

Review

Ensuring Safety and Reliability: An Overview of Lithium-Ion Battery Service Assessment

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Abstract: Lithium-ion batteries (LIBs) are fundamental to modern technology, powering everything from portable electronics to electric vehicles and large-scale energy storage systems. As their use expands across various industries, ensuring the reliability and safety of these batteries becomes paramount. This review explores the multifaceted aspects of LIB reliability, highlighting recent advancements and ongoing challenges. The importance of safety has been underscored by numerous incidents, such as the well-known smartphone battery explosions and more than 10,000 fires a year at facilities throughout Australia, both linked to LIB failures. These events emphasize the need for robust reliability and safety measures to ensure consistent performance and longevity. Factors like battery chemistry, design, manufacturing, and operating conditions can all influence the reliability of LIBs. Despite their widespread use, the mechanisms of failure, failure rates, and consequences of LIB failures are still not well understood, raising significant safety concerns. Current reliability assessment techniques include experimental methods, computational models, and data-driven approaches. Emerging trends, such as advanced characterization techniques and standardized testing protocols, advocate for improved practices to enhance the reliability and safety of LIBs across all applications.



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1. Introduction

Lithium-ion batteries (LIBs) have emerged as a key technology in the modern era, revolutionizing the way we store and use energy. Introduced commercially in the early 1990s, LIBs have rapidly become the preferred choice for a wide range of applications, from portable electronics such as smartphones, laptops, smart wearables, and power tools to electric vehicles (EVs), e-mobility devices (e-bikes, e-scooters), and large-scale energy storage systems (ESSs) for renewable energy integration. The widespread adoption of LIBs can be attributed to their high energy density, long cycle life, and relatively low self-discharge rates compared to other battery types [1]. While LIBs may dominate the energy storage landscape today, it was only in 1818 when the discovery and isolation of Li occurred, which marked the starting event that sparked the interest in its potential use for energy storage [2]. The history of LIBs comprises many important milestones, and come after the era of lead-acid, Ni-Cd ore Ni-MH batteries [3].

The importance of LIBs extends beyond their technical merits. In the context of global efforts to mitigate climate change and reduce dependence on fossil fuels, LIBs enable the

transition to cleaner energy systems. Electric vehicles powered by LIBs are at the forefront of reducing greenhouse gas emissions from the transportation sector. Simultaneously, energy storage systems using LIBs play a crucial role in stabilizing power grids and facilitating the integration of intermittent renewable energy sources like solar and wind power. Batteries can be classified based on their electrochemical processes, including flexible alkaline batteries, plastic or all-polymer batteries, polymer lithium-metal batteries with lithium foil anodes, and flexible rechargeable LIBs, among others. Flexible LIBs, in particular, are garnering growing interest, although they present greater manufacturing challenges compared to traditional rechargeable LIBs [4].

A key obstacle remained for the precipitation of Li on the anode in the form of dendrites that impact ion transport and interface, which could eventually cause a short-circuit [5]. Being an alkaline metal, Li has a high reactivity, and potential side-reactions add up to the thermal runaway problem of LIBs [3]. The current state of LIBs was actually introduced in 1985, with LiCoO_2 as the positive electrode and carbonaceous materials as the negative electrode [3]. After more than three decades, some reflections can be made on the maturity of lithium-ion technology [6]. With a gravimetric capacity and volumetric capacity surpassing that of other metals, lithium has the potential to be the best negative electrode (anode) [2]. The current state-of-the art of LIBs has been reviewed recently [7], and their pivotal role in EV applications has been acknowledged [8], along with key integration issues into EV market [9]. The quickly emerging and evolving EV market comprises batteries and fuel cells as primary energy sources [10,11]; however, the use of rechargeable LIBs does pose some key issues [12] related to the rechargeable process [13,14]. The body of knowledge built throughout the years facilitates a better understanding of LIBs and could consequently guide the engineers into building better batteries [15], ensuring a safer future where the main shortcomings of lithium-ion technology are addressed [16]. Overall, due to its high global consumption and upcoming conversion from traditional fuel to battery-powered vehicles and general electric transportation, some doubts were raised regarding the Earth's availability of lithium ores; however, the reserves are indeed sufficient, as Li_2CO_3 can be found in great amounts in South America or even countries like Afghanistan, or in sea water, although in lower amounts compared to sodium. Regardless, Li ranks the 27th most abundant metal on Earth, amounting to roughly 0.0065% of the Earth's crust; this order of magnitude can provide enough lithium for the foreseeable future where energy needs are covered by LIBs [16,17]. Other avenues have been explored recently in the pursuit for high energy storage devices, and Li-O_2 and Li-S battery design and development have gained momentum [18]. Flexible LIBs also face issues and challenges preventing widespread usage for practical applications [4].

As the reliance on LIBs grows, so does the necessity to ensure their reliable operation. Reliability, in the context of LIBs, refers to the ability of the battery to perform its intended function under specified conditions for a defined period without failure. Ensuring the reliability of LIBs is crucial for several reasons like safety [19], economic viability, performance consistency, and consumer confidence and satisfaction. Unreliable batteries pose significant safety risks, including the potential for thermal runaway, fires, and explosions. High-profile incidents involving battery failures have underscored the critical need for robust reliability assessments [20–22] and the proper evaluation of components of LIBs for commercial distribution [23]. For applications such as electric vehicles (EVs) and grid storage, consistent performance and risk assessment over the battery's lifecycle is essential [24]. Variability in battery performance can lead to reduced efficiency, unexpected downtimes, and increased operational costs due to premature battery degradation [25]. The economic benefits of LIBs are tied to their reliability; unreliable batteries require frequent replacements and maintenance, diminishing the overall cost-effectiveness of the technology.

and increasing operational costs. For the widespread adoption of technologies like EVs, consumer confidence in battery reliability is crucial. High reliability can enhance user trust and drive market growth towards a variety of applications [26].

This review overviews of the current state of reliability assessment in LIB service. The objectives of this review are to cover the main aspects of the current state-of-the art regarding LIBs, identify research gaps, and provide potential research directions. By compiling the existing literature on reliability assessment techniques [20,21], both experimental and computational [27–29], this review points out emerging trends and future directions, while highlighting the limitations and gaps in current methodologies. Additionally, this review can provide insights and recommendations that can inform future research directions and industry practices, ultimately contributing to the development of more reliable LIB systems.

2. Fundamentals of LIB Reliability

LIB reliability involves several aspects, such as performance and safety reliability, durability, and availability. Reliability defines the consistent ability of the battery to deliver the required power and energy over its expected service life, without causing harm, and avoiding hazardous situations such as thermal runaway, fires, and explosions. Moreover, the battery must be durable, i.e., it must maintain its performance characteristics over time, despite the degradation mechanisms [25,30]. Reinforcing safety standards and strictly following safety protocols can help limit fires and loss of human lives [31]. Sadly, even today, disasters are reported at LIB plants, such as the incident in July 2024 at Seoul, South Korea, where 22 workers were killed during the explosion at the battery plant, with specialists claiming that even a few inhalations from the toxic gases produced during the explosion could render an individual unconscious. Apparently, the incident was caused by a short-circuit occurring at one of the 35,000 cells present in the factory at the time, an incident that was traced to the compression of the inner layers making up the lithium cells. Industry professionals worldwide have been on the lookout for explosions and subsequent fires, reinforcing the need for strict protocols and safety measures, as well as clearly laid-out safety training.

Reliability is quantified through metrics such as failure rate, mean time between failures (MTBFs), and state of health (SOH). These metrics provide a framework for assessing and comparing the reliability of different battery systems. The reliability of LIBs is influenced by a myriad of factors that span battery chemistry, design, manufacturing processes, operating conditions, component materials [32], and external factors (thermal, mechanical, chemical) (Figure 1). Understanding these factors is crucial for developing strategies to enhance battery reliability.

The choice of materials and the electrochemical processes within the battery significantly impact its reliability. The components of the battery (cathode, anode, electrolytes, and separator materials) play an essential role in the battery chemistry. Typical cathode materials such as lithium cobalt oxide (LiCoO_2), lithium iron phosphate (LiFePO_4), and lithium nickel manganese cobalt oxide (NMC) [33,34] or nanostructured S-cathodes [35] have unique properties affecting energy density [36], cycle life, and thermal stability [33]. The anode materials are commonly comprised of graphite, the most widely used anode material, or other carbon-based materials. However, alternatives like silicon and lithium metal [37,38] are being explored for their potential to increase capacity [6]. The electrolyte composition [39] and used additives [40] affect ionic conductivity, stability, and the formation of solid electrolyte interphase (SEI) layers [41], which are crucial for long-term performance and safety [19]. Several materials have been explored for electrolyte components, such as gel polymers [42] and others [43]. Lastly, separators must maintain structural integrity while preventing short circuits; this imposes some conditions on the

interface [39]. Advances in separator technology aim to improve thermal stability and mechanical strength [44,45].

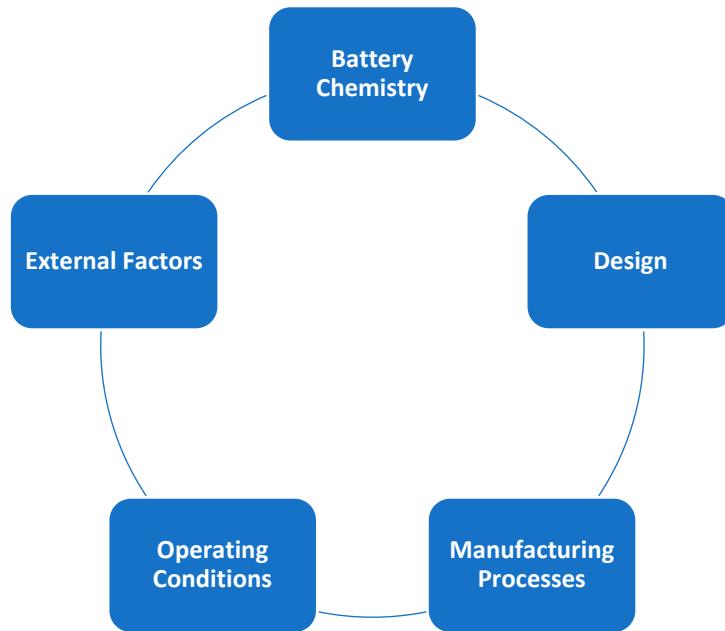


Figure 1. Main aspects affecting battery reliability.

The cell design and manufacturing quality control of LIBs are crucial in determining their reliability. The configuration of electrodes, electrolyte distribution, and cell geometry all play roles in ensuring uniform current distribution and mitigating localized degradation. Consistent production processes are essential to minimize defects such as particle contamination, electrode misalignment, and incomplete SEI formation. Additionally, rigorous testing and quality assurance protocols are necessary to detect and address defects early in the manufacturing process [28,46,47].

The conditions under which batteries are used greatly influence their reliability. Some key factors are operating temperature, the charge/discharge cycles (including overcharge and overdischarge). Extreme temperatures (both high and low) can accelerate degradation mechanisms such as electrolyte decomposition and thermal runaway. Effective thermal management systems are vital for maintaining optimal operating temperatures [48–50]. The rate and depth of charge/discharge cycles impact the rate of capacity fade and overall battery lifespan. Fast charging, in particular, can induce stress and accelerate wear [9]. Operating batteries within specified voltage limits is crucial to avoid overcharge and overdischarge conditions, which can lead to irreversible damage [51].

External factors, often beyond the control of the battery design, also affect reliability. In this regard, mechanical stress, environmental conditions, and usage patterns can significantly impact the battery performance and safety. Vibration, shock, and pressure changes can cause physical damage to battery components, leading to capacity loss or safety hazards [52]. Mechanical modeling aiming to minimize safety hazards of LIBs have been also explored [53,54]. Humidity, exposure to water, and atmospheric pressure variations can affect battery performance and safety [26]. Protective casings and environmental controls are important to mitigate these effects. Real-world usage can vary significantly from controlled conditions, necessitating robust designs that can handle diverse application scenarios.

A critical aspect of ensuring the reliability of LIBs is understanding the various degradation mechanisms that can occur over time, leading to failure [55]: electrolyte decomposition, SEI layer growth, lithium plating, cathode degradation, or mechanical degradation [22].

Failure mode analysis encompasses mechanism of failure assessment and analysis of effects (FMMEA) [55]. High temperatures and over-voltage conditions can cause the electrolyte to decompose, leading to gas generation, increased internal resistance, and capacity loss. The role of the electrolyte cannot be understated: using different types of electrodes can considerably increase LIB's efficiency: water-in-salt, polymeric, or based on ionic liquids. Among different types of polymers, the material offering the best stability and conductivity are gel polymer electrolytes. It has been documented that the growth of SEI layers on the anode surface (dendrites) can be detrimental to the operation of the LIB; however, excessive growth can increase impedance and reduce capacity and can even lead to short-circuiting. When charging patterns involve fast charging, or when operation is carried out at low temperatures, lithium ions are deposited as metallic lithium on the anode surface, leading to capacity loss and potential short circuits (Li plating). Lithium dendrite growth has been investigated experimentally by an XRD *operando* study by Yu et al. [56], and mechanistically by Foroozan et al., and are a main obstacle in the way of Li metal anode commercialization [57]. Cathode degradation is also possible due to time-related structural changes, like phase transitions and the dissolution of transition metals, reducing the capacity and thermal stability [33,34]. Repeated cycling and external mechanical stress can cause cracks and delamination in electrode materials, which add to mechanical degradation processes, affecting the structural integrity and performance of the battery [53].

Given the complex interplay of factors influencing battery reliability, an advanced approach is required to enhance the reliability of LIBs, spanning material innovation, advanced cell design, manufacturing technique, optimized battery management systems (BMSs) [58–60], advanced thermal management, and standardization and testing protocols [22,23]. Developing new materials with improved stability, higher capacity, and better thermal properties can mitigate many degradation mechanisms while providing a safer future for LIBs [61,62]. Precision manufacturing and strict quality control processes can reduce defects and enhance the consistency of battery performance. Using state-of-the-art materials can also provide optimized LIBs, where cost and performance are more evenly matched [63]. Advanced BMS algorithms can optimize charging protocols, monitor battery health in real-time, and provide early warnings of potential failures. Effective thermal management systems, including passive and active cooling strategies [49], can maintain optimal operating temperatures and prevent thermal runaway [50].

Moreover, reliable standardization, testing protocols, and up-to-date reliability benchmarks can ensure the consistent evaluation and comparison of different battery systems [28,46,47]. The reliability of LIBs is a critical determinant of their performance, safety [64], and economic viability across various applications [22]. By understanding the fundamental factors influencing reliability, the mechanisms of degradation [25,30], and advanced fault diagnosis [65], researchers and industry professionals can develop strategies to enhance the robustness and dependability of LIB systems.

3. Experimental Techniques for Reliability Assessment

The reliability of LIBs is crucial for their widespread adoption in various applications, from portable electronics to electric vehicles and grid storage. Ensuring this reliability requires robust experimental techniques that can accurately assess battery performance, identify potential failure modes, and predict longevity. Primary experimental methodologies used to evaluate the reliability of LIBs include accelerated aging tests, in situ diagnostics, failure mode analysis, and practical case studies.

Accelerated aging tests are designed to simulate the long-term usage of LIBs in a compressed timeframe. These tests help in understanding how batteries degrade over time

and under various conditions: high-temperature aging, cycle life testing, storage aging, or rate capability testing.

Since more accelerated degradation occurs due to increased temperature, aging at a high temperature becomes an important testing procedure. Elevated temperatures accelerate the chemical reactions within the battery, leading to faster degradation. By exposing batteries to higher temperatures, researchers can gather data on how temperature affects the battery's lifespan and performance. This method is particularly effective in identifying thermal stability issues and the formation of detrimental compounds within the battery [66]. Cycle life testing involves repeatedly charging and discharging the battery to simulate its usage over time. By increasing the rate of cycling, it is possible to observe the effects of wear and tear on the battery's components, such as the electrodes and electrolyte. Cycle life testing helps in understanding the mechanical and chemical changes that occur within the battery, providing insights into the factors that limit the battery's lifespan [5,24,25,67].

Storing conditions are also essential for maintaining the battery's specifications over time. Batteries are stored at different states of charge and environmental conditions to study how storage affects their performance and longevity [24,51]. This test helps in identifying self-discharge rates, capacity loss, and the formation of passivation layers on the electrodes. This can also create a broader context for stressors that can eventually lead to the failure of a LIB [51]. For instance, the storage of LIB at elevated altitude, under a lower temperature and pressure such as in an airplane, can also create conditions for battery failure and fire accidents [51].

Assessing the battery's performance under various discharge and charge rates provides insights into its ability to handle different power demands. This test is crucial for applications requiring high power outputs, such as electric vehicles, where batteries must deliver significant power over short periods, and charging data can make it easier to better assess the suitability of the battery to function as a second-life battery [68]. In situ diagnostic techniques provide real-time data on the internal state of the battery during operation, offering valuable insights into its reliability [59]. Among these techniques, the following are most utilized: electrochemical impedance spectroscopy (EIS), X-ray diffraction (XRD), scanning electron microscopy (SEM), nuclear magnetic resonance (NMR), and in situ Raman spectroscopy.

Electrochemical impedance spectroscopy (EIS) measures the impedance of the battery over a range of frequencies, providing information on the resistive and capacitive behavior of the battery components [69]. This technique helps in identifying issues such as increased internal resistance, electrolyte degradation, and SEI layer growth, offering a realistic estimation of the power delivery capability and state of health (SoH) of LIBs. Moreover, this nondestructive technique does not require the disassembly of the battery itself and provides accurate estimates under operating conditions. Other nondestructive ways to evaluate SoH for LIBs include impedance testing and voltammetry measurements, but each one has its shortcomings (limited information for impedance measurement, since it is usually applied at a specific frequency and does not account for all possible degradation pathways that may occur at low frequencies). Voltammetry is an electrochemical technique that measures current vs. applied voltage, and ampere hour (Ah) is the most commonly employed subset that is also time-consuming to implement. Unfortunately, EIS is not a widespread measure for checking the SoH of LIBs due to multiple variables in real-life scenarios: cell chemistries, construction and design, charging/discharging cycles, etc.

X-ray diffraction (XRD) is used to study the crystal structure of electrode materials in real-time. Changes in the crystal structure can indicate phase transitions, material degradation, and mechanical stress, all of which impact battery reliability and safety [70].

For instance, XRD was used to check the phase distribution in $\text{Li}_x\text{FeSO}_4\text{F}$ ($x = 1, 0.5, 0$) battery electrodes [70].

Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) help researchers to visualize the electrode surface morphology. It is used to detect physical changes such as cracks, dendrite formation, lithium plating, and particle agglomeration, which can lead to material accumulation at the micro-scale and eventually to battery failure [55,70]. Nuclear magnetic resonance (NMR) provides information on the chemical environment within the battery. It can detect changes in the electrolyte composition, identify degradation products, and monitor lithium distribution within the battery [55]. Fourier transform infrared (FTIR) and *in situ* Raman spectroscopy provide molecular information about the battery's materials such as thickness, composition of the SEI layer, or valuable morphology data. They are particularly useful for detecting changes in the chemical composition and structure of the electrodes and electrolyte during cycling [26,55].

Understanding the mechanisms behind battery failure is crucial for improving reliability. Failure mode analysis involves identifying, analyzing, and categorizing the different ways in which batteries can fail. In this regard, researchers perform various tasks such as thermal runaway, mechanical stress, overcharge/overdischarge, and post mortem analysis in order to elucidate the most important factors leading to battery failure. This complex investigation protocol can ease the way to further enhance the reliability of LIBs.

Thermal runaway is a critical failure mode where an increase in temperature leads to uncontrollable exothermic reactions, potentially causing fires or explosions. By inducing thermal runaway in a controlled environment, researchers can study the conditions that trigger it and develop strategies to prevent it [50,51,62]. Batteries are subjected to mechanical stress such as vibration, shock, and compression to simulate real-world conditions. These tests help in identifying weaknesses in the battery's design and construction that could lead to failure, while providing a thorough estimation of the LIB's SoH [71].

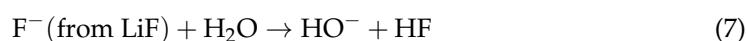
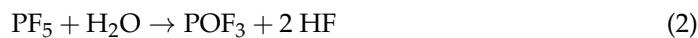
The battery's usage pattern may strongly affect the battery's capacity and performance over time; therefore, overcharge and overdischarge testing protocols can elucidate the behavior of batteries under real-life conditions [9,22]. Exposing batteries to overcharge and overdischarge conditions helps in understanding the limits of their safe operation, by identifying the potential for lithium plating, electrolyte decomposition, and other detrimental effects that occur when batteries are pushed beyond their recommended operating ranges. After a battery has failed, a detailed examination of its components can reveal the root causes of failure (post mortem analysis) [72]. Techniques such as disassembly, microscopy, and spectroscopy are used to analyze the electrodes, electrolyte, and separator for signs of degradation, mechanical damage, and chemical changes. Real-world case studies provide valuable insights into the practical challenges and solutions in ensuring LIB reliability.

Several insights related to electrolyte behavior in LIBs have surfaced in the recent literature. There are five types of electrolytes that are typically used in LIB technology: solid, liquid (aqueous) solid polymer, gel polymer, and ionic liquid electrolytes. While aqueous electrolytes are safer, non-flammable, and more economical, they also have downsides like side-reactions, H_2 gas evolution, and corrosion [73]. The current trend is to utilize solid-state LIBs that feature more stable electrochemical behavior by the introduction of the solid electrolyte interface. The electrolytes are responsible for the ion movement between electrodes, and contribute to overall cell stability, underscoring their key role in defining the LIBs' efficiency (Table 1).

Table 1. Main properties of carbonate-based electrolytes used in LIBs.

Electrolyte Type	Features	Advantages	Disadvantages
dimethylene carbonate (DMC)			Structure-dependent physical properties (dielectric constant, viscosity); high volatility; electrolyte decomposition at anode
diethylene carbonate (DEC)	Low viscosity, high ionic conductivity	Reduced overall viscosity	
ethyl methyl carbonate (EMC)			
ethylene carbonate (EC)	High thermal stability, high dielectric constant, low volatility, film forming ability	High usability for LIBs. Widespread use; SEI film forming at graphite anode preventing exfoliation	High viscosity, high melting point (36 °C), low ionic conductivity thus cannot be used at room temp
fluorinated ethylene carbonate (FEC)	Enhanced SEI forming ability, reduced flammability, higher thermal stability	High coulombic efficiency; reversible lithiation of graphite anode	Higher viscosity, reduced ionic conductivity
propylene carbonate (PC)	Similar dielectric constant to EC	Lower mp (−48.8 °C)	Cannot create SEI film; fewer chemical gases released during a fire (slower kinetics); flammable
LiPF ₆ (Li salt)/EC (electrolyte)	Wide electrochemical stability window	High ionic conductivity, chemical stability, passive towards cathodic current collector (Al)	Thermally unstable, proneness to hydrolysis (producing PF ₅ , LiF, and HF)

LiPF₆ is a lithium salt and can easily be found under its ionic form in solutions, namely producing Li⁺ and PF₆[−] ions. While LiPF₆ is the most commonly used Li salt utilized in LIBs, it is not without shortcomings, mainly due to its thermal degradation profile, but also the moisture sensitivity, which further degrades the Li⁺ salt into corrosive HF corrosion [73]. Despite its widespread use, the detailed mechanistic insights into LiPF₆ degradation due to temperature and water are not fully understood, and recent research papers shed some light on this process.



A typical composition found in LIBs consists of 1M LiPF₆ in the EC/DEC electrolyte. The thermal decomposition (1) leads to breaking LiPF₆ into the two constitutive salts, LiF and PF₅, a strong Lewis acid, and can be followed by different hydrolysis pathways (2)–(6). The reaction of POF₃ in the presence of diethyl carbonate (DEC) at 60 °C can even produce CO₂ gas (reaction (3)), which accumulates inside the cell, leading to additional safety concerns [73]. Recently, the spectroscopic investigation of PF₅ hydrolysis by ion chromatography (IC), coulometric Karl–Fischer titration (cKFT) and acid–base titration revealed the production of HPO₂F₂ and HF, according to reaction (4) [74]. Last but not least, even though LiF has a relatively poor water solubility (0.134 g/100 mL at 25 °C), the resulting fluoride anion can hydrolyze, being a strong conjugated base, with the release of HF and HO[−] anions according to reaction (7). Moreover, the formation of LiF at the electrode surface is also detrimental to the fast-charging ability of the LIB, due to its resistive properties. Considering the number and nature of hydrolysis and thermal decomposition of LiPF₆ (reactions (1) to (7)), one may conclude that hydrolysis is detrimental not only to the normal and sustained performance of LIBs, but it can pose serious health hazards when powering everyday mobile devices and more.

The complex hydrolytic behavior of LiPF₆ when in contact with moisture can raise important safety questions, highlighting the need for strict quality control regarding LIBs that come in contact with water, either through insufficient LIB cell sealing or the improper use of electrolyte materials that have not been properly dried before use. Still, compared to potential replacements like LiBF₄ or LiClO₄, LiPF₆ has the best mixture of advantages related to conductivity and ionic mobility. However, progress has been made in order to overcome the side-reactions related to the presence of water in the electrolyte, such as the use of inhibitors that block the further decomposition of PF₅ by forming a complex with it [75]. For this purpose, trimethylsilyl(isothiocyanate) (TMSNCS) has been employed and it showed good scavenging properties for LiF, while stabilizing the PF₅ by suppressing further HF formation (Figure 2). The enhanced electrochemical stability was achieved even under minor TMSNCS concentrations of 0.1%, with a superior discharge capacity of 144 mAh/g and 91.8% capacity retention over 300 cycles.

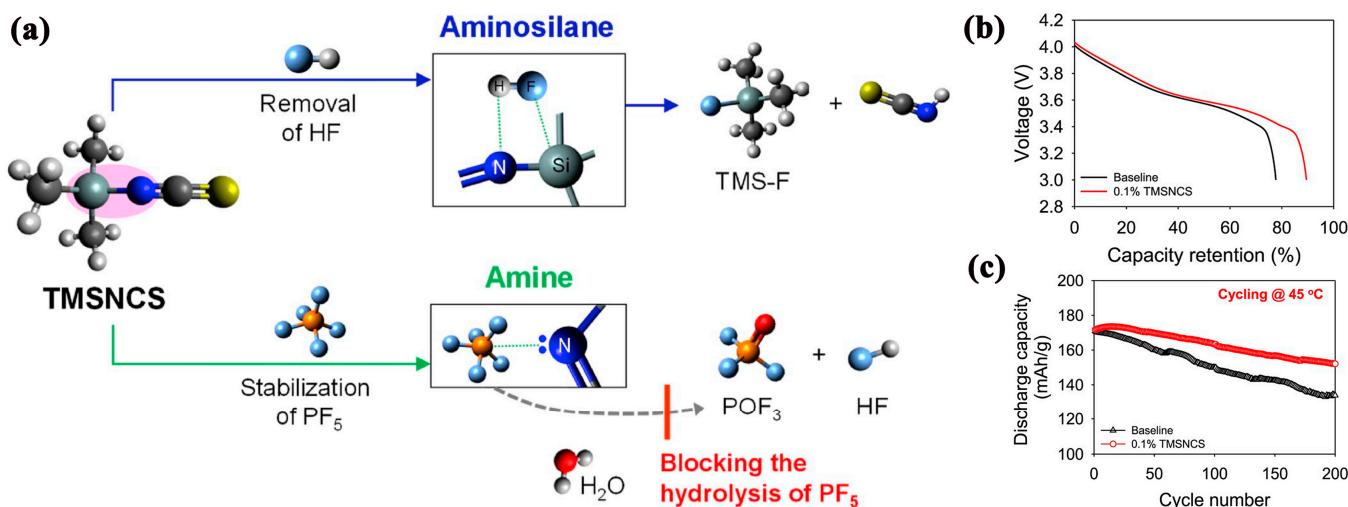


Figure 2. (a) Illustration of HF scavenging and stabilization of PF₅ by TMSNCS additive. (b) Comparison of capacity retention of NCM622/graphite full cells with and without the TMSNCS additive after storage at 60 °C for 14 days. (c) Cycle performance of the NCM622/graphite full cells with the baseline electrolyte and 0.1 wt% TMSNCS-containing electrolyte at 45 °C, a 2C charge rate, and a 1C discharge rate during 200 cycles. Reprinted with permission from [75].

As a strong Lewis acid, PF_5 has pronounced electron-withdrawing properties; therefore, it would easily bind to electron-donating atoms such as N and P that possess a lone electron pair at their disposal. Using trimethylsilyl)isothiocyanate (TMSNCS) with aminosilane and isothiocyanate functional groups, Han et al. have provided a dual-intention additive able to bind HF through the N-Si moiety, but also the PF_5 through a strong Lewis acid (PF_5)–Lewis base (TMSNCS) interaction [75].

The formation of a stable solid electrolyte interface (SEI) remains essential for overcoming the electrolyte degradation and originates from the reaction carbonate— LiPF_6 in LIBs. The DFT modeling of such interactions showed that alternative pathways can be imagined, but the energetics are somewhat unfavorable. Spotte-Smith et al. have shown that the reactivity of LiPF_6 can be tuned by varying the inorganic/organic carbonate species and by limiting the ionic transport of the PF_6^- anion through the SEI [76]. The authors modeled the reaction between POF_3 and inorganic carbonate species (H_2CO_3 , LiHCO_3 , and Li_2CO_3), and found that reactivity was much more likely to occur for Li_2CO_3 (more negative ΔG) due to the more negative partial charges for oxygen atoms [76] (Figure 3).

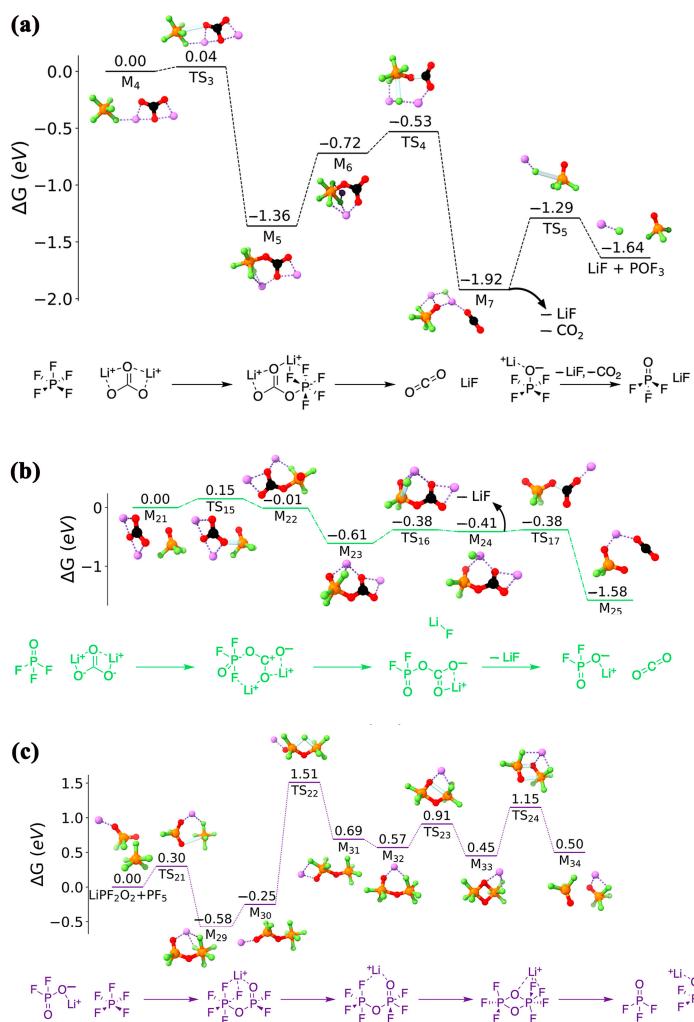


Figure 3. (a) Energy diagrams for the formation of POF_3 from PF_5 and Li_2CO_3 . LiPOF₄ forms via simultaneous elimination of LiF and CO_2 from a $\text{PF}_5\text{-Li}_2\text{CO}_3$ adduct. LiPOF₄ can then eliminate LiF to form POF_3 . (b) Reactions between POF_3 and simple inorganic carbonates Li_2CO_3 to form CO_2 and LiPF_2O_2 . (c) Possible routes for the re-formation of POF_3 from LiPF_2O_2 [76]. Color codes: red (oxygen), violet (lithium), orange (phosphorus), green (fluorine), black (carbon). Copyright © 2022 The Authors. Published by American Chemical Society. This publication is licensed under CC-BY 4.0.

The regeneration of catalytically active species POF3 could proceed by pathway Figure 3c, but the mechanism is kinetically limited due to an extremely unfavorable intramolecular fluorine transfer step ($M30 \rightarrow M31$, high activation energy $\Delta G = 1.76$ eV), which makes POF3 autocatalysis unlikely at modest temperatures [76].

Studies on electric vehicle (EV) battery packs have shown that thermal management is crucial for maintaining reliability [8,11]. For example, the use of liquid cooling systems has been effective in preventing overheating and ensuring a uniform temperature distribution within the battery pack. These studies also highlight the importance of robust battery management systems (BMSs) that can monitor and control the charging and discharging processes to extend battery life.

In grid-scale energy storage systems [52], the reliability of LIBs is critical for ensuring an uninterrupted power supply [22]. Case studies have demonstrated the effectiveness of advanced monitoring systems that use real-time data analytics to predict and prevent failures. These systems can detect anomalies in battery performance and trigger maintenance actions before failures occur.

Reliability assessments of batteries in consumer electronics, such as smartphones and laptops, focus on issues like swelling, reduced capacity, and safety risks [77]. Practical examples include the development of protective circuits that prevent overcharging and the use of advanced materials that enhance the thermal stability of the batteries.

LIBs used in aerospace applications face unique challenges due to extreme temperatures, pressure variations, and high reliability requirements. Case studies have highlighted the importance of rigorous testing and quality control processes in ensuring the reliability of batteries used in satellites, aircrafts, and space missions [26].

Experimental techniques for reliability assessment are critical for understanding and improving the performance and safety of LIBs [77]. Accelerated aging tests, in situ diagnostics, failure mode analysis, and real-world case studies provide comprehensive insights into the factors affecting battery reliability. By employing these techniques, researchers and industry professionals can develop strategies to enhance the robustness and dependability of LIBs, ensuring their safe and effective use across a wide range of applications.

4. Computational and Data-Driven Approaches

As the complexity of LIBs continues to evolve, the need for advanced methods to predict and enhance their reliability becomes increasingly critical. Computational and data-driven approaches offer powerful tools to model, analyze, and optimize battery performance, providing insights that are difficult to achieve through experimental methods alone. There are several examples where actual reported failures of LIBs have been documented, and the corresponding lessons taught, such as the case of the 787 Dreamliner [78].

Physics-based models provide a detailed understanding of the underlying electrochemical processes and physical phenomena occurring within LIBs. These models (electrochemical, thermal, mechanical, and degradation models) simulate the behavior of batteries under various conditions and stress, helping to predict performance and identify potential failure mechanisms. Electrochemical models, like the Doyle–Fuller–Newman (DFN) model, simulate the transport of ions and electrons within the battery, with further tuning by means of reparametrizing by normalization and grouping, sensitivity, and parameter estimation analysis; Khalik et al. concluded that the estimation of 12 out of 22 model parameters can accurately lead to an accurate model description [79]. They consider factors like electrolyte concentration, potential distribution, and reaction kinetics. By solving the governing equations of mass and charge conservation, electrochemical models can predict voltage profiles, state of charge (SoC), and state of health (SoH) under different operating conditions.

Thermal models are based on thermal management optimizations [48], which are crucial for battery reliability, as temperature significantly affects battery performance and safety [19,80]. Thermal models simulate thermal dynamics (heat generation and dissipation within the battery), incorporating parameters such as heat capacity, thermal conductivity, and convective heat transfer. These models help in designing effective cooling systems and in understanding the impact of temperature on battery degradation.

$$\rho c_p \left(\frac{\partial T}{\partial t} + v_e + \nabla T \right) \approx \frac{\partial (\rho c_p T)}{\partial t} = \nabla \cdot \lambda \nabla T + q \quad (8)$$

The cell temperature could be obtained by solving the heat transfer Equation (8), where ρ is the average density, c_p is the heat capacity at a constant pressure, v_e is the electrolyte velocity (limited mobility of electrolyte in LIBs, hence neglectable), λ is the average thermal conductivity, and q is the heat generation rate [48].

On the other hand, mechanical models consider the mechanical/physical factors that may affect the LIBs' performance [53]. Mechanical stresses can cause deformation and damage to battery components, leading to capacity loss and failure. Mechanical models simulate the mechanical behavior of electrodes and other components under various loading conditions, showing interconnected values of SoC, SoH, and stack level mechanical stress [71]. Depending on the level they address, mechanical models refer to the micro- and meso-scale, macro-scale (cell level), or macrosystem scale (battery modules) [53]. Finite element analysis (FEA) and representative volume element (RVE) are commonly used to study stress distribution, deformation, and fracture mechanics; however, FEA requires considerable computational resources, as there could be more than 100,000 elements for this model and possibly even more for local fracture prediction. These models are essential for designing robust battery structures that can withstand mechanical stresses during operation.

Degradation models aim to predict the long-term performance of batteries by simulating the various degradation mechanisms, such as SEI layer growth, lithium plating, and particle cracking [25,30]. These models often couple electrochemical, thermal, and mechanical effects to provide a comprehensive view of battery aging. By understanding how different factors contribute to degradation, these models can inform strategies to extend battery life.

Machine learning (ML) algorithms have emerged as powerful tools for the predictive maintenance and reliability assessment of LIBs [81]. These data-driven techniques can analyze large datasets to identify patterns and make predictions about battery performance and failure with increased accuracy [82]. These algorithms include supervised learning, unsupervised/semi-supervised learning, reinforcement learning, and hybrid models.

Supervised learning algorithms, such as regression models, support vector machines (SVMs), and neural networks, are trained on labeled data to predict specific outcomes. For battery reliability, these algorithms can predict parameters like remaining useful life (RUL), capacity fade, and internal resistance based on historical data. Supervised learning models require large, high-quality datasets to achieve accurate predictions [83].

Unsupervised learning techniques, such as clustering and principal component analysis (PCA), are used to identify underlying patterns and anomalies in the data without predefined labels [84]. These methods can help in detecting early signs of battery degradation or identifying distinct operational modes. For example, clustering algorithms can group similar usage patterns, aiding in understanding different stress factors affecting battery life [82].

Reinforcement learning algorithms learn optimal strategies through trial and error, making them suitable for dynamic and adaptive battery management systems (BMSs) [85]. These algorithms can optimize charging and discharging protocols to maximize battery life

and performance. By continuously learning from the battery's operational data, reinforcement learning models can adapt to changing conditions and improve reliability over time, while also providing more accurate estimations regarding the aging process of LIBs [86].

Combining physics-based models with machine learning techniques led to the development of hybrid models that can enhance predictive accuracy and reliability assessment. For instance, machine learning algorithms can be used to calibrate and update parameters in physics-based models based on real-time data. This hybrid approach leverages the strengths of both methodologies, providing more robust and accurate predictions [87,88]. The vast amount of data generated by batteries during operation present an opportunity to improve reliability through advanced data analytics (Figure 4).

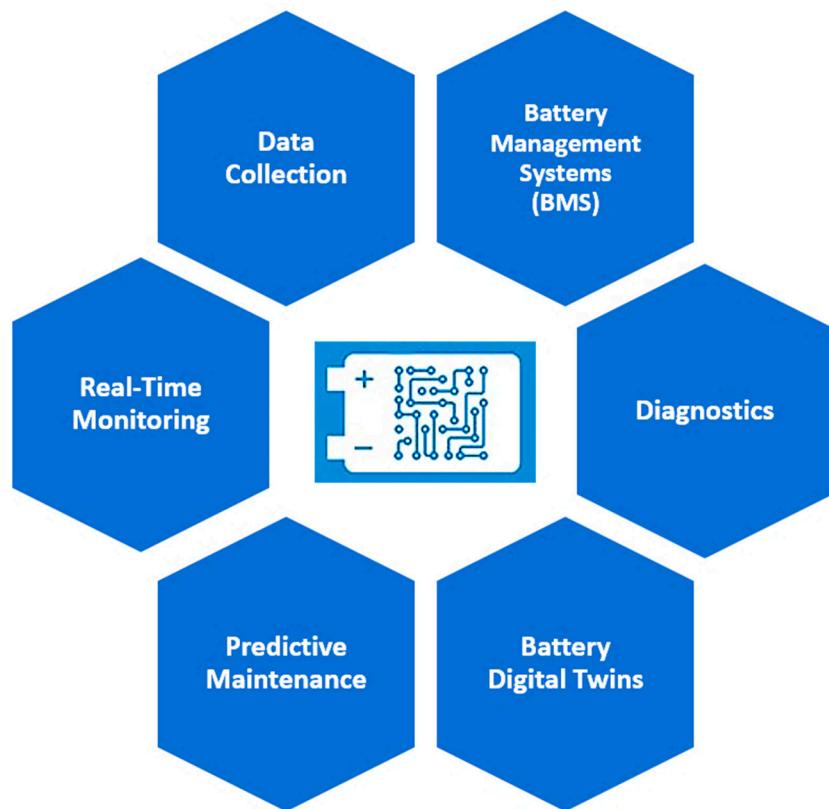


Figure 4. Key point in battery data workflow.

Effective data collection and management are essential for leveraging operational data. This includes data from sensors, battery management systems (BMSs), and external sources. Ensuring data quality and integrity is crucial, as poor-quality data can lead to inaccurate predictions and assessments [89].

Real-time monitoring systems continuously track key performance indicators (KPIs) such as voltage, current, temperature, and impedance. Advanced diagnostic algorithms can analyze these data to detect anomalies, predict failures, and trigger maintenance actions [66]. For example, real-time impedance spectroscopy can identify changes in internal resistance, indicating potential degradation. Implementing advanced diagnosis methods can ultimately lead to high safety LIBs [66].

Predictive maintenance strategies use data analytics to forecast when maintenance should be performed, preventing unexpected failures and reducing downtime. By analyzing trends and patterns in operational data, predictive maintenance algorithms can provide early warnings and optimize maintenance schedules, enhancing overall reliability [90].

A digital twin is a virtual replica of a physical battery that simulates its behavior under various conditions [91]. By integrating real-time data with physics-based models,

digital twins can provide accurate predictions of battery performance and health. This approach enables the proactive management and optimization of battery systems, improving reliability and extending the lifespan of LIBs towards diverse applications [92].

Combining computational and experimental approaches offers a comprehensive framework for assessing and improving battery reliability. This strategy implies the simultaneous use of model validation and calibration, experimental design optimization, and in situ monitoring and simulation (Figure 5).

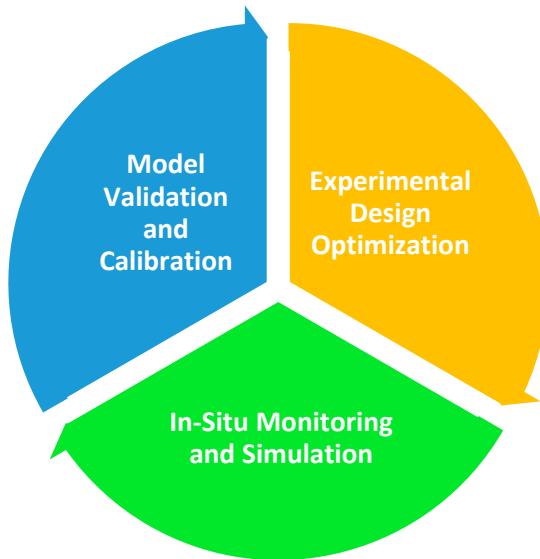


Figure 5. Comprehensive framework from combined experimental and computational data.

Experimental data are essential for validating and calibrating computational models [93]. By comparing model predictions with experimental results, researchers can refine model parameters and improve accuracy. This iterative process ensures that models accurately reflect real-world battery behavior. Computational models can guide the design of experiments by identifying the most critical parameters and conditions to test, fostering the experimental design optimization approach. This approach reduces the number of experiments needed, saving time and resources. For example, simulations can identify the optimal temperature ranges and cycling protocols to study, ensuring that experiments focus on the most relevant scenarios [94].

Integrating in situ monitoring techniques with real-time simulations provides a powerful tool for assessing battery reliability [95]. For instance, real-time data from in situ diagnostics can be fed into computational models to simulate future performance and predict potential failures. This integration enables dynamic adjustments to operating conditions, optimizing reliability in real-time.

Computational and data-driven approaches are indispensable for assessing and enhancing the reliability of LIBs. Physics-based models provide detailed insights into the electrochemical, thermal, and mechanical behavior of batteries, while machine learning algorithms offer powerful tools for predictive maintenance and anomaly detection. Advanced data analytics and the utilization of operational data further enhance the ability to monitor and optimize battery performance in real-time. By integrating these computational methods with experimental techniques, researchers and industry professionals can develop robust strategies to ensure the reliability and longevity of LIBs.

When evaluating the reliability of LIBs, several key experimental methodologies can be employed. These include accelerated aging tests, in situ diagnostics, failure mode analysis, and practical case studies, each providing insights into battery degradation mechanisms, operational safety, and longevity.

Accelerated aging tests are used to simulate long-term usage over a shorter period, subjecting LIBs to high temperatures, increased charging/discharging rates, and stress cycles beyond standard operational conditions. These tests reveal degradation patterns, capacity fade, and internal resistance growth, enabling predictions of the battery lifespan. As a key performance indicator, the LIBs' capacity can be traced by plotting a capacity fade curve. The capacity fade over several charging/discharging cycles can shorten the useful LIBs' lifespan. Thus, modeling and experimental approaches are combined. Carnovale et al. have developed and validated such a model based on the growth of the SEI layer, and the active material loss at the anode and cathode [96]. Their result confirms that, when temperature is increased, there is a sharp decrease in battery capacity due to accelerated aging at elevated temperatures. However, the main factor contributing to the capacity fade was the growth of the SEI layer at the negative electrode, followed by the accumulation and immobilization of the active component at the anode. The degradation model follows an Arrhenius law-type $k = k_0 e^{-\frac{E}{RT}}$, where the reference reaction rate, k_0 , refers to the negative electrode SEI film growth (1.3×10^{-18}), the positive electrode SEI film growth (3.1×10^{-8}), and the negative electrode active material isolation (3.47×10^{-14}), and E is the corresponding activation energy for the same process [96].

The proposed model fits reasonably well with experimental data and shows that as the discharge/charge cycles increase, the battery capacity decreases steadily; however, there is a more pronounced reduction in capacity over the first 40 cycles (larger slope of the graph), followed by a steadier reduction within the first 40–300 cycles, followed again by a faster capacity loss beyond the first 300 cycles (Figure 6a). The proposed model agrees well for the operating temperature of 35 °C and a discharge/charge rate of 1C, pointing to the fact that the assumptions related to material isolation at the negative electrode and the growth of the SEI layer at both electrodes are valid model assumptions [96].

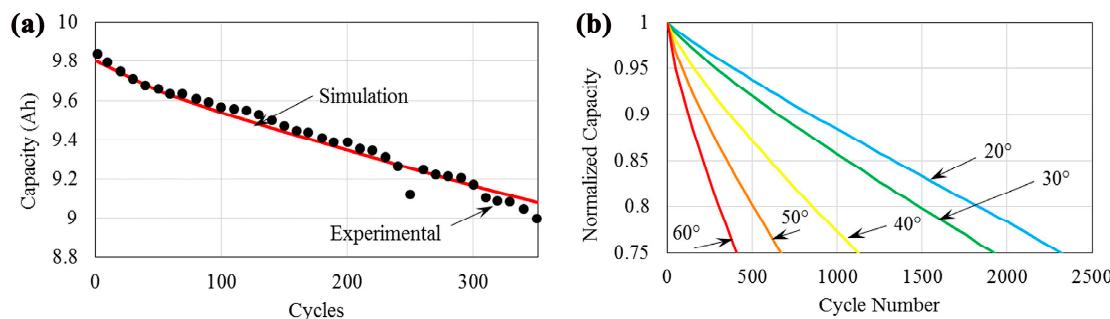


Figure 6. (a) Comparison between the model predicted and experimental battery capacity at 1C charge/discharge cycling at the battery operation temperature of 35 °C. (b) Degradation of battery capacity as a function of the discharge and charge cycles for isothermal discharge/charge rate at 1C at various battery operation temperatures, at normalized capacity. Reproduced with permission from [96].

The *capacity fade curve* (Figure 6b) shows the normalized battery capacity over the cycle life at different temperature conditions (20 °C to 60 °C). The figure highlights the faster degradation at elevated temperatures (especially at 50 °C and 60 °C), demonstrating the negative impact of thermal stress on capacity retention. The trend in capacity fade may be due to the accelerated tests and is correlated with typical battery chemistries and conditions under which batteries may experience such stresses. The capacity fade correlates to the number of charge/discharge cycles and the operating temperature; the initial battery capacity of 10 Ah reduces to 7.5 Ah after 2000 cycles when operating at 20 °C, but it only takes 400 discharge/charge cycles for it to reach the same 7.5 Ah capacity when operated

at 60 °C. This aspect shows the importance of proper battery thermal management for an enhanced battery lifespan.

In situ diagnostics monitor LIBs in real-time during operation, allowing researchers to observe degradation mechanisms as they occur. Techniques like in situ X-ray diffraction (XRD), neutron imaging, and electrochemical impedance spectroscopy (EIS) reveal structural and compositional changes in electrode materials and electrolyte degradation. Recently, several material advances have been made in order to enhance the cyclic performance of oxidic materials utilized as cathode materials for LIBs. For instance, LiFePO₄ (LFP)-coated LiNi_{0.6}Co_{0.2}Mn_{0.2}O₂ (NCM622) has been shown to alleviate the shortcomings of NCM622, namely the electrochemical behavior. In the voltage range of 3–4.3 V, LFP@NCM622 showed a retention capacity of 92.4% when cycling at 1C for 100 cycles [97]. This behavior represents a marked improvement over the untreated NCM622, which had a more pronounced capacity fade under the same testing conditions. Interestingly, the XRD analysis of NCM622 and LFP@NCM622 show subtle differences as a result of LFP coating (Figure 7).

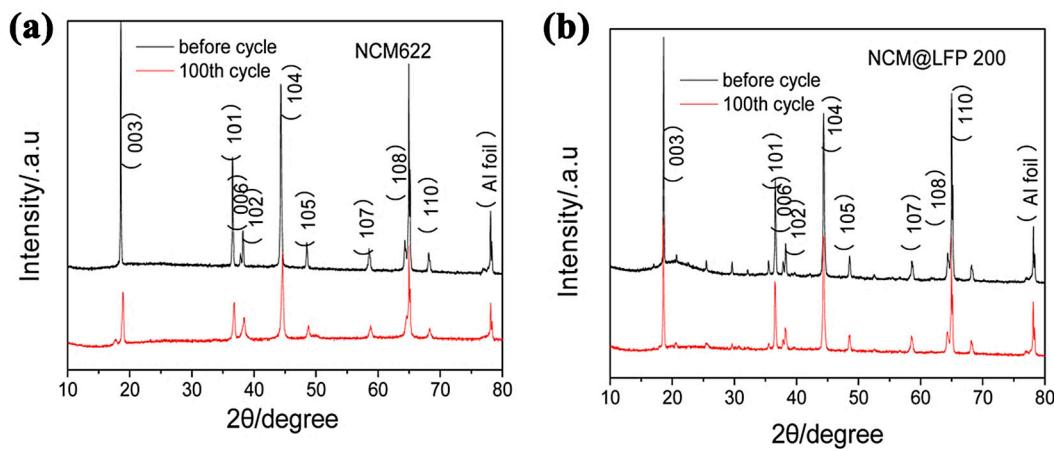


Figure 7. XRD patterns of different cathodes after 1 and 100 charge/discharge cycles: (a) bare NCM622, (b) NCM@LFP. Reproduced under a Creative Commons Attribution-Noncommercial 3.0 Unported License from [97].

When cycled at 55 °C, the peaks corresponding to layered LiNi_{0.6}Co_{0.2}Mn_{0.2}O₂ showed a marked collapse of the crystalline structure over long-term cycling (Figure 7a), with a strong reduction in peak intensity on the (003) attributed to Li⁺/Ni²⁺ ion mixing. By contrast, the peaks corresponding to NCM@LFP were largely unchanged, attesting to the superior thermal stability of the coated electrode material. Moreover, the split (102)/(006) is strongly affected after cycling, meaning that the NCM becomes a poorly layered material, whereas the same split in the coated NCM@LFP remains largely unchanged, attesting to the superior morphological characteristics even after 100 cycles [97]. The XRD pattern evolution (Figure 7) over cycling shows the phase transitions in the cathode material. The split (102)/(006) confirms material degradation over 100 cycles.

In other cases, the phase transitions can correlate with capacity loss and reduced cycling efficiency. These could help identify irreversible reactions or transformations that impact battery performance. Comparing the in situ data with post mortem analysis (if available) could enrich the insights by connecting observed changes with specific failure modes.

Failure mode analysis seeks to identify, classify, and understand the specific mechanisms causing LIB failures. Techniques such as scanning electron microscopy (SEM), focused ion beam (FIB) cross-sections, and thermal runaway tests reveal physical and chemical causes of failure, from dendrite formation to separator damage.

Methods such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM), or in situ optical microscopy (Figure 8) can be utilized to obtain live data on the dendrite growth status. Dendrite growth does not plague only batteries based on the Li anode, but also LIBs, especially under high charging rates and at lower temperatures. The cross-section SEM image (Figure 8e) of a cycled lithium battery cell shows dendrite growth on the anode and/or separator damage. This reveals the impact of factors such as high current density or extreme cycling on the internal battery structure.

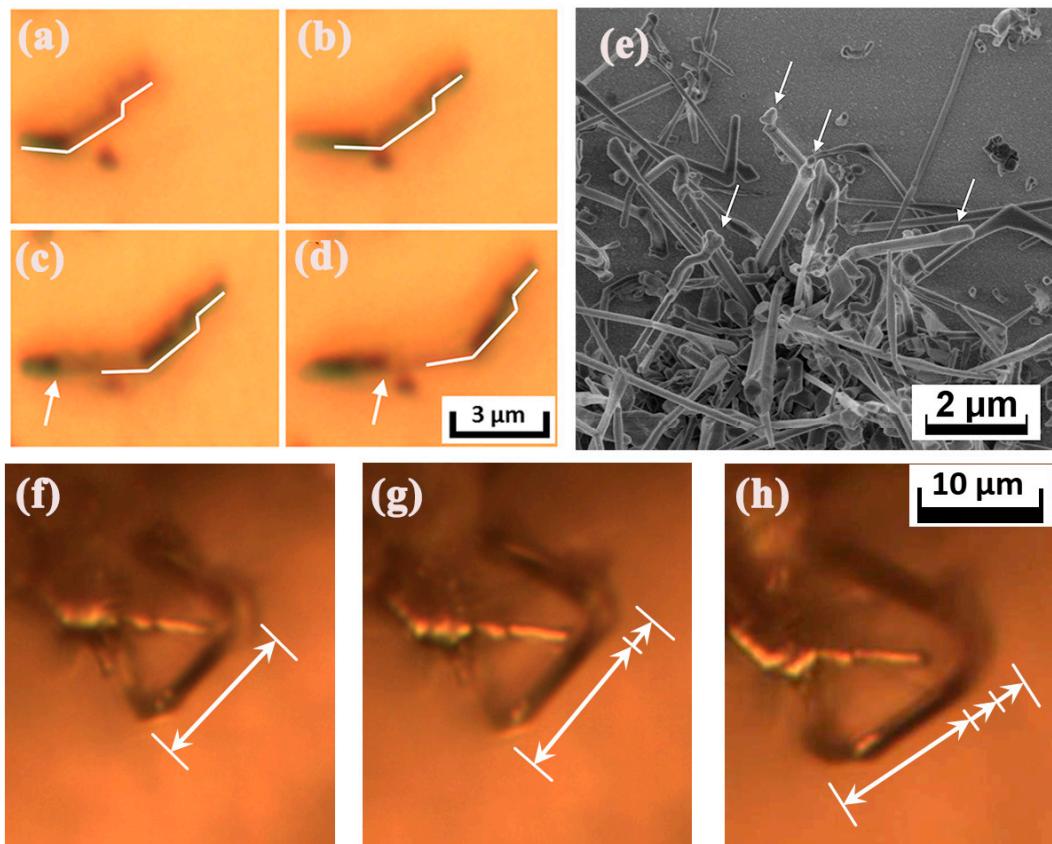


Figure 8. (a) In situ light microscopy of needle-like lithium growth in 1 M LiPF₆ electrolyte. The structure of image (a) (traced in white) remains unchanged, while more segments are added at the base of the structure as shown in the subsequent pictures, i.e., the images demonstrate that in this case, the growth occurred exclusively at the base of the needle. A kink forms in (c) and is marked by an arrow. Image (b) was taken 15 s, (c) 180 s, and (d) 450 s after figure (a) was recorded; (e) SEM image (1 kV) of lithium filaments deposited on tungsten at -100 mV. Several filaments show structures at the tip, e.g., contrast changes, contaminants such as particles, or a broadening of the tip. (f) In situ light microscopy of needle-like growth in 1 M LiPF₆ on a lithium substrate. The view on the tip and the base of the needle is obstructed by other lithium structures; three straight segments connected by two kinks can be seen. Images (g,h) show that the segment between the kinks grew in length (marked by white arrow). Image (g) was taken after 45 s, and (h) after 135 s. Reproduced with permission from [98].

The dendrite formation can cause internal short circuits or thermal runaway, a critical safety hazard in LIBs. Increased stress influences dendrite growth rates, causing further separator wear.

Practical case studies on LIB failures in real-world applications—like EV batteries, smartphones, or stationary storage systems—provide context to lab findings and validate experimental results under actual operating conditions. Shu et al. have proposed a model

for a real-world degradation profile (Figure 9), comparing the capacity fade of LIBs from electric vehicles under varying climatic conditions.

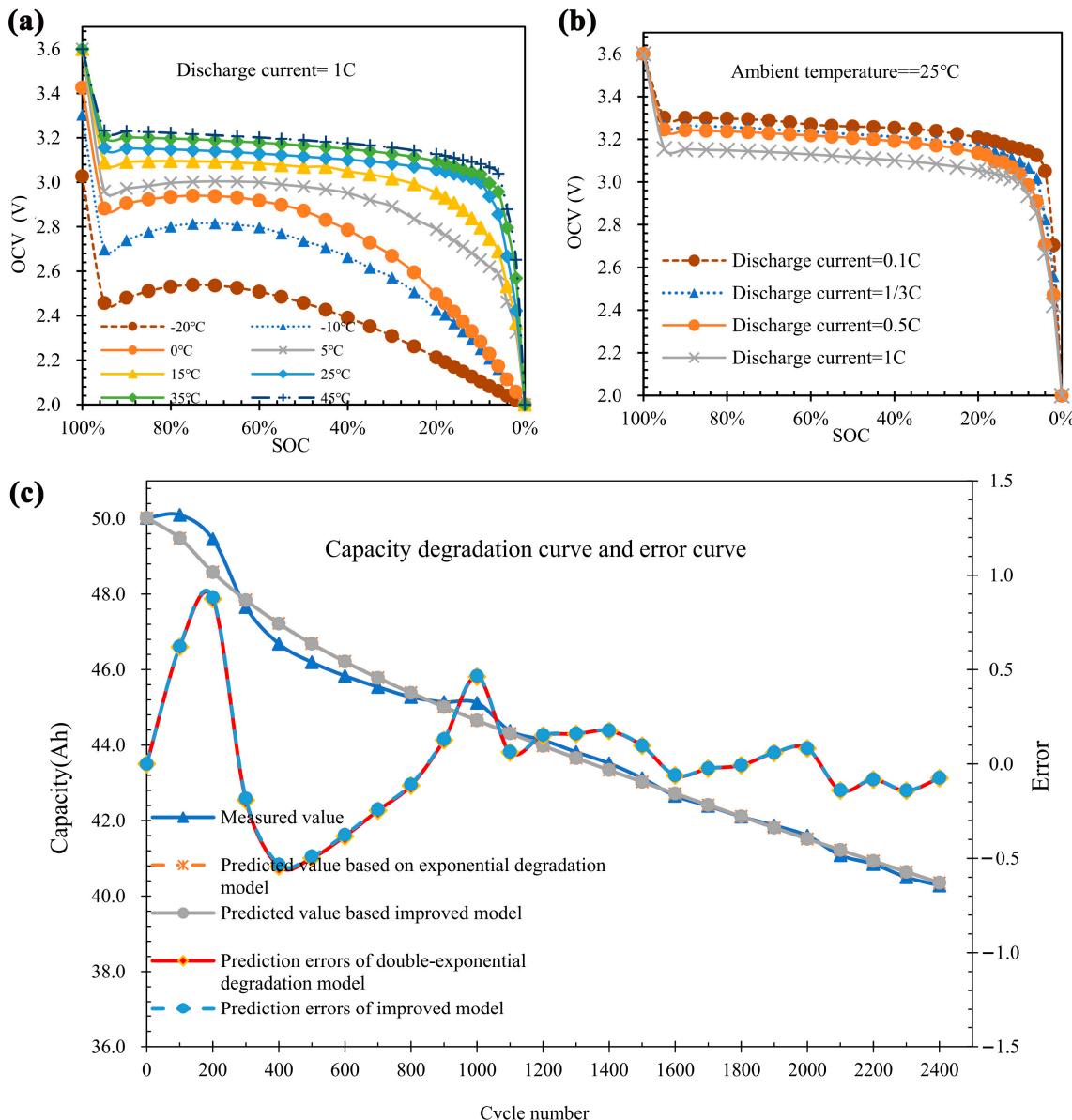


Figure 9. The SOC-OCV curves of the LIBs obtained under different discharge conditions: (a) when the battery is discharged at 1C, and (b) when the battery is discharged with a different current; (c) degradation prediction results obtained when the cells operate at a constant temperature. Reproduced with permission from [99].

Figure 9 illustrates that batteries in hot climates or operating under increased temperatures degrade faster than those in cooler regions, emphasizing the environmental impact on battery reliability. However, when the temperature decreases to $-20\text{ }^{\circ}\text{C}$, the performance of LIBs decreases to about one-third of their capacity at $25\text{ }^{\circ}\text{C}$ [99]. Moreover, temperature changes further contribute to capacity fading over time, highlighting the need to account for temperature when developing a predictive model for LIB degradation. The OCV is dependent on the temperature, decreasing as the temperature decreases. Figure 9a reveals three stages in the degradation of LIBs: a first stage when the SOH is between 100% and 95% (the initial degradation stage), when $95\% < \text{SOH} < 15\%$ (stable degradation stage) and finally, when $\text{SOH} < 15\%$ (the final and rapid degradation stage). Notably, the OCV drops

sharply when the SOH decreases, in the region when the SOH is between 100 and 95% and below 15%. The model proposed by Shu et al. showed a better fit to the experimental data. With a much better error of 2.34% compared to 11.18% of the traditional dual exponential model, the model proposed by Shu et al. paves the way for a more reliable design for future EV batteries.

The degradation trends observed in different climates correlate with the accelerated aging and in situ diagnostic results. The real-world validation of lab results highlights the importance of environmental factors and reinforces the relevance of reliability studies.

5. Policy, Regulation, and Standards for Ensuring LIB Reliability

The widespread adoption of LIBs across various sectors—from consumer electronics and electric vehicles to grid storage and renewable energy systems—necessitates stringent policies, regulations, and standards to ensure their reliability, safety, and sustainability [77,80]. The existing regulatory landscape shows a critical role in shaping international and national standards, and future policy directions to enhance the reliability and safe deployment of LIBs (Figure 10). With a 100% market increase in the LIB market from USD 50 billion in 2020 to an estimated USD 100 billion in 2025, the LIB technology continues to evolve into covering more environmentally sustainable goals.

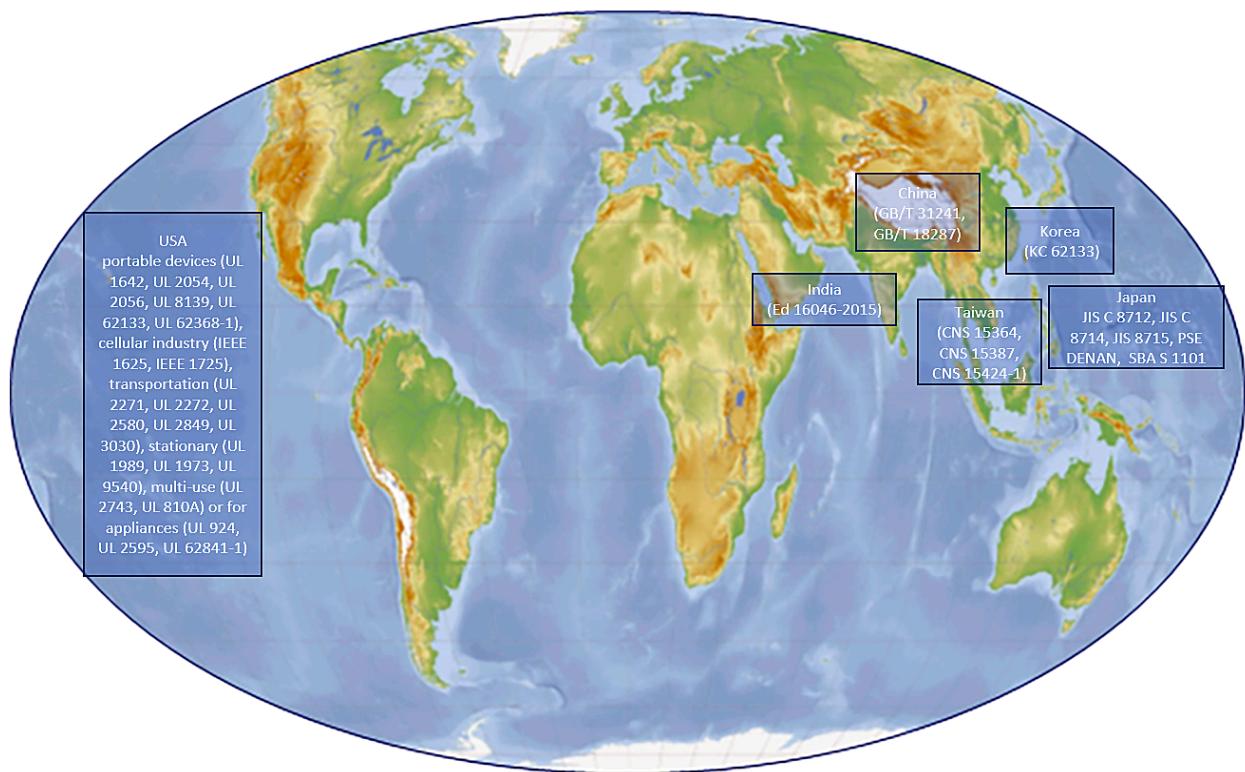


Figure 10. World map with representative safety standards in highly industrialized countries.

The regulatory framework governing LIBs is multifaceted, encompassing safety standards, environmental regulations, and guidelines for performance and reliability. Depending on the geographical region, different standards may apply; for instance, in the US, there are standards for portable devices (UL 1642, UL 2054, UL 2056, UL 8139, UL 62133, UL 62368-1 developed by UL Solutions), cellular industry (IEEE 1625, IEEE 1725 developed by IEEE Standards Association), transportation (UL 2271, UL 2272, UL 2580, UL 2849, UL 3030), stationary (UL 1989, UL 1973, UL 9540), multi-use (UL 2743, UL 810A), or for appliances (UL 924, UL 2595, UL 62841-1). In Japan, for instance, some of the common standards are JIS C 8712, JIS C 8714, JIS 8715, PSE DENAN, or SBA S 1101. Other coun-

tries may use specific standards: Taiwan (CNS 15364, CNS 15387, CNS 15424-1), China (GB/T 31241, GB/T 18287), Korea (KC 62133), or India (Ed 16046-2015). Apart from these nation-specific standards, there is also the world's first widespread IEC system, i.e., the Conformity Assessment Schemes for Electrotechnical Equipment and Components (IECEE) Certification Body (CB) scheme. Using globally accepted standards, the CB scheme relies on testing in their CB laboratories (CBTLs). With more than 50 participating countries, the CB scheme offers manufacturers a simplified way of obtaining multiple national safety certifications for their products. The CB scheme is not restricted to batteries only, and covers other appliances like cords, cables, capacitors, medical equipment, switches and so on. Among these standards, some specific tests offer compliance certification for LIBs, such as those for portable devices (IEC 62133-1, IEC 60086-1, IEC 61960, IEC 61951-1, IEC 62188, IEC 62368), for stationary use (IEC 60896, IEC 62040-1, IEC 62485, IEC 62619, IEC 62933, IEC 62660, IEC 62620, IEC 60335-2-114), multi-use (IEC 62281), and appliance use (IEC 60745-1, IEC 62841-1).

Safety regulations remain paramount in the use of LIBs, given their potential for thermal runaway, fires, and explosions. LIB integration into an end product should tackle safety and reliability by implementing software and external factor control (Figure 11).

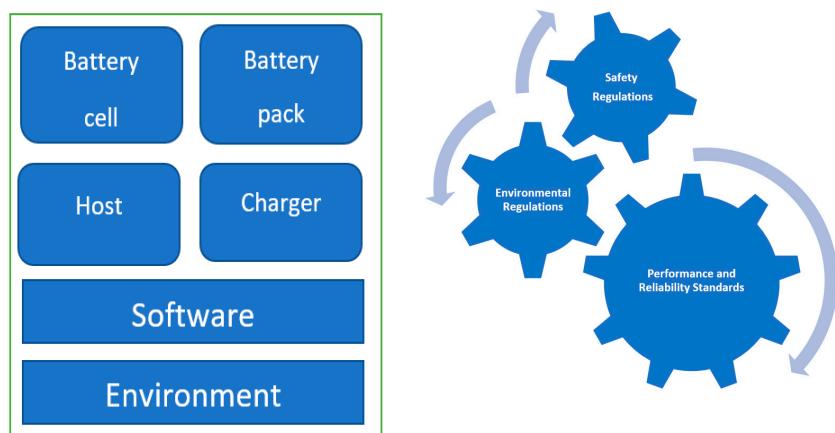


Figure 11. Main factors related to LIB integration into an end product and the two major influences on its overall performance, safety, and reliability: software control and environment/external factors.

For instance, in the period 2013–2018, more than 25,000 incidents related to LIBs have been reported in USA, making it clear that action must be taken by regulatory bodies. The widespread nature of this fire hazard should not be underestimated; incidents have also occurred during air flights where more than 250 incidents have been reported by the Federal Aviation Administration for the period 2006–2020. Moreover, due to the outburst of e-mobility devices, these incidents are even more widespread than previously reported. Regulatory bodies such as the International Electrotechnical Commission (IEC), Underwriters Laboratories (UL), and various national agencies have established safety standards to mitigate these risks.

International and national standards play a crucial role in harmonizing battery testing and ensuring consistent performance across different markets. There are several international standards organizations (the IEC, ISO, and SAE) that have been tasked with development of comprehensive standards to be widely adopted across the globe. These standards ensure that batteries meet minimum safety and performance criteria, facilitating international trade and cooperation, and national standards and regulations oftentimes complement or even add more stringent requirements based on their specific needs and regulatory environments. All possible aspects have been tackled by regulatory bodies, covering all aspects of battery manufacture, storage, transport, and international trading.

For this reason, national standards and regulations have been adopted by different countries, that may enforce additional or more stringent requirements based on their specific needs and regulatory environments. For instance, China has developed its own standards for electric vehicle batteries (GB/T 31484, GB/T 31485) that include tests for vibration, mechanical shock, and thermal management [100]. These standards are critical for the rapidly growing EV market in China. Japan's standards (JIS C 8715) focus on the safety and performance of LIBs, with specific requirements for testing methodologies and criteria for consumer electronics. Having a broad view over the whole landscape of regulatory standards throughout the globe may be overwhelming. However, some specific standards are more often encountered (Table 2).

Table 2. A brief overview of standards more often used in LIB industry.

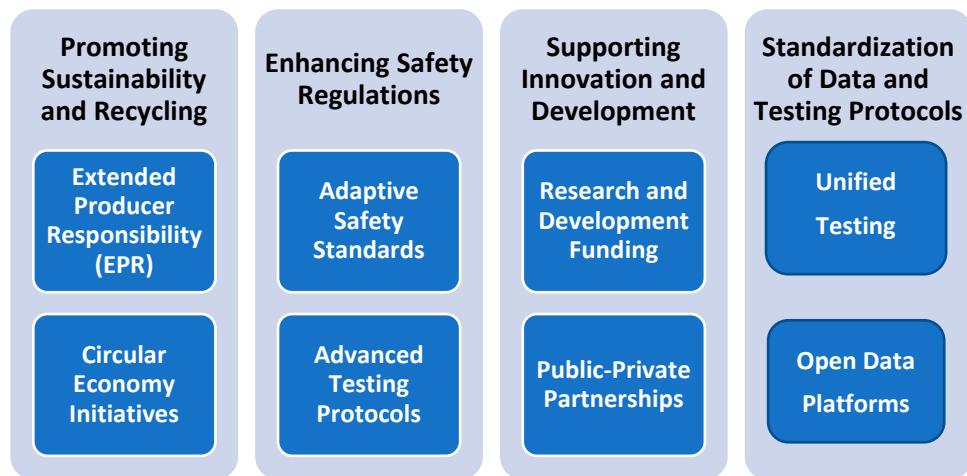
Standard	Specific Details
IEC 62133	The standard outlines safety requirements for secondary cells and batteries containing alkaline or other non-acid electrolytes. It includes tests for overcharging, external short-circuiting, and mechanical abuse to ensure battery design, performance, and safety.
IEC 62281	Regulates safety of primary and secondary cells and batteries during transport.
UL 1642	Underwriters Laboratories' standard for lithium batteries includes rigorous testing for potential hazards such as thermal runaway, mechanical shock, and exposure to extreme temperatures.
SAE J2464	The Society of Automotive Engineers (SAE) has developed standards specifically for electric vehicle batteries, addressing issues like crush, fire exposure, and overcharging.
2006/66/EC	The EU Battery Directive from 6 September 2006 aims to reduce the environmental impact of batteries by promoting the collection and recycling of battery waste. It sets targets for recycling efficiencies and restricts the use of hazardous substances in batteries.
RCRA	The US Resource Conservation and Recovery Act (RCRA) regulates the disposal of hazardous waste, including certain types of batteries, to ensure environmentally responsible handling and recycling.
IEC 61960	This standard specifies performance testing for LIBs used in portable applications, including criteria for capacity, cycle life, and energy density. The revised version IEC 61960-4:2020 specifies performance tests, designations, markings, dimensions, and other requirements for coin secondary lithium cells and batteries for portable applications and backup power supply such as memory backup applications.
ISO 12405	This series of standards outlines testing methods for electric vehicle batteries, focusing on performance, reliability, and safety under various operating conditions. The standard ISO 12405-4:2018 refers to test specifications for LIB packs and systems that propel road vehicles.
GPSD	General Product Safety Directive (GPSD) provides standards for product safety to protect consumers from potential hazards, by means of EN standards.
EN 60086-4	Safety aspects of LIBs offering a reference point for specifications and technical solutions at the product design stage.
EN 61960	Performance tests, designations, and dimensions for LIBs.

Third-party battery testing provides clear test results and documentation that could ensure compliance with all regulations related to safety standards and substance restrictions (type of elements, concentration limits). Reliance on pre-existing test reports could come with some shortcomings; those requiring and accepting these tests should only rely on renowned wholesale resellers and verifiable sources, to avoid fake batteries that may be found along the supply chain itself. Any update to a safety standard related to LIBs involves independent lab testing, which may cost several thousand dollars.

Different regulations tackle various aspects related to batteries: safety, environment, and performance being the most common ones. The environmental impact of LIBs, from production to disposal, is regulated to minimize ecological damage and promote sustainability. Performance and reliability standards ensure the long-term performance and reliability of LIBs, which is critical for their effective use in various applications.

There are several specifics to battery management in European countries. The battery directive initiative states concrete upper limit concentrations for the inclusion of toxic metals in LIBs, such as Pb (<0.0004 wt%, labelling requirement), Hg (<0.0005 wt%), or Cd (0.002 wt%). Batteries should carry a special carry symbol and should not be discarded along with regular waste. The battery capacity typically states the voltage (V) and capacity (mAh or Ah). The European Commission elaborated the General Product Safety Directive (GPSD), which, using harmonized and non-harmonized standards, regulates the safety aspects of all components in consumer products, including batteries. It is recommended to follow EN standards; however, they are not mandatory.

The rapid evolution of battery technology necessitates continuous updates to policies and regulations to address emerging challenges and opportunities (Scheme 1).



Scheme 1. Further innovation expected for LIB technology.

There are other representative LIB standards, such as those described in ADR—an EU document regulating the transport of hazardous goods over land. Batteries are classified as Class 9, receiving UN number 3480. Additional labelling is required to clarify the state in which the LIB is found; for instance, the label might read ““lithium-ion battery” when new or used LIBs are transported for reuse, “lithium-ion battery for recycling” when undamaged LIBs are transported, or “damaged/defective lithium-ion batteries” for batteries found in this latter state [101]. The ADR book regulates the battery manufacturing process and requires a quality management program, while the testing protocols are stipulated under the Manual of Tests and Criteria, Part III, sub-section 38.3 [101]. Other environmental aspects like pollutants to aquatic systems are also described within the same EU initiative, covering aspects like acute aquatic toxicity (using a fish 96 h LC50, or 50%

lethal concentration, which is the concentration of a substance in water that causes the death of 50% of a group of test animals), chronic aquatic toxicity (OECD Test Guidelines 210, Fish Early Life Stage) and bioaccumulation (according to OECD Test Guideline 107 or 117).

With ever-growing energy needs, the demand for LIBs is on the rise. As with most user electronics and devices, the LIB is bound to meet its expected end-of-life timestamp, a crucial moment when effective recycling and sustainable practices need to properly regulate LIBs components. Extended producer responsibility (EPR) policies hold manufacturers accountable for the entire lifecycle of their batteries, from production to end-of-life disposal. These policies incentivize the design of more recyclable batteries and the establishment of take-back/buy-back programs. Since the components of LIBs could soon face shortages, circular economy initiatives must be enforced by promoting a circular economy that encourages the reuse, refurbishment, and recycling of batteries, reducing waste and conserving resources. This includes support for research into second-life applications for used batteries [68], such as repurposing EV batteries for grid storage.

Considering the large number of incidents that have been traced back to LIBs, safety regulations need to be continuously enhanced. New or updated safety standards must evolve to address new risks associated with higher energy densities and new materials [70]. Developing adaptive safety standards that can be updated rapidly in response to new findings and technological advancements is crucial. These standards should incorporate the latest research on thermal management [100], material stability, and failure modes. Safety standards need to be doubled by advanced testing protocols that simulate real-world conditions to more accurately improve safety assessments, including tests for extreme temperatures, rapid cycling, and multi-cell interactions in battery packs.

Policies that foster innovation in battery technology can drive advancements in reliability and performance. Government funding for R&D in battery technology can accelerate the development of more reliable and efficient batteries. This includes support for basic research, as well as applied projects aimed at commercializing new technologies. Encouraging collaboration between industry, academia, and governments can facilitate the sharing of knowledge and resources, driving innovation. Initiatives like the U.S. Department of Energy's Innovation Center for Battery500 Consortium exemplify the benefits of such partnerships among national labs and academia for more reliable, high-performing vehicle batteries.

The lack of standardization in data collection and testing methodologies can lead to inconsistent results and hinder progress; therefore, a key aspect is standardization of data and testing protocols. Developing unified testing protocols that are accepted globally can reduce variability and improve the comparability of results. These protocols should cover all aspects of battery performance, including capacity, cycle life, safety, and environmental impact. Furthermore, establishing open data platforms where researchers and industry professionals can share performance data, failure modes, and best practices can accelerate learning and improvement. Such platforms can facilitate the development of more accurate predictive models and reliability assessments. "Voltaiq", for instance, offers enterprise cloud-based platform aggregating battery performance and quality data from across the battery lifecycle. International and national standards play a critical role in harmonizing testing and performance criteria, while future policy directions should focus on sustainability, safety, innovation, and standardization.

Ensuring and enhancing the reliability of LIBs require a multifaceted approach involving robust policies, regulations, and standards. There is a continuous need for ongoing adaptation and collaboration to keep pace with technological advancements. The regulatory

landscape must continuously evolve to address the challenges posed by new technologies and applications.

While powering diverse applications ranging from household appliances to inclusion in high energy systems harnessing renewable energy, LIBs can provide energy in a safe manner as long as the usage pattern is correct and they are stored properly. Batteries remain prone to damage when operating temperatures rise; hence, LIBs should not be exposed to extreme temperatures (direct sunlight for instance), and their charging current must be correlated to their thermal profile so that overcharging does not occur. Utilizing a proper charger could help mitigate the temperature issue, as modern chargers cut off the charge when the battery is fully charged, and this can prevent further overheating. There has been a debate over the charging of a LIB's potential and the battery health over time [67], and most authors agree that charging to 80% could be the sweet spot for prolonging the batteries' lifespan, while avoiding excessive heating and degradation processes that stem from this.

There are several risks associated with any energy storage system, and LIBs are no exception. LIBs have gained popularity due to their high energy storage capacity in a small footprint, and due to their high performance. They contain a liquid electrolyte embedding Li⁺-salts, and a solvent like ethylene carbonate, which facilitates the necessary Li⁺ mobility. The solvent itself is flammable and volatile, which increases the risk of a fire when exposed to high temperatures. During operation, LIBs also produce heat, which again adds to the potential dangers of battery failure. And if failure leads to fire, it cannot be easily contained, since the fire is self-sustaining.

The physical state of the LIB should be kept intact, as even the slightest damage sustained during dropping, for instance, can lead to problems like leakage. Moreover, if a fire occurs as a result of battery failure, LIBs are known to pose a high risk for reigniting (even after days, in some cases); therefore, large size batteries should be stored safely to prevent fire spreading to other surrounding areas. The danger of LIBs stems from the so-called thermal runaway, also known as overheating [100]. This temperature increase further leads to other chemical reactions that generate even more heat, which in turn leads to unforeseeable effects related to battery failure. Excessive heat could also be generated by some battery malfunctions, such as a shortcut. Once a fire ignites as a result of LIB failure, the fire extinguishers are difficult to use and their effect is limited: the fire itself on the battery cannot be fully extinguished until the end of the reaction using water-based fire extinguishers, while other more targeted types (lithium-ion gel types) are more expensive and less utilized as a result. To add to the injury, LIBs emit poisonous gases upon failure, and moreover, they can explode due to the excess heat generated.

Implementing battery management systems (BMSs) could allow for the collection of data regarding temperature, cell current, voltage, and charge, ensuring a proper working state in a safe manner. BMSs could also help by reducing cell temperature if temperature data deem it necessary due to excessive heating. As with other interconnected systems, BMSs could also fail, which in turn leads to failure of the LIB, and the cost involved in implementing BMSs could still be too high for smaller household appliances.

The integration of training programs and ongoing research and development outcomes could provide necessary knowledge for understanding the dangers and mitigation actions one must take in the case of LIB failure. The importance of safety protocols remains paramount for the proper utilization of LIBs. While other technologies have been on the market for decades (Ni-Cd or lead-acid) and are still used today, newer chemistries make their way into replacing LIBs; for instance, solid-state electrolyte batteries have fewer associated dangers and similar performance to LIBs; however, they are currently cost-prohibitive. Given that LIBs can hold a charge for a reasonable amount of time, offering

high-power density and also fast charging capabilities, we can expect them to dominate the market for years to come.

6. Emerging Trends and Future Directions

The rapid advancements in LIB technology have ushered in an era of unprecedented innovation and transformation. As the demand for reliable and efficient energy storage solutions grows across various sectors, the need for enhancing the reliability of LIBs becomes even more pressing [22]. Advanced characterization techniques are crucial for understanding the intricate details of battery operation and identifying factors that affect reliability, such as in situ and operando techniques, synchrotron X-ray and neutron diffraction imaging, high resolution electron microscopy (HR-TEM), or rapid 3D X-ray computer tomography powered by AI technology (detection of anode overhang, Nikon, 2023). In situ and operando techniques allow for the real-time monitoring of batteries during operation, providing insights into dynamic processes. Techniques such as in situ X-ray diffraction (XRD), in situ Raman spectroscopy, and in situ nuclear magnetic resonance (NMR) enable the observation of structural and chemical changes within the battery, offering invaluable information for studying the formation and evolution of the solid electrolyte interphase (SEI) layer, phase transitions in electrode materials, and lithium-ion transport mechanisms [26].

Neutron imaging offers a unique advantage in studying lithium distribution and dendrite formation within batteries. Unlike X-rays, neutrons are highly sensitive to light elements like lithium, providing detailed images of lithium-ion movement and accumulation, which aids in understanding the causes of lithium plating and developing strategies for mitigation [70]. High-resolution transmission electron microscopy (HRTEM) and scanning transmission electron microscopy (STEM) provide atomic-level images of electrode materials. These techniques are crucial for studying defects, particle size distribution, and structural changes at the nanoscale, revealing insights into degradation mechanisms such as particle cracking, dissolution, and agglomeration [45]. Very recently (2023), X-ray CT enabled the three-dimensional imaging of battery components, allowing for nondestructive examinations of internal structures, and predictions of anode overhauls. This technique is particularly useful for identifying mechanical defects, electrode alignment issues, and the distribution of active materials. X-ray CT can guide improvements in battery design and manufacturing processes to enhance reliability.

The development and implementation of standardized testing protocols are essential for ensuring the consistent and reliable assessment of LIBs, and include international standards, harmonized testing procedures, accelerated testing, and multi-scale testing [26,60]. Harmonizing testing procedures across different regions and industries can reduce variability and improve the comparability of test results [27,50,62,80]. Organizations such as the International Electrotechnical Commission (IEC) and the Society of Automotive Engineers (SAE) have developed standardized testing protocols for batteries, with multiple updates being released annually. These standards cover performance, safety, and environmental testing. Adherence to these standards ensures that batteries meet minimum reliability and safety requirements.

Unified protocols consider diverse operating conditions and usage scenarios. For example, harmonized cycling tests can simulate different usage patterns, from consumer electronics to EVs, providing a comprehensive assessment of battery reliability. Accelerated testing protocols aim to simulate long-term usage in a shortened timeframe. These tests expose batteries to extreme conditions, such as high temperatures, high charge/discharge rates, and mechanical stress, to induce failure mechanisms quickly. By studying the outcomes of accelerated tests, researchers can predict the long-term reliability of batteries and identify potential failure modes. The results show that thermal processes occurring

at or above 90 °C can be held responsible for solid electrolyte interphase (SEI) decomposition [61].

Multi-scale testing involves assessing battery performance and reliability at different scales, from individual cells to full battery packs [53]. This approach helps in understanding how interactions between cells, thermal management systems [100], and mechanical structures impact overall reliability. Multi-scale testing provides a holistic view of battery performance, guiding improvements in design and integration.

Innovative strategies to enhance the reliability of LIBs focus on addressing the root causes of degradation and improving overall performance; the usage of advanced materials, evolution towards solid-state batteries, electrolyte additives, and implementing advanced battery management systems (BMSs) [48] are key to bring further innovations to the field of batteries. The development of new materials with enhanced properties is a key strategy for improving battery reliability. High-capacity anode materials, such as silicon and lithium metal, are being explored to replace conventional graphite. These materials offer higher energy densities but require innovations in electrolyte composition and SEI formation to prevent degradation. Similarly, advanced cathode materials with improved stability and capacity, such as nickel-rich layered oxides and lithium-rich compounds, are being developed.

Solid-state batteries, which use solid electrolytes instead of liquid electrolytes, offer significant advantages in terms of safety and reliability [64]. Solid electrolytes are less prone to leakage and thermal runaway, enhancing the overall safety of the battery [5]. Additionally, solid-state batteries can support the use of high-capacity anode materials, further improving energy density and lifespan. The use of electrolyte additives can enhance the stability and performance of LIBs [51]. Additives such as fluorinated compounds, phosphorus-based compounds, and ionic liquids can improve SEI formation, reduce electrolyte decomposition, and enhance thermal stability. These additives help in mitigating degradation mechanisms and extending battery life.

The use and continuous sophistication and evolution towards cloud-based services [60] of advanced battery management systems (BMSs) are essential for monitoring and optimizing battery performance [58–60]. These systems use real-time data to adjust charging and discharging protocols, balance cell voltages, and manage thermal conditions [48]. Advances in artificial intelligence and machine learning enable BMSs to predict failures, optimize energy usage, and extend battery lifespan [60].

The integration of new materials and emerging technologies is essential for advancing the reliability of LIBs; these encompass the use of nanomaterials (2D and 3D materials), the use of AI, and the shift towards smart batteries [62]. Two-dimensional materials, such as graphene and transition metal dichalcogenides (TMDs), offer unique properties that can enhance battery performance [8,70]. These materials have high electrical conductivity, a large surface area, and mechanical flexibility, making them ideal for use in electrodes and interfacial layers. Incorporating 2D materials can improve charge/discharge rates, enhance mechanical stability, and mitigate degradation. Nanotechnology enables the design of electrode materials at the nanoscale, optimizing their structure and performance. Nanostructured electrodes can improve ion transport, increase the active surface area, and enhance mechanical resilience. For example, silicon nanoparticles can be used in anodes to accommodate volume changes during cycling, reducing mechanical stress and improving longevity. The shift towards Si/C batteries has been implemented even by some phone manufacturers, where capacities of 5000–6000 mAh could become the norm in the flagship territory, while providing more screen-on time (SoT) and cooler operating temperatures than conventional LIBs.

With the advent of artificial intelligence (AI) and machine learning (ML), the analysis of large datasets from battery testing and operation become much easier. These technologies can identify usage patterns, predict failures, and optimize performance. AI-driven models can simulate different operating scenarios, guiding the design of more reliable batteries, while also helping operating systems better implement the use of hardware resources for a more consistent battery performance. Additionally, ML algorithms can enhance BMSs by providing real-time insights and adaptive control strategies, with a higher degree of confidence [50].

Smart batteries incorporate sensors and communication technologies to provide real-time data on battery health and performance [26]. These batteries can communicate with external systems, enabling predictive maintenance and remote diagnostics. Smart batteries enhance reliability by allowing for proactive management and timely interventions.

The future of LIB reliability lies in the continuous advancement of materials, technologies, methodologies, testing protocols, and standard implementation strategies. Developing sustainable materials that reduce environmental impacts and improve battery performance is a key research direction. This includes exploring bio-based materials [44], recycling technologies [24,68], and environmentally benign electrolytes. Beyond lithium-ion batteries, next-generation batteries such as lithium-sulfur [35], lithium-air [18], and sodium-ion batteries hold promise for higher energy densities and improved reliability. Research into these technologies focuses on overcoming current challenges related to stability, cycle life, and safety.

The integration of batteries into smart grids, renewable energy systems, and distributed energy resources requires reliable and efficient energy storage solutions [9,52]. Advanced grid integration techniques and energy management systems will enhance the reliability and performance of these integrated systems. Collaborative efforts between academia, industry, and regulatory bodies are essential for advancing battery technology. The standardization of testing protocols, data sharing, and joint research initiatives will drive innovation and ensure the development of reliable and safe batteries [46,47].

Emerging trends and future directions in LIB reliability focus on leveraging advanced characterization techniques, standardized testing protocols, innovative materials, and cutting-edge technologies [8]. These approaches aim to address the complex challenges of battery degradation and performance, ensuring the development of reliable, safe, and efficient energy storage solutions. Exploring these trends and integrating new methodologies can pave the way for the next generation of LIBs, meeting the growing demands of various applications and contributing to a sustainable energy future.

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