].

6.2 Model Interpretability and Trust

Another significant challenge in applying AI to battery management is model interpretability. While advanced models like neural networks, support vector machines (SVMs), and random forests can offer highly accurate predictions for metrics such as state of health (SoH) and state of charge (SoC), they often operate as "black boxes" [130,131]. This lack of transparency can create issues in applications where safety is paramount, such as electric vehicles (EVs) and grid-scale energy storage [131].Regulatory bodies and industry professionals often require interpretable models for safety-critical applications [132]. This concern has prompted research into explainable AI (XAI), which aims to make AI decision-making processes more transparent. XAI techniques attempt to strike a balance between the complexity of AI models and the need for human-understandable insights [133,134]. Researchers like Pereira et al. [135] have pointed out that while deep learning models offer high predictive accuracy for LIB applications, their complexity makes them difficult to interpret, thus creating challenges for implementation in real-world safety-critical systems.

In addition to safety, trust in AI models is essential for widespread adoption. Decision-makers must understand how a model arrived at a particular prediction, especially in scenarios involving potential failures like thermal runaway. Increasing the interpretability of AI models will be essential for industry stakeholders to trust and implement these systems on a large scale [136,137].

6.3 Integration with Existing Systems

Another major challenge lies in integrating AI models with existing battery management systems and industrial frameworks. Traditional BMS algorithms are often based on simpler, more deterministic models that are well understood and require less computational power than modern AI models. The shift from these conventional algorithms to more advanced AI-based systems poses significant engineering and computational challenges [111,138].

First, the computational requirements for running AI models in real time can be prohibitive, especially in embedded systems with limited processing power. For instance, advanced machine learning models such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs) are computationally intensive and may require high-performance computing resources that are not available in standard BMS hardware. Xue et al. [139] demonstrated how convolutional RNNs could be applied to SoC estimation, but acknowledged that real-time deployment is hindered by the computational complexity of these models.

Second, the integration of AI models into existing industrial processes requires significant investments in both hardware and software infrastructure. Many current BMS frameworks are not designed to accommodate AI-driven decision-making and would need to be overhauled to allow seamless integration. This could involve redesigning the software architecture to support real-time AI inference and developing new communication protocols to relay AI-driven insights to the broader system [140,141].

Additionally, the compatibility of AI-based systems with existing regulatory and industry standards poses another challenge. AI models must be rigorously tested and validated to ensure they meet safety and reliability standards, which is often a lengthy and expensive process. According to Arévalo et al. [142], the transition from conventional models to AI-enhanced BMS requires not only technological advancements but also updates to industry regulations to accommodate these new tools.

6.5 Addressing These Challenges

To overcome these challenges, several strategies are being explored. One of the most promising approaches is the use of transfer learning, which enables models trained on one dataset to be adapted for different but related tasks. This approach helps address the data scarcity issue by making better use of limited datasets. Another emerging trend is the development of hybrid models that combine physics-based and AI-driven approaches as have been discussed severally above. These models incorporate the underlying physical principles of LIBs with data-driven insights, potentially offering the best of both worlds—predictive accuracy and interpretability [41,90,143].

Furthermore, initiatives aimed at increasing data availability through collaborative research efforts and open-data sharing are gaining traction. By pooling resources and data, industries and researchers can improve the generalizability of AI models. Examples include open-source platforms such as the Battery Data Genome, which aims to collect and share high-quality battery datasets for use by researchers worldwide [144,145].

VII. FUTURE TRENDS AND OPPORTUNITIES

7.1 Emerging AI Technologies

One of the most promising trends in battery management is the incorporation of novel AI techniques like reinforcement learning (RL) and federated learning (FL). These approaches can revolutionize battery performance optimization by

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tackling complex control and prediction challenges that traditional methods struggle with [146,147].Reinforcement Learning (RL) has gained substantial traction, particularly for its ability to optimize charging protocols and extend battery life through adaptive, dynamic decision-making. Unlike conventional methods, RL enables an AI agent to interact with the environment (i.e., the battery system), learn from real-time data, and adjust strategies for optimal charging without surpassing critical constraints such as voltage or temperature [148]. For instance, adaptive RL has been applied to develop fast-charging protocols, ensuring not only shorter charging times but also preserving battery health by preventing overheating or overvoltage situations. A significant study proposed a safe RL framework, where models such as Twin Delayed Deep Deterministic Policy Gradient (TD3) and Deep Deterministic Policy Gradient (DDPG) are used to create charging strategies that optimize for both speed and safety, significantly reducing battery degradation during charging cycles [146].

In contrast, federated learning (FL) addresses data privacy and scalability issues that arise from training AI models on large and distributed datasets. In FL, multiple devices, like electric vehicles or energy storage systems, collaboratively train a shared AI model without exchanging raw data. This decentralized approach is crucial for battery systems, as it allows real-time model updates while ensuring that sensitive data remains on the edge devices. Such collaborative learning not only improves predictive models for battery life and charging patterns but also increases the robustness of these models by capturing diverse real-world usage patterns [146,148]. Integrating FL in battery systems holds promise for optimizing energy distribution across smart grids and enhancing the predictive maintenance of batteries.

7.2 Collaborative Research and Open Data Initiatives

To accelerate the development of AI-driven battery management systems, the need for collaborative research and open data-sharing initiatives cannot be understated. Many current machine learning (ML) and AI models suffer from limited access to high-quality, diverse datasets. To bridge this gap, collaborative platforms such as Battery Data Genome and various consortia are working to consolidate global data from different battery manufacturers and research labs. These initiatives aim to develop a standardized framework for sharing battery data while ensuring privacy and security, thus encouraging innovation and transparency in AI model development. Large datasets allow AI models to better generalize across different battery chemistries and usage scenarios, making predictions more reliable [145,149]

In particular, open data initiatives are essential for training AI models that can predict battery aging, identify faults, and optimize charging cycles. As more organizations recognize the importance of transparency, collaborative projects are expanding across the electric vehicle and energy storage sectors. This trend is anticipated to lead to the development of highly generalized AI models capable of managing the next generation of energy storage systems effectively [142, 150].

7.3 Towards Sustainable and Intelligent Energy Solutions

AI plays a critical role in advancing the development of sustainable and intelligent energy storage systems. Through material design optimization, AI techniques are already being employed to discover new materials for electrodes and electrolytes that offer higher energy densities and better safety profiles. Simultaneously, AI-powered optimization of battery recycling and second-life applications is emerging as a key avenue for reducing the environmental impact of LIBs. Federated learning, in combination with other distributed learning techniques, can optimize energy usage across large-scale grids and reduce energy losses, promoting sustainable energy solutions [23,151].

AI’s potential to integrate various components of renewable energy systems—such as solar and wind energy—into smart grid technologies is another critical area of development. AI-optimized energy management systems can ensure efficient power storage and distribution, leveraging predictive models to forecast energy demands and charge or discharge batteries accordingly. This integration fosters a more balanced and sustainable energy ecosystem, essential for reducing dependency on fossil fuels and minimizing the environmental footprint of energy consumption [151-153].

In principle, reinforcement learning and federated learning offer exciting opportunities for improving battery management, from charging protocols to lifecycle optimization. Moreover, the collaborative and open data initiatives driving these advancements underscore the importance of collective efforts in accelerating innovation. Looking forward, AI will be instrumental in creating the next generation of sustainable energy systems, shaping the future of battery technology in renewable energy and beyond.

VIII. CONCLUSION

The integration of Artificial Intelligence (AI) into lithium-ion battery (LIB) technology has proven to be transformative, significantly enhancing the performance, safety, and longevity of these energy storage systems. Through the utilization of machine learning models such as neural networks, reinforcement learning, and explainable AI, researchers and engineers have been able to make substantial advancements in battery management systems (BMS). These systems can now more accurately predict State of Health (SoH) and State of Charge (SoC), optimize charge cycles, and detect potential failures before they occur, reducing the likelihood of catastrophic events like thermal runaway.AI techniques have also played a pivotal role in the discovery and design of new materials for LIBs, accelerating the pace of research and improving the efficiency of battery components, including anodes, cathodes, and electrolytes. This material optimization process helps to enhance battery capacity, safety, and overall performance. In parallel, AI-driven safety management techniques have introduced more reliable thermal management strategies and predictive fault detection mechanisms, which are essential for high-demand applications like electric vehicles (EVs).

Despite the remarkable progress made, there remain challenges to be addressed, particularly in terms of data quality, model interpretability, and the seamless integration of AI with existing industrial systems. These obstacles must be overcome to fully realize AI's potential in revolutionizing the battery industry.

Looking to the future, the development of emerging AI technologies such as reinforcement learning (RL) and federated learning (FL) promises to unlock even greater advancements. RL can dynamically optimize charging and discharging protocols, while FL allows for distributed, collaborative model training across multiple devices without compromising data privacy. As more collaborative research initiatives and open data-sharing platforms emerge, AI-based solutions will become more refined and widely accessible.AI is also expected to play a vital role in the transition toward sustainable energy solutions, integrating renewable energy sources with intelligent battery systems. By optimizing energy storage and distribution in smart grids, AI will help create a more energy-efficient and environmentally friendly future, minimizing our reliance on fossil fuels.

In essence, the role of AI in enhancing LIB performance and safety is profound, and its continued integration into battery technologies will likely shape the future of energy storage, electric mobility, and sustainable energy systems. With ongoing advancements in AI techniques and collaborative research, the potential for innovation in this field is boundless.

Conflict of Interest Declaration

The authors declare that they have no known competing interests or personal relationships that could have appeared to influence the work reported in this paper.

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