

Engineering

Special Topic: Artificial Intelligence and Energy Revolution

Revolutionizing batteries based on digital twin through AI-simulation synergy for design, manufacturing, operation, and recycling

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Abstract: Optimizing lithium-ion batteries (LIBs) is pivotal for advancing sustainable energy solutions, particularly for portable electronics, electric vehicles and renewable energy storage systems. This review explores state-of-the-art strategies that integrate advanced digital simulations with comprehensive lifecycle management, assisted by artificial intelligence (AI), to overcome critical challenges in battery performance, safety, and durability. Our approach combines computational materials science with multi-scale modeling, bridging atomic-scale phenomena to system-level dynamics. This synergy provides new insights into materials behavior and electrochemical processes. Physics-based simulation techniques and AI-driven optimization technologies underpin these methods, enabling them to achieve accurate predictions and drive the design of next-generation batteries. Furthermore, the integration of cloud-based battery management systems (BMS) with edge computing facilitates real-time monitoring, predictive diagnostics, and proactive control, while the adoption of the “Battery Passport” concept enhances lifecycle traceability, promoting recycling and reuse. Collectively, these strategies establish a robust framework centered on standardization, modularization, and digitization, driving innovation across design, manufacturing, maintenance and recycling processes. This industry-academia-research collaborative battery large model has not only accelerated the industrialization of next-generation battery technologies but also provided strong support for the sustainable development of the sector. This review underscores the transformative potential of these integrated approaches, laying the groundwork for future breakthroughs in energy technologies and advancing global sustainability goals.

Keywords: artificial intelligence, digital twin, battery large model, multi-scale simulation, battery design, manufacturing, operation and recycling

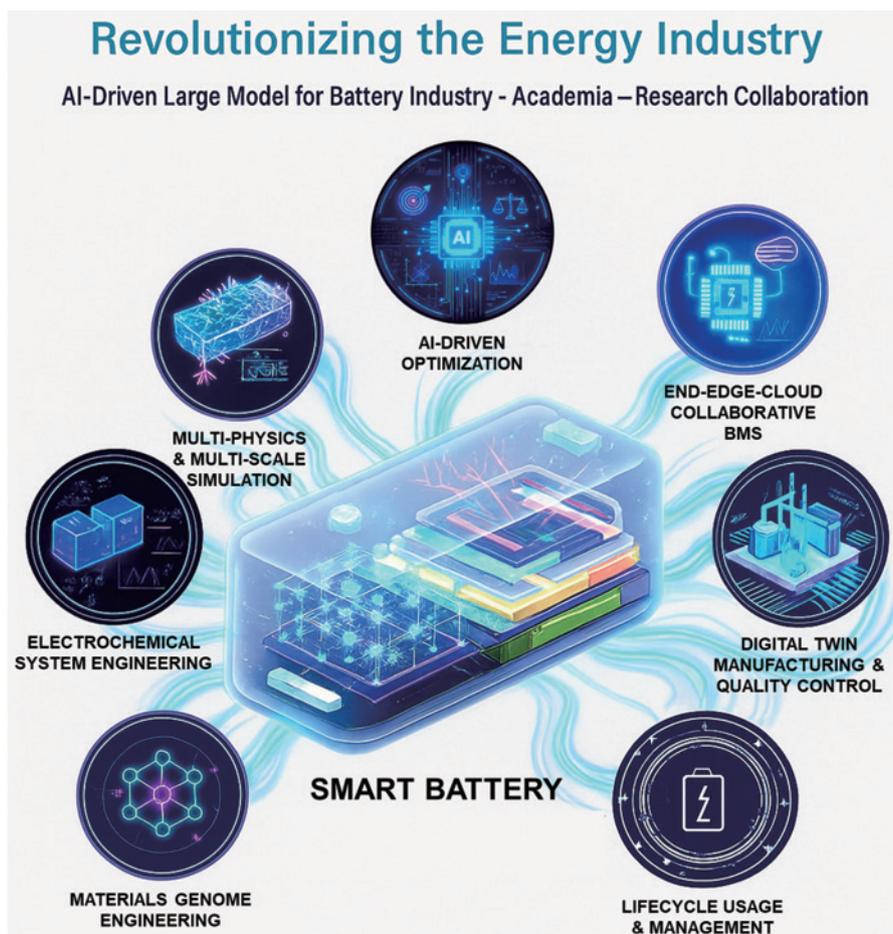
INTRODUCTION

Lithium-ion batteries (LIBs) have become vital in energy storage, powering portable electronics, electric vehicles (EVs), and large-scale energy systems. As the world increasingly prioritizes environmental protection and sustainable development, renewable energy has emerged as a key force in the energy transition. The pioneering work of John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino revolutionized energy storage and shaped modern society [1–17].

Thanks to supportive policies and rapid technological progress, global EV sales have surged—from a few thousand units in 2010 to 2.1 million in 2019. In 2024, China’s EV sales reached 12.88 million units, contributing to a global total of 18.24 million—a 24.4% increase year-over-year (data referenced from the research institution EV Tank). By 2040, global EV sales are projected to hit 54 million units annually, accounting for 58% of new car sales. Automakers plan to invest over \$300 billion in the next five years toward batteries and EV development. This rapid growth in the new energy industry is driving demand for power batteries, expected to exceed 4 TWh by 2030, with energy storage batteries surpassing 1 TWh. Increasing adoption of renewables like solar and wind further highlights the urgent need for advanced energy storage [18–21]. Energy storage systems (ESS) are becoming a critical enabler for large-scale energy storage, powering AI data centers, and driving the ongoing global energy transition. Emerging sectors in the low-altitude economy also present new opportunities and challenges for LIB technologies [22,23].

Despite their impact, LIBs face critical challenges [24–32]. Safety risks such as thermal runaway, overheating, and fire hazards persist—especially under extreme conditions or due to manufacturing defects. Performance degradation over time further limits battery longevity and reliability. Traditional trial-and-error approaches for performance improvement are inefficient and resource-intensive. Environmental and economic concerns also arise from raw material extraction, notably lithium, cobalt, and nickel, which cause significant ecological damage. At the end of life, LIBs recycling, resource recovery, and disposal remain challenging. To tackle these issues, Scheme 1 presents an AI-driven battery large model as a unified intelligence hub spanning the battery value chain. It integrates materials, electrochemical systems, battery design, manufacturing and quality control, and operational data (including lifecycle), combining multi-physics and multi-scale simulations with materials genome engineering to accelerate material discovery and predict properties efficiently. Electrochemical system engineering and digital twin manufacturing link virtual design with real-world production, while an end-edge-cloud collaborative battery management system (BMS) delivers real-time feedback and adaptive optimization across hierarchical levels. Lifecycle management closes the loop from laboratory innovation to field deployment, enabling continuous learning from operational data and fostering a sustainable and intelligent battery ecosystem.

Artificial intelligence (AI) is accelerating LIBs development [33–39], particularly in material discovery [40–42], design optimization [43], and performance prediction [44–49]. Machine learning and deep learning models analyze vast datasets to uncover complex relationships between material properties, design parameters, and electrochemical performance. This reduces reliance on time-consuming experimentation and expedites identification of high-performance materials and efficient designs. AI-driven simulations improve prediction accuracy for battery behavior under charge/discharge cycles, temperature variations, and aging. These advances enable optimization of electrodes, electrolytes, separators, and structures—yielding batteries with higher energy density, longer cycle life, and enhanced safety. Furthermore, AI enhances real-time



Scheme 1 AI-driven battery large model for battery industry-academia-research collaboration. The framework positions an AI-driven large model as a unified intelligence hub, connecting materials, electrochemical systems, battery design, manufacturing/quality control, and operation across the battery value chain. By integrating multi-physics and multi-scale simulations with materials genome engineering, it accelerates materials discovery and enables efficient property prediction. Electrochemical system engineering and digital twin manufacturing link virtual design with real-world production. An end-edge-cloud collaborative BMS provides real-time feedback and adaptive optimization, allowing battery working for the people and continuous learning from operational data. Lifecycle management closes the loop between laboratory innovation and field deployment, fostering an intelligent and sustainable battery ecosystem.

monitoring and predictive maintenance through integrated BMS, ensuring reliability from EVs to grid-scale storage.

Significant progress has been made in digitizing new energy battery research and development through strong collaboration between academia and industry. Universities drive innovation with fundamental research, while enterprises invest heavily in integrating digital intelligence into battery development, production, management, and recycling. This synergy accelerates the industrialization of advanced battery technologies and supports sustainable societal growth.

To address these multifaceted challenges and unlock LIBs potential, this review proposes an integrated framework combining digital modeling, intelligent management, and life-cycle optimization. At its core is an advanced digital tool—the “Battery Passport”—which consolidates comprehensive battery data throughout its life cycle, from manufacturing and usage history to health monitoring. By deeply integrating real-time data with multi-physics simulation models, the Battery Passport enables a closed-loop system for perfor-

mance degradation prediction, maintenance optimization, and lifespan extension. This approach systematically tackles long-standing issues in material development and safety management.

However, implementing the Battery Passport faces three major challenges. First, data standardization: heterogeneous data formats—such as manufacturing data in Excel, BMS data in JSON, and recycling data in CSV—impede cross-platform interoperability. Recent advances in AI-driven battery management have leveraged deep generative transfer learning to address data scarcity and heterogeneity in second-life LIBs [50]. Such frameworks not only facilitate reliable second-life battery deployment but also provide a foundation for standardized data reporting, secure cross-stakeholder information sharing, and integration with Battery Passport initiatives, supporting both operational decision-making and lifecycle management. Second, data privacy: the exchange of sensitive information, such as proprietary electrode formulations and vehicle operation data raises security concerns. Federated learning provides a promising route for privacy-preserving collaboration across the battery value chain. A recent study developed a federated machine-learning framework enabling the sorting of retired LIBs for direct recycling without sharing raw data, achieving 99% and 97% accuracy under homogeneous and heterogeneous conditions, respectively, through an innovative Wasserstein-distance voting strategy. This approach demonstrates how privacy-preserving AI can enhance recycling efficiency and sustainability, establishing a scalable paradigm for secure data collaboration in the circular battery economy [51]. Third, cross-stakeholder adoption: manufacturers, automakers, and recyclers often operate under misaligned incentives; for instance, manufacturers may be reluctant to disclose defect data. Policy instruments such as the EU Battery Regulation, combined with economic incentives, like enhanced recycling subsidies for Passport-compliant batteries, are likely to be decisive in accelerating widespread adoption.

Moreover, the framework fosters a paradigm shift in battery life cycle management through standardized data interfaces, modular system architectures, and intelligent algorithms. Collaborative deployment of cloud-based BMSs, edge computing, and AI-driven optimization engines creates an operation and maintenance platform with real-time responsiveness and autonomous decision-making capabilities. This platform enhances energy efficiency, cycle stability, and service life by enabling precise health assessments. Crucially, this technological advancement aligns with global goals to meet growing energy demand, protect the environment, and promote economic sustainability. By improving resource utilization efficiency and delivering substantial environmental and economic benefits, it provides strong impetus for sustainable development in the energy sector.

The remainder of this review is organized as follows. The Section “Digital simulation empowers the full-lifecycle optimization of smart batteries” presents multi-scale modeling approaches spanning atomic to pack levels and their coupling with intelligent BMSs. The Section “Innovations in battery management and maintenance practices” highlights innovations in the Battery Passport initiative and AI-enabled optimization of disassembly and material recovery. The Section “Perspective: driving the future of the battery industry through digital twin integration and AI innovation” explores the convergence of standardization, digitization, and AI, with an emphasis on strategies to enhance model generalization. The Section “AI driving comprehensive upgrades and transformative development of LIBs” explores the transformative role of AI in reshaping lithium-ion battery research and development. Finally, the Section “Future and outlook” discusses persisting challenges, prospective solutions, and the extension of the framework toward beyond-lithium chemistries.

DIGITAL SIMULATION EMPOWERS THE FULL-LIFECYCLE OPTIMIZATION OF SMART BATTERIES

As LIBs become increasingly central to energy storage and EVs applications, advanced digital simulation technologies have emerged as transformative tools for optimizing their design, manufacturing, and lifecycle management. LIBs simulation models encompass a wide range of types, including density functional theory (DFT), molecular dynamics (MD), pseudo-two-dimensional (P2D) model, equivalent circuit model (ECM), computational fluid dynamics (CFD), phase-field model, thermal-electrochemical coupling model, stress-electrochemical coupling model, mechanical model, and fatigue life analysis model, as summarized in Table 1. These models enable comprehensive analysis across scales, from atomic-level material properties to system-level performance and safety optimization. These simulations, which span from material development to end-of-life (EOL) recycling, enable significant advancements in performance, safety, and cost efficiency. By addressing challenges across the entire battery value chain, they drive innovation and sustainability in both established and emerging applications (Figure 1).

Multi-scale modeling for comprehensive optimization

Digital simulations utilize multi-scale, multi-physics modeling and AI-driven optimization to provide precise insights into the complex processes that govern LIBs performance. By bridging the gap between microscopic material behavior and macroscopic system performance, these tools create a seamless framework for designing and improving battery components. This hierarchical methodology encompasses atomic, molecular, particle, electrode, electrolyte, cell, module, and pack levels, ensuring a comprehensive understanding of the physical, chemical, and mechanical interactions within batteries.

At the atomic and molecular levels, advanced computational tools such as first principles calculations, MD, and quantum chemistry offer insights into the fundamental properties of battery materials. These techniques enable accurate predictions of thermodynamics, electronic structures, and mechanical behaviors, accelerating the discovery and design of materials with enhanced ionic conductivity, reduced charge transfer resistance, and improved interfacial stability [52–60]. Simulations of nickel-rich NMC cathodes have predicted voltage profiles while addressing oxygen evolution, thereby improving both performance and safety [61,62]. Similarly, MD simulations have elucidated the volumetric expansion mechanisms in silicon anodes during lithiation, guiding the development of nanoscale architectures and binder systems that enhance mechanical stability and extend cycle life [63,64]. Solid-state battery development also benefits from DFT studies of lithium superionic conductors such as garnet-type LLZO ($\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$), which exhibit high ionic conductivity and electrochemical stability [65–67]. Together, these methods facilitate the rapid identification of candidate materials, streamlining the development of next-generation electrodes, conductive agents, electrolytes, binders and separators, and reducing reliance on experimental trial-and-error processes.

Particle-level modeling focuses on optimizing material morphology and surface characteristics. These simulations stabilize the solid electrolyte interphase (SEI) and cathode electrolyte interphase (CEI), mitigating undesirable growth and electrode corrosion. Controlling particle size distribution and material formulations enhances electrode packing density, a critical factor for achieving higher energy density, extended cycle life, and improved safety.

Table 1 Summary of lithium battery simulation methods, including computational material science, electrochemical simulation, thermal simulation and mechanical simulation

Methods/Models	Descriptions	Applications	Software
Computational material science	<ul style="list-style-type: none"> Based on quantum mechanics, density functional theory (DFT) describes the electronic structure of materials by solving the Schrödinger equation in an approximate form. It replaces the complex many-electron wavefunction with an electron density functional, significantly reducing computational complexity. The method is parameter-free, meaning it does not rely on experimental data, and can provide fundamental insights into electronic structures, bonding interactions, energy levels, and material stability. 	<ul style="list-style-type: none"> Electronic structure analysis Interface stability Ion intercalation/Extraction 	<ul style="list-style-type: none"> VASP Quantum ESPRESSO Materials Studio PWmat
Molecular dynamics	<ul style="list-style-type: none"> Uses Newton's laws of motion to simulate the time evolution of a system of atoms or molecules. Each atom's motion is determined by interatomic forces derived from a predefined force field, which describes the potential energy as a function of atomic positions. MD allows for the study of atomic-scale dynamic processes such as diffusion, solvation, thermal stability, and mechanical deformation. Simulations can be either classical (using empirical force fields) or <i>ab initio</i> MD (where forces are calculated from quantum mechanical principles like DFT). 	<ul style="list-style-type: none"> Ion diffusion in solid/Liquid electrolytes SEI film formation and solvation effects Electrode-electrolyte interface stability 	<ul style="list-style-type: none"> LAMMPS GROMAC Materials Studio
Monte Carlo	<ul style="list-style-type: none"> A stochastic (random sampling) method based on probability theory and statistical mechanics. MC is used to explore the energy landscape and thermodynamic properties of a system by generating many random configurations and accepting or rejecting them based on an energy criterion (e.g., Metropolis algorithm). Unlike MD, MC does not simulate time-dependent processes but excels at predicting phase transitions, equilibrium states, and material stability in large-scale systems. 	<ul style="list-style-type: none"> Electrode materials phase transitions and stability Electrode particle structural evolution 	<ul style="list-style-type: none"> Gibbs LAMMPS
Calculation of phase diagrams	<ul style="list-style-type: none"> A thermodynamic modeling approach that integrates experimental data and theoretical calculations to determine the phase stability and thermodynamic properties of multi-component systems. It relies on Gibbs free energy minimization and uses empirical databases to predict phase diagrams, material compositions, and reaction equilibria. CALPHAD is widely used for designing battery materials with optimized stability and performance. 	<ul style="list-style-type: none"> Phase diagrams of battery materials Battery materials thermodynamic stability 	<ul style="list-style-type: none"> Thermo-Calc JMatPro
Phase field method	<ul style="list-style-type: none"> A continuum modeling approach that describes the evolution of phase boundaries using partial differential equations (PDEs). PFM represents different phases within a system using a continuous order parameter, which changes smoothly across interfaces. The method incorporates thermodynamic and kinetic equations (such as Cahn-Hilliard or Allen-Cahn equations) to model microstructural evolution, phase transformations, stress distributions, and interfacial dynamics. PFM is particularly useful for studying electrode microstructure evolution, mechanical degradation, and SEI layer growth in lithium batteries. 	<ul style="list-style-type: none"> Particle cracking, stress distribution Electrode microstructural changes 	<ul style="list-style-type: none"> COMSOL Multiphysics MOOSE OpenPhase

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Electrochemical simulations	Methods/Models	Descriptions	Applications	Software
	Pseudo-two-dimensional (P2D) model	<ul style="list-style-type: none"> The Pseudo-two-dimensional (P2D) model combines porous electrode theory and concentrated solution theory. It simplifies the three-dimensional lithium-ion battery system to two dimensions, mainly considering ion transport in the electrode thickness and particle radial directions. P2D describes lithium-ion movement in electrolyte pores and solid-phase diffusion within electrode particles, along with electrochemical reactions at the electrode-electrolyte interface. 	<ul style="list-style-type: none"> Electrode material screening Charge-discharge behavior simulation Low/High-temperature performance analysis SEI growth dynamics Lifetime degradation mechanism research Aging model analysis 	<ul style="list-style-type: none"> COMSOL Multiphysics Simcenter STAR-CCM+ Battery Design Studio (BDS) PyBaMM Electroder
	2D/3D porous electrode model	<ul style="list-style-type: none"> The porous electrode model is based on porous electrode theory, treating the electrode as a porous medium with solid active materials and pores. It uses equations like Nernst-Planck to describe ion transport in the liquid-phase electrolyte within pores, considering concentration gradients and electric fields. Fick's laws are applied to model solid-phase diffusion of lithium ions inside electrode particles. 	<ul style="list-style-type: none"> Electrode microstructure optimization Solid-phase diffusion limitation analysis Electrode polarization analysis 	<ul style="list-style-type: none"> COMSOL Multiphysics Simcenter STAR-CCM+ Simcenter Amesim Electroder
	Reduced-order electrochemical models	<ul style="list-style-type: none"> Reduced-order electrochemical models (ROMs) are simplified versions of high-fidelity electrochemical models (e.g., P2D model) that retain key physical mechanisms while significantly reducing computational complexity. Classic ROMs include the single particle model (SPM), which assumes electrodes are represented by a single spherical particle and ignores electrolyte concentration gradients, making it suitable for real-time state estimation and control. The extended single particle model (ESPM) enhances SPM by incorporating electrolyte dynamics, improving accuracy. Polynomial approximation models further simplify calculations by fitting lithium-ion concentration profiles with polynomials. 	<ul style="list-style-type: none"> Real-time state estimation Fault diagnosis Charge-discharge control State estimation algorithm development 	<ul style="list-style-type: none"> COMSOL Multiphysics MATLAB/Simulink GT-AutoLion Battery Design Studio (BDS) VEBsim
	Equivalent circuit models (ECMs)	<ul style="list-style-type: none"> Equivalent circuit models (ECMs) represent a battery as an electrical circuit made up of basic elements like resistors, capacitors, and voltage sources. Rooted in circuit theory, they use Kirchhoff's laws to describe the relationship between battery voltage, current, and state-of-charge. For instance, the Randles circuit, a common ECM, includes elements such as charge-transfer resistance and double-layer capacitance, which are used to fit electrochemical impedance spectroscopy data. ECMs simplify the complex electrochemical processes in a battery, enabling quick and practical analysis of battery behavior, especially in battery management systems for tasks like state-of-charge estimation. 	<ul style="list-style-type: none"> State of charge (SOC) estimation State of health (SOH) monitoring State of power (SOP) prediction Fast charging control Polarization analysis Battery life prediction 	<ul style="list-style-type: none"> MATLAB/Simulink GT-AutoLion Simcenter Amesim PyBaMM

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	Methods/Models	Descriptions	Applications	Software
Mechanical simulations	Cell structural mechanics simulations	<ul style="list-style-type: none"> Structural mechanics simulations, often using finite element methods, analyze the mechanical behavior of battery components. They apply principles like Hooke's law for elastic materials and consider factors such as stress, strain, and loading conditions. 	<ul style="list-style-type: none"> Vibration simulation Impact simulation Extrusion simulation 	<ul style="list-style-type: none"> Abaqus ANSYS Mechanical LS-DYNA RADIOSS
	Expansion force model	<ul style="list-style-type: none"> Expansion force models in the context of lithium-ion batteries aim to describe and predict the forces generated due to volume changes during battery operation. These models consider factors such as lithium-ion insertion/extraction in electrode materials, which cause expansion and contraction. They typically use principles of material mechanics and electrochemistry, taking into account parameters like electrode porosity, particle size, and the mechanical properties of materials. By quantifying expansion forces, these models help in understanding the mechanical stress on battery components, crucial for designing batteries with enhanced structural integrity and lifespan. 	<ul style="list-style-type: none"> Mechanical safety evaluation Capacity fade prediction SOC and SOH estimation 	<ul style="list-style-type: none"> COMSOL Multiphysics ANSYS Mechanical Abaqus GT-Autolion
	Pack extrusion model (multi-scale contact mechanics model)	<ul style="list-style-type: none"> The lithium-ion battery extrusion simulation model is based on continuum mechanics. It uses the finite element method to discretize the model, takes into account the non-linear characteristics of materials, contact and friction phenomena, and through the multi-physics coupling theory (such as electro-chemical-mechanical coupling), it simulates the mechanical response and performance evolution of lithium-ion batteries under extrusion. 	<ul style="list-style-type: none"> Battery pack structural integrity assessment Internal short circuit and thermal runaway prediction Safety standard compliance verification 	<ul style="list-style-type: none"> Abaqus ANSYS Mechanical LS-DYNA
	Pack vibration model (modal-fatigue coupling model)	<ul style="list-style-type: none"> The battery pack vibration model provides critical insights into the dynamic behavior of battery systems, enabling robust design and compliance with industry standards. By combining advanced simulation tools with experimental validation, engineers can ensure the reliability and durability of battery packs under real-world vibration conditions. 	<ul style="list-style-type: none"> Battery pack modal analysis Random vibration analysis Fatigue life assessment Electrical performance analysis under vibration environment 	<ul style="list-style-type: none"> Abaqus ANSYS Mechanical LS-DYNA
	Pack impact model (ball impact transient impact-damage model)	<ul style="list-style-type: none"> The lithium battery ball impact model theory aims to simulate the dynamic response and damage behavior of battery packs under high-speed impacts, such as steel ball collisions. The model is based on explicit dynamics theory, incorporating elastoplastic constitutive equations (e.g., the Johnson-Cook model) to describe material deformation characteristics under high strain rates. It predicts shell fracture and internal short-circuit risks using failure criteria (e.g., equivalent plastic strain or stress thresholds). The model typically employs the finite element method (FEM) or smoothed particle hydrodynamics (SPH) to capture key phenomena during the transient impact process, including stress wave propagation, material failure, and electrolyte leakage, providing quantitative insights for battery pack protection design. 	<ul style="list-style-type: none"> Battery pack structural integrity assessment Electrolyte leakage risk assessment Safety standard compliance verification 	<ul style="list-style-type: none"> Abaqus ANSYS Mechanical LS-DYNA

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	Methods/Models	Descriptions	Applications	Software
Thermal simulations	Bernardi heat generation model	<ul style="list-style-type: none"> The Bernardi heat generation model calculates heat generation in batteries by considering three main sources. Ohmic heating results from the resistance to current flow. Reaction heating comes from electrochemical reactions at the electrodes. Entropy-change heating is due to the entropy change associated with the reactions. By combining these components, the model provides a comprehensive way to estimate the total heat generation rate in a battery under various operating conditions, crucial for predicting thermal behavior and preventing thermal runaway. 	<ul style="list-style-type: none"> Total heat generation calculation Cell thermal runaway critical conditions 	<ul style="list-style-type: none"> COMSOL Multiphysics MATLAB/Simulink ThermoLi
	Cell thermal model	<ul style="list-style-type: none"> Battery cell thermal simulation focuses on analyzing the thermal behavior of individual battery cells during operation, including charging, discharging, and resting states. The temperature distribution within a cell significantly impacts its performance, safety, and lifespan. Key factors influencing cell temperature include internal heat generation (due to electrochemical reactions, Joule heating, and polarization) and external heat dissipation (via conduction, convection, and radiation). 	<ul style="list-style-type: none"> Fast charging strategy optimization Battery temperature distribution calculation Current overload analysis of cell connectors 	<ul style="list-style-type: none"> COMSOL Multiphysics Simcenter STAR-CCM+ GT-AutoLion ThermoLi
	CFD thermal model (pack)	<ul style="list-style-type: none"> CFD thermal simulations employ computational fluid dynamics techniques to solve the Navier-Stokes equations governing fluid flow and the energy equation for heat transfer simultaneously. By discretizing the fluid domain into a mesh, these simulations calculate the flow field of the cooling medium (air or liquid) around the battery. They also determine the temperature distribution within the battery and its surroundings. 	<ul style="list-style-type: none"> Air/liquid cooling flow field optimization Battery pack thermal balance analysis 	<ul style="list-style-type: none"> Simcenter STAR-CCM+ ANSYS Fluent Simcenter BDS Icepak ThermoLi
	Thermal runaway model	<ul style="list-style-type: none"> The lithium battery thermal runaway model theory aims to simulate the coupled thermal-electrochemical behavior of batteries under overheating conditions, providing critical insights into the initiation and propagation of thermal runaway. Thermal runaway temperature simulation captures the heat transfer within the cell and module using heat conduction equations, while gas generation models predict the release of flammable gases (e.g., electrolyte vapor) and their impact on internal pressure. 	<ul style="list-style-type: none"> Heat propagation analysis Thermal runaway temperature rise calculation Gas generation and pressure management 	<ul style="list-style-type: none"> COMSOL Multiphysics STAR-CCM+ Simcenter BDS Icepak ThermoLi
	Multi-physics coupling model	<ul style="list-style-type: none"> The lithium battery multi-physics model theory aims to comprehensively describe the coupled electrochemical, thermal, and mechanical behaviors of batteries under complex operating conditions. The electro-mechanical coupling model analyzes the volume changes in electrodes caused by lithium-ion intercalation/deintercalation (e.g., silicon anode expansion up to 300%) and the resulting stress distribution, revealing the correlation between electrode crack propagation and capacity degradation. The thermo-mechanical coupling model incorporates thermal expansion coefficients and thermal stress equations to quantify material deformation and interface delamination risks induced by temperature gradients (e.g., tensile stress in NCM cathodes at high temperatures). The electrochemical-mechanical-thermal coupling model further integrates the Butler-Volmer equation, heat generation models (e.g., Bernardi equation), and stress-diffusion equations to simulate the interactions among electrochemical reactions, heat generation, and mechanical stresses during charge/discharge processes, providing theoretical support for battery performance optimization and safety design. 	<ul style="list-style-type: none"> Operating condition adaptability assessment Research on aging mechanism Mechanical abuse simulation Thermal runaway analysis 	<ul style="list-style-type: none"> LS-DYNA COMSOL Multiphysics GT-AutoLion Simcenter BDS LIONSIMBA



Figure 1 This figure illustrates the role of digital simulations in optimizing smart battery design for efficient full-lifecycle utilization and management. The upper section maps the progression from materials, electrodes/cells, and modules/battery packs to BMS and recycling, alongside their corresponding simulation methods and real-world applications. The lower section emphasizes how multi-scale modeling and simulations drive LIBs research and optimization, spanning scales from the atomic level (10^{-10} m) to the battery pack level (10^0 m), with key research areas at each scale. The bottom portion highlights the diverse applications of LIBs in energy storage systems, consumer electronics, and low-emission vehicles, underscoring their pivotal role in the global energy transition.

Electrochemical modeling is vital for understanding charge transfer mechanisms, ion diffusion, and interface stability within LIBs. These models simulate the electrochemical processes that govern battery charging and discharging, providing a predictive framework for optimizing battery performance and longevity.

By applying the Butler-Volmer equation and diffusion models, researchers can analyze charge transfer

kinetics, exploring the relationship between overpotentials, current densities, and charge transfer rates to optimize electrode materials for faster charge/discharge cycles and improved efficiency. Additionally, modeling the formation and evolution of SEI layers at the electrode-electrolyte interface is essential for designing stable electrodes and electrolytes, reducing side reactions, and enhancing cycle life and performance. Electrochemical impedance spectroscopy (EIS) is also integrated into electrochemical models to assess internal resistance, ion diffusion, and electrochemical behavior under various operational conditions, providing insights into optimizing battery efficiency and reliability. These simulations bridge the gap between fundamental material properties and practical battery performance, enabling accurate predictions of capacity, cycle stability, and charge/discharge rates.

Physics-based modeling at the electrode and cell levels addresses critical challenges related to electrochemical performance, structural integrity, and safety [68–78]. Multi-scale modeling techniques such as phase-field modeling, Monte Carlo simulations, and finite element analysis (FEA), guide the design of gradient electrode structures with tailored porosity and stress distribution. These designs enhance ionic and electronic conductivity while mitigating stress accumulation during cycling, resulting in improved energy density and mechanical robustness.

At the cell level, advanced simulations predict key behaviors such as thermal runaway dynamics, lithium plating, and swelling forces. These models provide actionable insights for optimizing thermal management strategies and structural resilience. Modeling lithium-ion distribution within cells identifies plating-prone areas and guides the development of charging protocols and electrode surface modifications to mitigate dendrite formation, enhancing both safety and cycle life. Additionally, thermodynamic and mechanical models inform the design of electrodes and separators that accommodate volumetric changes, ensuring long-term durability under extreme cycling conditions.

As LIB systems scale up to modules and packs, multi-physics simulations play a pivotal role in addressing thermal, mechanical, and electrochemical challenges. Effective thermal management is essential for safe and reliable operation, and simulations support the design of cooling systems such as liquid cooling pathways and phase-change materials to ensure uniform temperature distribution. Predictive modeling also identifies pathways for thermal runaway propagation, enabling the incorporation of thermal barriers and advanced insulation layers that contain thermal events and improve system safety [79–83]. Beyond thermal management, mechanical durability is a crucial determinant of module-level reliability, influencing both safety and longevity in LIB systems. High-fidelity multi-physics simulations enable a comprehensive assessment of vibration, impact, and compressive forces, guiding the development of lightweight yet structurally robust pack architectures [84–88]. For EV applications, these models facilitate design optimization to withstand road-induced vibrations, accidental impacts, and crash scenarios, ensuring mechanical integrity under real-world operating conditions. By integrating predictive insights from multi-physics simulations, pack architectures can be systematically engineered to enhance structural resilience, failure resistance, and energy efficiency, thereby ensuring long-term operational reliability across diverse environments.

Intelligent BMS with digital simulation

As depicted in Figure 2, the intelligent BMS has achieved full lifecycle intelligent management of LIBs by integrating digital simulation and AI technologies, becoming a core pillar for the efficient operation of EVs

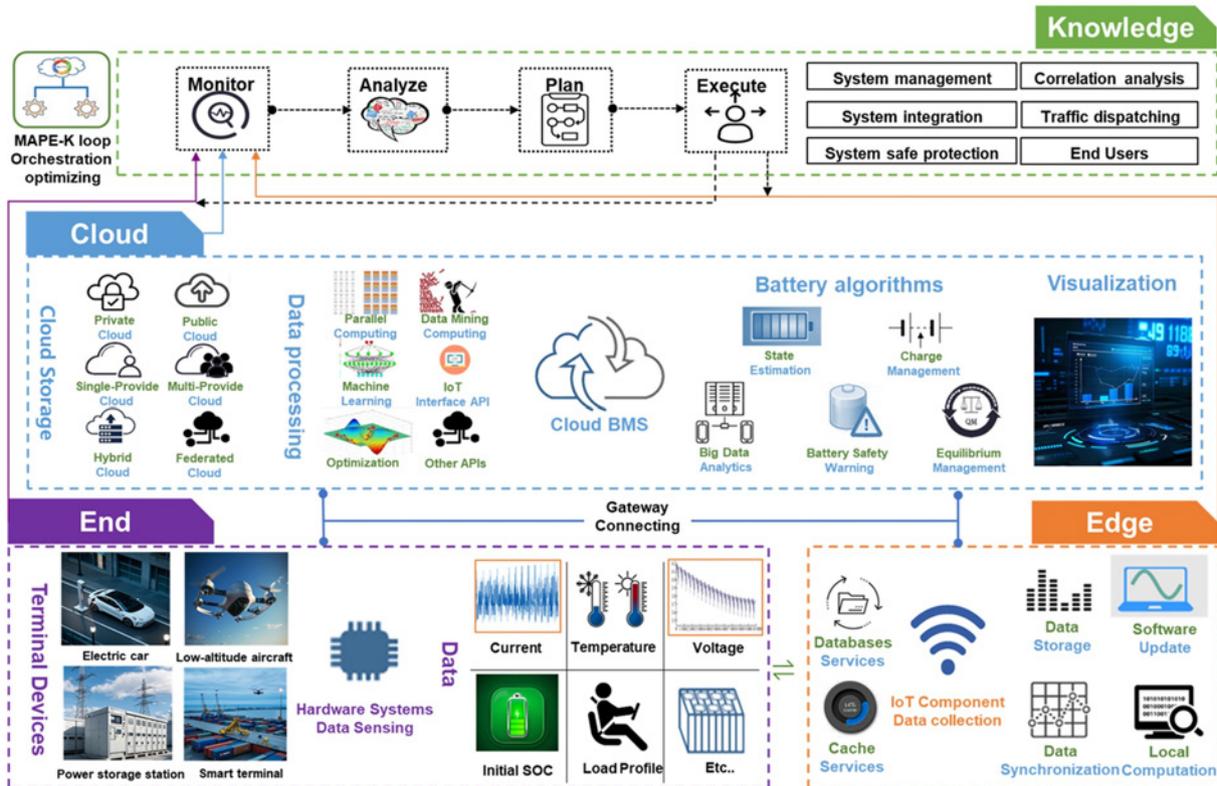


Figure 2 This figure illustrates a cloud BMS framework, which consists of four subsystems: the end layer (real-time battery data acquisition via sensors and embedded controllers), the edge layer (localized processing and anomaly detection using lightweight AI models), the cloud layer (centralized data storage, digital twins, and predictive analytics), and the knowledge layer (AI-driven optimization and adaptive decision-making). Data flows bidirectionally across layers, enabling scalable, real-time, and intelligent battery lifecycle management.

and energy storage systems [89–94]. Its core architecture combines multi-physics modeling, distributed edge computing, and cloud collaboration into a three-tier technical system: the terminal layer deploys a high-density multi-physics sensor network to collect multi-dimensional data such as voltage, temperature, and stress in real time, constructing a comprehensive operational profile of the battery; the edge computing layer, based on physics-informed neural networks (PINNs) and model predictive control (MPC), enables millisecond-level accurate estimation of state of charge (SOC) and state of health (SOH), as well as adaptive charging and discharging strategy optimization [95,96]. Simultaneously, it dynamically tracks lithium-ion transport, electrode expansion stress, and thermal runaway propagation paths through electrochemical-thermal coupling models, combined with deep learning-based degradation pattern recognition capabilities, to predict capacity fade, lithium plating risks, and internal short-circuit faults in real time, ensuring battery safety [97–99].

In the cloud, digital twin technology constructs high-fidelity electrochemical-thermal-mechanical coupling models, synchronously analyzing multi-physics behaviors within the battery. Integrated with big data analytics and AI algorithms, it forms an intelligent knowledge graph encompassing voltage characteristics, thermal distribution, and mechanical deformation [100–104]. Cloud computing platforms provide elastic computing power, leveraging federated learning to continuously optimize multi-scale models, achieving

closed-loop optimization from material design to system integration [105–107]. Through thermal field reconstruction and stress tracking, BMS dynamically balances energy efficiency and thermal stability, optimizing cooling strategies and preventing hotspot formation. Predictive maintenance algorithms enable early identification of battery degradation trends, facilitating proactive maintenance planning, significantly extending battery lifespan, and reducing operational costs.

The autonomous decision-making system based on the MAPE-K (monitor-analyze-plan-execute-knowl-edge) framework further enhances the intelligence level of BMS [108–111]. This system processes real-time data streams and employs online AI to dynamically construct feature spaces, autonomously optimizing resource allocation and task scheduling. Additionally, a central knowledge repository integrates historical operational data, fault signatures, and predictive models, supporting cross-system intelligent sharing and collaborative optimization, driving the battery ecosystem toward higher safety and adaptability.

Looking ahead, with the deep integration of 5G communication, edge computing, and AI technologies, BMS will further evolve toward intelligent and networked development. By building a collaborative computing architecture spanning terminals, edge, and cloud, BMS will achieve a leap from single-cell to battery-pack optimization and from local to global coordination, providing more efficient and safer energy management solutions for EVs, smart grids, and industrial energy storage systems. This will propel energy storage technology toward higher performance, longer lifespan, and lower costs in the future.

INNOVATIONS IN BATTERY MANAGEMENT AND MAINTENANCE PRACTICES

Battery passport: a digital framework for lifecycle management

The rapid evolution of LIB technologies has accelerated advancements in battery management and maintenance practices. The battery passport provides comprehensive traceability for LIBs throughout their lifecycle [112–118]. By consolidating manufacturing and operation data, it enhances operational efficiency, ensures safety compliance, and promotes sustainable recycling and reuse.

The passport records key manufacturing details such as material composition, electrode formulations, and assembly processes, alongside operational data like performance metrics, charging cycles, and temperature profiles. These data enable real-time monitoring, identifying potential risks and supporting maintenance decisions. Advanced encryption methods protect sensitive data, ensuring integrity and confidentiality.

Through continuous tracking of usage data, the battery passport enables precise assessment of remaining capacity, degradation patterns, and energy efficiency. These data also support EOL management and recycling, contributing to a circular economy in battery manufacturing. The implementation of the battery passport requires integrating real-time data acquisition with AI algorithms to predict degradation, thermal risks, and safety thresholds.

The integration of simulation technology and the battery digital passport (DP) creates a comprehensive decision-making system for battery lifecycle management. During the design phase, multi-scale modeling and simulations enable precise decoupling of material-structure-performance relationships. Multiphysics-coupled FEA, integrated with phase-field theory, simulates lattice strain and stress during lithiation/delithiation. High-fidelity CFD models, combined with electrochemical-thermal algorithms, predict thermal distribution under high-rate charge/discharge conditions. Simulation data are integrated into the battery DP,

forming a dynamic digital twin that tracks mechanical integrity, thermal safety, and other key performance metrics.

In the operational phase, a monitoring system based on the DP and real-time simulation forms a feedback loop. By integrating multi-source data (voltage, temperature, SOC, etc.) from the BMS and using Kalman filtering, a digital twin model of battery SOH is constructed. This enables early warnings for potential hazards such as lithium plating or thermal runaway. The system also dynamically optimizes charging parameters (e.g., current/voltage switching point) through real-time simulations, improving lithium-ion diffusion and deposition kinetics. This suppresses dendrite growth and enhances battery life by 18%–25%, while reducing thermal runaway risks to 10^{-6} .

Sustainable EOL management: optimizing LIBs recycling

EOL management is critical for LIB technology, driven by the urgent need for resource efficiency and environmental sustainability [119–124]. Advanced digital simulations are transforming the recycling value chain, from automated disassembly and selective material recovery to secondary applications, closed-loop system optimization, and second-life utilization, accelerating the transition to a circular battery ecosystem [125–128].

In the disassembly phase, physics-based simulations inform the design of robotic systems for efficient material separation, minimizing component damage [126,127]. Digital twin technology enables the virtual prototyping of disassembly sequences, balancing throughput, cost, and material recovery rates.

Material recovery is optimized through multiscale simulations that bridge atomic-scale reaction dynamics with macroscopic process engineering. Hydrometallurgical and pyrometallurgical models refine solvent selection and metal extraction processes, while electrochemical degradation simulations guide targeted material regeneration strategies. These high-fidelity models enable performance-tiered material reuse, facilitating the reintroduction of refurbished components into applications ranging from EV batteries to stationary energy storage systems [112,127]. Second-life applications for degraded batteries are crucial for reducing environmental impact. Refurbished batteries can be utilized in low-power demand applications such as home energy storage, commercial storage, and grid stabilization, which extend the battery's lifespan and reduce resource wastage.

Integrated life-cycle simulation platforms dynamically balance environmental impact, economic feasibility, and process efficiency, optimizing recycling pathways and energy consumption. Emerging computational paradigms, including AI-driven process optimization and MD-based electrolyte recovery modeling, are unlocking new opportunities in second-life battery applications, fostering adaptive, self-optimizing recycling systems. Accurate modeling of battery degradation enables the prediction of residual battery life at different stages of their lifecycle, facilitating optimal second-life utilization strategies.

By integrating advanced simulation frameworks, sustainable EOL management can be systematically enhanced, supporting the LIBs industry's shift toward a fully circular economy while ensuring long-term resource security, environmental compliance, and the growth of a second-life battery market. Second-life utilization not only promotes efficient battery reuse but also provides a new economic growth avenue for the battery industry, contributing to the long-term sustainable development of green energy.

PERSPECTIVE: DRIVING THE FUTURE OF THE BATTERY INDUSTRY THROUGH DIGITAL TWIN INTEGRATION AND AI INNOVATION

The battery industry is undergoing a significant transformation, driven by the convergence of standardization, digitization, modularization, intelligence, networking, and visualization. These principles are revolutionizing the design, manufacturing, and operational phases of battery systems, facilitating improvements in efficiency, sustainability, and innovation across the entire lifecycle. This paradigm shift is crucial for advancing global electrification and renewable energy solutions, as illustrated in Figure 3. It lays the groundwork for the integration of intelligent, data-driven approaches, underpinned by digital twin technologies and large-scale AI models.

Standardization serves as the foundational pillar of this transformation by ensuring consistency and reliability across the production process. By establishing standardized protocols for material selection, cell architecture, and manufacturing techniques, the industry reduces variability, enhances quality control, and enables scalable production. Additionally, standardized testing protocols ensure safety, performance, and compliance with regulations, which strengthens consumer trust. This standardization also facilitates the seamless integration of digital twin models, enabling real-time monitoring and simulation throughout the manufacturing process, ensuring data consistency and enhancing decision-making.

Digitization is revolutionizing the industry by incorporating digital technologies such as the internet of things (IoT), big data analysis, and cloud computing into the battery lifecycle. Notably, digital twin technology creates virtual replicas of battery systems that simulate diverse operational conditions. This enables designers to optimize parameters and refine system designs prior to constructing physical prototypes, thereby reducing development time and costs while minimizing inefficiencies. In addition, real-time performance monitoring, powered by embedded sensors and advanced algorithms, allows for predictive maintenance, optimizing battery lifespan and operational efficiency through proactive, data-driven strategies.

Intellectualization has brought profound innovations to battery technology. The application of AI algorithms enables precise optimization of battery design and performance by analyzing large datasets, including adjustments to material formulations and performance predictions under various conditions. AI models can identify degradation patterns and potential failure mechanisms, providing strategies to extend battery life. In the manufacturing process, intellectualized quality control systems can detect defects in real time, improving production efficiency and reducing waste. These systems are further enhanced through large pre-trained models, enabling efficient decision-making and playing a key role within the digital twin framework.

Modularization is facilitating the scalability and adaptability of battery systems. By segmenting battery systems into standardized modules, manufacturers can customize and scale solutions rapidly without disrupting the entire system. This modular approach significantly reduces downtime, lowers maintenance costs, and supports fast-paced technological advancements. Moreover, IoT-enabled batteries are creating interconnected systems that provide continuous performance data, enabling real-time health monitoring. For example, in EV fleets, this data-driven approach optimizes charging schedules, reduces operational costs, and extends the lifespan of battery systems through predictive maintenance.

This integrated framework is bolstered by AI-powered technology platforms and comprehensive databases. Materials databases aggregate data from simulations, mechanical property evaluations, and material research, offering a solid foundation for innovation in material science. Cell databases catalog design speci-

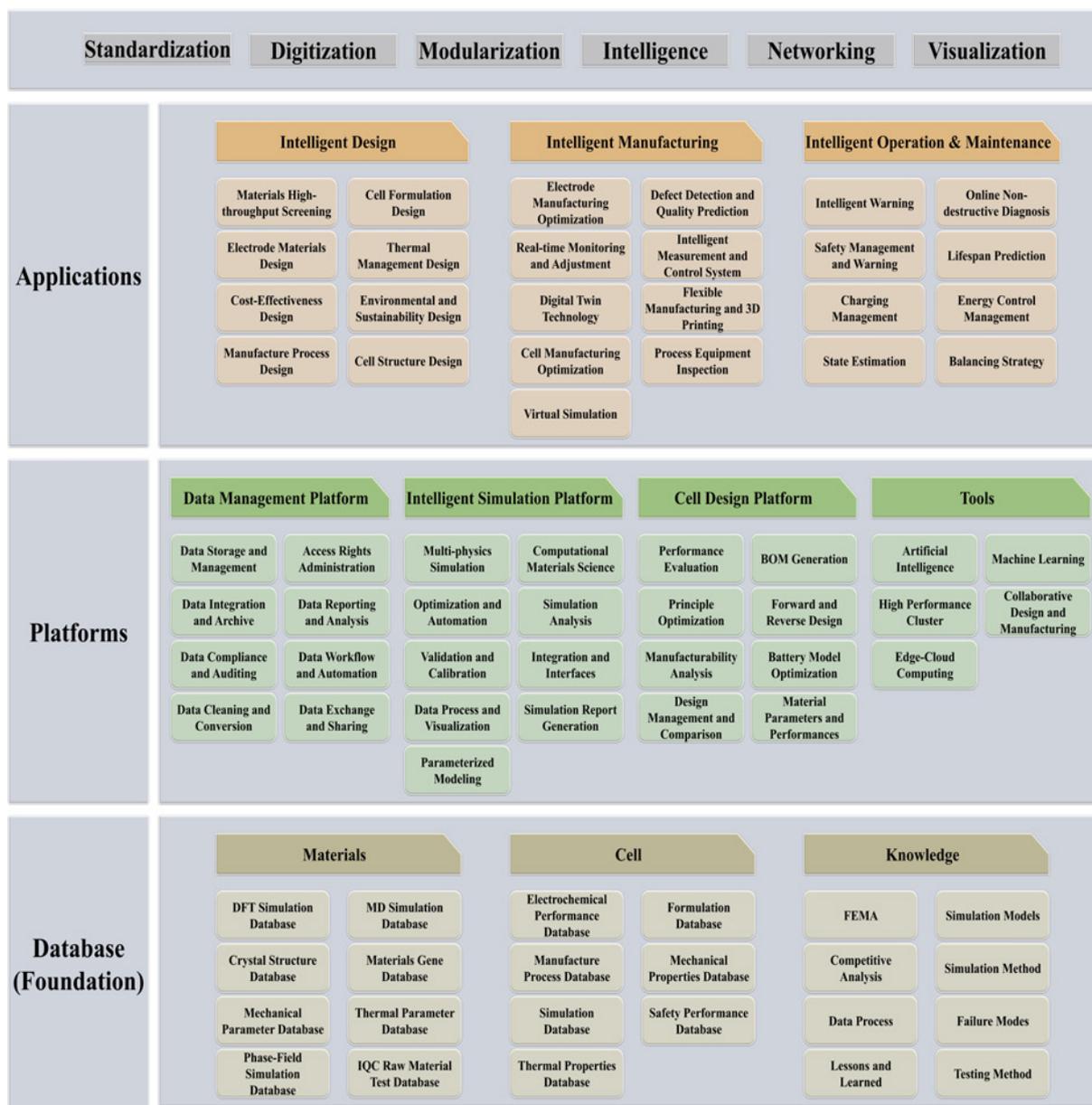


Figure 3 This figure illustrates the system architecture for intelligent lithium battery design, manufacturing, and lifecycle management, structured across three layers: database, platform, and application. It emphasizes six core dimensions—standardization, digitization, modularization, intellectualization, networking, and visualization—which drive innovation and efficiency across the battery ecosystem. The database layer integrates materials and cell-related databases with knowledge modules such as simulation databases and failure modes and effects analysis (FMEA), enabling data-driven insights. The platform layer provides essential tools for data management, intelligent simulation, and cell design, supporting model-driven optimization. The application layer encompasses intelligent design, advanced manufacturing, predictive maintenance, and operational optimization, ensuring seamless integration from development to end-of-life strategies.

fications and performance data to aid in optimizing existing technologies and developing new ones. Knowledge repositories compile research findings to support ongoing improvements. Technology platforms, including advanced simulation and design optimization tools, facilitate the seamless implementation of AI-driven solutions across the battery lifecycle, ensuring efficiency and consistency from design to EOL

management.

In contrast to previous reviews that have examined AI-enabled BMS or digital-twin technologies in isolation [45,118,129–131], this Perspective presents a unified, closed-loop framework that integrates these paradigms across the entire battery value chain—from atomic-scale materials discovery and intelligent manufacturing to operation and EOL recycling. Rather than classifying AI applications by function (for example, prediction, control, or diagnostics), our approach highlights the synergistic coupling of data-driven and physics-based modeling within a multi-scale digital-twin architecture. Specifically, we propose a feedback-driven system that links PINNs, generative design models, and reinforcement learning (RL) with real-time sensor data and multi-physics simulations, enabling adaptive learning, continuous model updating, and cross-domain knowledge transfer throughout the full battery lifecycle.

Distinct from earlier efforts that focused primarily on data-driven performance prediction (such as SOC/SOH estimation [45]) or standalone digital-twin implementations in manufacturing [129], our framework establishes a closed-loop optimization system that unifies materials science, manufacturing intelligence, and system-level operation within a single data-centric architecture. A central feature of this framework is the Battery Passport, conceived as a unifying digital thread that connects fragmented lifecycle data—including manufacturing parameters, operational metrics, and recycling information—to enable transparent data exchange, traceability, and sustainability assessment across stakeholders. By explicitly combining physics-based simulations (for example, DFT and phase-field modeling) with advanced AI methodologies (such as PINNs and transfer learning), the framework addresses the limited generalizability of purely data-driven models and enhances interpretability and physical consistency. Beyond operational management, this Perspective further broadens the scope to encompass materials design, intelligent manufacturing, and lifecycle sustainability—dimensions that remain underexplored in existing literature. Collectively, the proposed AI-digital twin-multiscale framework provides both conceptual and methodological advances, establishing a cognitive, self-evolving digital ecosystem for the next generation of intelligent battery systems.

By leveraging AI-driven pre-trained models, multi-modal analytics, and intelligent applications, the battery industry is entering a new era of intelligent, high-efficiency, and sustainable development. These large models are essential to the entire digital twin ecosystem, enabling optimized simulations, system-wide analyses, and predictive capabilities. From materials discovery to intelligent manufacturing and lifecycle management, AI is redefining industry standards, fostering innovation, and driving the long-term success of battery technologies. This digital and intelligent approach is crucial to maintaining competitive advantages in the rapidly evolving global market while supporting the transition to electrification and renewable energy solutions. Overall, this Perspective articulates a forward-looking roadmap in which AI and digital-twin technologies converge within a closed-loop, self-evolving system—driving continuous enhancements in performance, reliability, and sustainability of next-generation battery technologies.

AI DRIVING COMPREHENSIVE UPGRADES AND TRANSFORMATIVE DEVELOPMENT OF LIBS

The integration of AI across industries has sparked unprecedented innovation, and nowhere is this more evident than in the development of LIBs. AI is fundamentally transforming LIBs technology by accelerating

Table 2 State-of-the-art AI algorithms applied in lithium ion batteries

Application area	Descriptions	Relevant algorithms
Material screening	<ul style="list-style-type: none"> Identifying materials with high energy density and excellent cycle life by analyzing material properties and electrochemical performance 	<ul style="list-style-type: none"> CNNs, SVMs, random forests, GNNs
Performance prediction	<ul style="list-style-type: none"> Predicting battery characteristics such as capacity retention, cycle life, charging/discharging efficiency, and aging behavior 	<ul style="list-style-type: none"> LSTMs, RNNs, Bayesian network, DQNs, linear regression
Defect detection	<ul style="list-style-type: none"> Detecting defects in lithium batteries during production and usage, such as internal delamination, cracks, and thermal runaway risks 	<ul style="list-style-type: none"> CNNs, GANs, K-means
Optimization design	<ul style="list-style-type: none"> Enhancing battery performance by optimizing anode and cathode materials, electrolyte composition, and structural design 	<ul style="list-style-type: none"> GA, Bayesian network, random Forests, GNNs, PINNs
Data analysis & classification	<ul style="list-style-type: none"> Performing pattern recognition, classification, and clustering of experimental data to support performance consistency analysis and anomaly detection 	<ul style="list-style-type: none"> K-NNs, K-means

advancements in material discovery [132–135], design optimization [133,134,136], and performance prediction [137,136,138–140], thereby enhancing efficiency and reducing development timelines.

AI-driven approaches profoundly impact multiple stages of LIBs development. Cutting-edge algorithms, as summarized in Table 2, including convolutional neural networks (CNNs), recurrent neural networks (RNNs), and long short-term memory (LSTM) networks, are extensively applied to LIBs research. Table 3 further provides detailed insights into the specific applications, descriptions, advantages, and limitations of these advanced AI techniques. CNNs excel at analyzing microstructural images, enabling the detection of defects and anomalies that may otherwise go unnoticed. RNNs and LSTMs, with their ability to process time-series data, capture degradation trends and performance fluctuations over multiple charge-discharge cycles. RL and deep Q-networks (DQNs) optimize battery management by adjusting operational parameters to maximize efficiency and prolong lifespan. Additionally, support vector machines (SVMs) and transformer-based models enhance predictive modeling, enabling more accurate estimations of battery state under a variety of operating conditions.

A particularly promising AI approach gaining traction in LIBs research is PINNs [141]. PINNs combine the strengths of AI with fundamental physical laws, such as the conservation of mass, momentum, and energy. By directly incorporating these governing equations into the AI training process, PINNs improve the accuracy and generalization of predictions, particularly in systems governed by complex physics like the electrochemical processes in LIBs. This integration ensures that AI models respect core physical principles, which is invaluable for optimizing battery performance and reducing reliance on experimental data alone.

In material discovery, AI methods such as graph neural networks (GNNs) and transformer architectures are revolutionizing the identification of new materials. These deep learning models predict key material properties, such as ionic conductivity, lithium-ion diffusion barriers, and interfacial stability, with near DFT accuracy, but at substantially reduced computational costs. Combined with Bayesian optimization and active learning strategies, AI has accelerated the screening of high-potential materials, such as novel electrolyte additives with enhanced thermal stability and ionic conductivity. This integration of AI with first-principles

Table 3 The specific allocation, descriptions, advantages, and limitations of AI algorithms in the research and development of lithium ion batteries

AI algorithms	Specific applications	Descriptions	Advantages	Limitations
Linear regression	<ul style="list-style-type: none"> Battery performance prediction 	<ul style="list-style-type: none"> Linear regression is a fundamental statistical and machine learning algorithm used to model the relationship between a dependent variable (battery performance metrics) and one or more independent variables (such as charge/discharge cycles, temperature, and current density). 	<ul style="list-style-type: none"> Simple, interpretable, and effective for identifying key trends. 	<ul style="list-style-type: none"> Assumes linear relationships; limited for complex, non-linear behaviors.
Convolutional neural networks (CNNs)	<ul style="list-style-type: none"> Image analysis and defect detection 	<ul style="list-style-type: none"> Convolutional Neural Networks (CNNs) are a class of deep learning models specifically designed for analyzing image data. They excel in detecting patterns, textures, and structural anomalies, making them highly effective for battery defect detection using imaging techniques like Computed Tomography (CT), Scanning Electron Microscopy (SEM), and X-ray imaging. 	<ul style="list-style-type: none"> Excels in image-based tasks; automated defect detection. 	<ul style="list-style-type: none"> Requires large datasets and high computational power.
Recurrent neural networks (RNNs)	<ul style="list-style-type: none"> Battery behavior prediction 	<ul style="list-style-type: none"> Recurrent Neural Networks (RNNs) are a type of neural network designed for processing sequential data. They are particularly well-suited for predicting the dynamic behavior of lithium-ion batteries over time, such as charge/discharge cycles, state of charge (SOC), state of health (SOH), and long-term degradation. RNNs have the ability to maintain a "memory" of previous inputs, making them effective at modeling time-dependent battery behavior, which is crucial for battery lifecycle prediction and performance tracking. 	<ul style="list-style-type: none"> Captures temporal dependencies in sequential data. 	<ul style="list-style-type: none"> Suffers from vanishing gradients in long sequences; resource-intensive.
Long short-term memorys (LSTMs)	<ul style="list-style-type: none"> Long-term behavior prediction 	<ul style="list-style-type: none"> Long short-term memory (LSTM) is a specialized form of recurrent neural networks (RNNs) designed to solve the issues of learning long-term dependencies in sequential data. LSTMs are particularly effective for tasks that require modeling long-term behavior over extended periods, such as battery lifecycle prediction, and for capturing voltage/current dynamics under varying operating conditions. 	<ul style="list-style-type: none"> Solves vanishing gradient issues; ideal for long-term analysis. 	<ul style="list-style-type: none"> Computationally demanding; complex to tune.
Deep Q-networks (DQNs)	<ul style="list-style-type: none"> Charging strategy optimization 	<ul style="list-style-type: none"> Deep Q-network (DQN) is a reinforcement learning (RL) algorithm that combines Q-learning (a value-based RL method) with deep neural networks to optimize decision-making in complex environments. In the context of battery charging strategy optimization, DQN is used to determine the most efficient charging protocols that maximize battery lifespan, improve charging speed, and optimize performance under various conditions. 	<ul style="list-style-type: none"> Real-time decision-making; handles complex, high-dimensional data. 	<ul style="list-style-type: none"> Requires extensive training data; sensitive to hyperparameters.
Support vector machines (SVMs)	<ul style="list-style-type: none"> Classification and prediction 	<ul style="list-style-type: none"> Support vector machine (SVM) is a supervised machine learning algorithm widely used for classification and regression tasks. In the context of battery performance classification and prediction, SVM is leveraged to classify various operational states of a battery (such as healthy, degraded, or faulty) and predict critical metrics like cycle life, capacity retention, and state of charge (SOC) based on high-dimensional data. 	<ul style="list-style-type: none"> Handles non-linear and small datasets effectively. 	<ul style="list-style-type: none"> Computationally expensive for large datasets; kernel selection is critical.
Physics-informed neural networks (PINNs)	<ul style="list-style-type: none"> Optimization of battery design 	<ul style="list-style-type: none"> PINNs are neural networks that integrate physical laws, typically in the form of partial differential equations (PDEs), into the learning process. This allows the network to respect known physics while learning from data, ensuring that predictions align with fundamental physical principles. 	<ul style="list-style-type: none"> Physically grounded prediction, reduction data requirements and higher accuracy in complex systems. 	<ul style="list-style-type: none"> High computational cost, complexity in model formulation and difficulty in incorporating relevant physical laws.

calculations and high-throughput screening technologies is transforming material discovery, enabling a shift toward autonomous research workflows and significantly shortening innovation cycles.

AI is also reshaping battery design optimization. Through RL and multi-objective optimization algorithms, AI enables the rapid exploration of complex design parameters, balancing key factors such as energy density, safety, lifespan, and cost. PINNs bridge machine learning with electrochemical principles to simulate battery behavior under varying configurations, yielding faster and more accurate insights into design performance. Generative models, including generative adversarial networks (GANs) and variational autoencoders (VAEs), generate optimized electrode architectures and composite material structures, delivering superior electrochemical properties. These AI-driven strategies reduce reliance on trial-and-error experimentation, accelerating prototyping and refining battery design processes.

Predicting battery performance and degradation across a range of operating conditions is another area where AI excels. Hybrid models that integrate CNNs with physics-based degradation models offer enhanced defect detection and enable real-time reliability assessments throughout the manufacturing and operational phases. RNNs and LSTMs process extensive time-series data to provide accurate predictions of cycle life, capacity retention, and failure modes. Additionally, transfer learning techniques leverage data from established chemistries to expedite the commercialization of emerging battery formulations, reducing the need for extensive new datasets. AI-driven digital twin frameworks further enhance real-world applicability by continuously refining predictive models through real-time feedback from embedded sensors, optimizing BMS, and enabling proactive interventions to extend battery lifespan.

Recent studies illustrate the transformative power of AI in practical battery research [142–147]. For instance, combining AI with AIMD simulations has enabled in-depth exploration of interfacial reactions, providing molecular-level insights that guide electrode-electrolyte design [142]. Generative AI-driven molecular design has facilitated the efficient discovery of novel electrolytes with enhanced oxidative stability, reducing experimental screening efforts by over 60% [144]. Hybrid models integrating deep learning and DFT have accelerated materials discovery pipelines by more than 70%, demonstrating measurable efficiency gains and improved interpretability [145].

In addition, SES's Xu Kang team has developed an AI-driven “molecular universe” platform for designing lithium-ion battery electrolytes and optimizing their formulations, achieving targeted performance improvements in conductivity and electrochemical stability. Similarly, the Materialize AI initiative led by Shyue Ping Ong is building an interdisciplinary framework that leverages theory, experiments, and AI to accelerate the discovery of breakthrough materials across next-generation batteries, aerospace alloys, and semiconductors, highlighting the flexibility and scalability of AI-enabled materials innovation.

These examples collectively underscore how AI-simulation integration provides quantifiable performance gains, reduces trial-and-error in experimentation, and enhances interpretability across multiple stages of battery R&D.

To enhance robustness and generalization of AI models across chemistries and operating conditions, recent work has emphasized a three-pronged strategy—transfer learning, physics-informed approaches, and task/domain adaptation (including few-shot/multi-task learning and survival-analysis frameworks)—and these strategies are naturally integrated into digital-twin architectures to improve resilience under varying temperature, current and cycling regimes. Transfer learning allows models pretrained on abundant data from one chemistry or operating regime to be efficiently adapted to another with minimal new data. Recent studies

have further explored explainable transfer-learning frameworks for battery lifetime and SOH prediction, showing significant improvements in cross-domain performance and interpretability [148,149]. PINNs integrate electrochemical laws and degradation physics into the learning process, enabling stable modeling of battery degradation trajectories and reliable transfer across chemistries and operating conditions. Notably, recent frameworks have demonstrated robust SOH estimation and strong performance under limited data and cross-domain scenarios [150,151]. Complementary algorithmic strategies—few-shot and multi-task learning, domain adaptation, and survival-analysis hybrids—improve prediction across operating conditions (different temperatures and C-rates) and enable second-life/remaining-value assessments for retired cells; recent work on few-shot LSTMs adaptation and hybrid survival-analysis/machine-learning pipelines illustrates how these methods can predict capacity trajectories or time-to-failure with high fidelity even when target data are sparse [152].

Integrated into a digital-twin, these methods form a practical workflow: pretrained models (or physics-constrained priors) are embedded in the twin's simulation/estimation modules, few-shot fine-tuning is performed at deployment with minimal new measurements, and survival- or RUL-oriented modules drive second-life decisioning and recycling prioritization. This combined strategy mitigates failure modes arising from domain shift, reduces required retraining effort, and improves interpretability and uncertainty quantification—key requirements for industrial adoption and regulatory acceptance.

Looking to the future, AI is poised to continue driving transformative changes in LIBs research. The development of specialized knowledge repositories, coupled with the integration of vast experimental datasets and industry insights, will provide AI algorithms with richer learning resources, further accelerating material discovery and design optimization. Expert systems will translate industry expertise into AI-understandable rules, enabling more scientifically informed decision-making in battery research. The emergence of autonomous material agents, which use AI to search and filter material databases, will further accelerate the discovery and optimization of new materials, ultimately driving the next wave of innovation in LIB technology.

FUTURE AND OUTLOOK

New industrial paradigm: AI-driven transformation of the LIBs industry

The integration of AI is fundamentally reshaping the LIBs industry, enabling data-driven decisions, automation, and lifecycle optimization. AI algorithms are increasingly applied from electrode formulation and material selection to electrochemical performance prediction. ML models identify degradation pathways and failure mechanisms, informing strategies for enhanced longevity. AI-powered quality control systems further improve manufacturing efficiency through real-time defect detection, minimizing waste and optimizing production yield. This AI-driven framework, as illustrated in Figure 4, revolutionizes lithium battery development, paving the way for data-driven innovation, autonomous optimization, and intelligent manufacturing.

This transformation unfolds across three key dimensions. First, AI-driven knowledge graphs unify materials science, electrochemistry, manufacturing, and diagnostic data, improving predictive accuracy and process optimization. Second, multi-modal AI models integrate diverse data sources—text, images, videos,

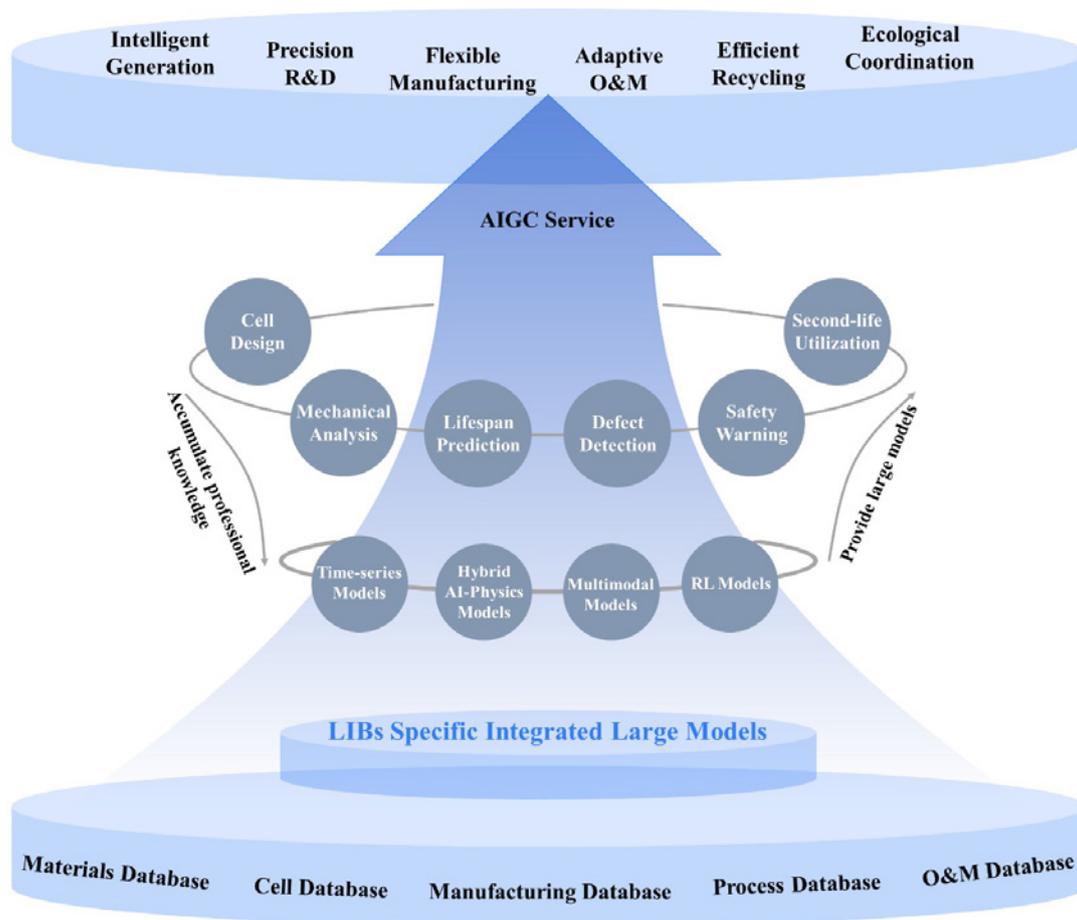


Figure 4 A new AI-driven paradigm for LIBs' innovation. We propose an industry-level pretrained AI model tailored for lithium-ion batteries, battery large model, driving intelligent upgrades across research and development (R&D), manufacturing, and lifecycle management. Foundation layer: integrates material, cell, manufacturing, process and operation and maintenance (O&M) databases, constructing a comprehensive industry-specific knowledge graph. Intermediate layer: employs time-series models, hybrid AI-physics models, multimodal AI models (text, images, etc.) and reinforcement learning (RL) models to enhance cell design, lifespan prediction, and process optimization. Application layer: leverages AI-generated content (AIGC) to autonomously generate design solutions, predict battery performance, and detect defects, enabling full-lifecycle optimization. This AI-driven framework transforms lithium battery development, paving the way for data-driven innovation, autonomous optimization, and intelligent manufacturing.

and sensor signals—into specialized frameworks for cell design, mechanistic simulations, lifespan forecasting, and fault diagnostics. Third, AI-generated content (AIGC) automates tasks such as design optimization, performance forecasting, defect analysis, and EOL resource management, contributing to full lifecycle efficiency.

These AI-driven innovations have catalyzed six key advancements: accelerated material discovery and optimized cell architectures for improved thermal management; high-fidelity multi-physics simulations and zero-shot lifespan predictions, reducing reliance on costly experiments; real-time process optimization via AI and edge computing, enhancing yield and adaptive manufacturing; digital twin models for predictive maintenance and battery health diagnostics, improving reliability; AI-powered recycling strategies, optimizing resource recovery and circular economy practices; cross-domain AI integration, fostering standardization, open-source development, and collaborative innovation.

New scientific paradigm: AI battery large models and multi-scale integration

The adoption of large AI models, such as DeepSeek and Grok3, is poised to enhance problem-solving efficiency in LIBs research. These models leverage advanced language understanding, knowledge integration, and logical reasoning to accelerate materials discovery and design optimization.

Future advancements will emerge from the fusion of multi-scale modeling, AI optimization, and PINNs, enabling seamless integration from atomic-scale interactions to macroscopic performance. By bridging fundamental material properties with system-level engineering, AI will provide deeper scientific insights and guide next-generation battery design.

Mainstream AI models for scientific and industrial applications and their potential applications in LIBs research are summarized in Table 4. AI diffusion models further enhance virtual material design, microstructure prediction, and data completion, significantly lowering experimental costs while accelerating innovation. Hybrid AI architectures—combining deep learning methods such as CNNs, RNNs, and GNNs—enable the fusion of microstructure imaging, experimental data, and simulation results, improving material simulations, process optimization, and lifecycle prediction. Transformer-based models, specialized in processing structured and textual data, facilitate automated literature analysis, patent mining, and time-series forecasting, optimizing experimental planning and battery health assessments.

Notably, the proposed framework is not confined to LIBs but is inherently extensible to emerging energy storage systems through modular reconstruction and data-driven model transfer. By preserving the universal architecture while adapting to system-specific physicochemical features, the framework enables cross-chemistry generalization and lifecycle-level optimization.

For lithium-sulfur (Li-S) batteries, whose performance is limited by the polysulfide shuttle effect and sluggish sulfur reduction kinetics, rational catalyst design remains a long-standing challenge. Recent work [153] developed a machine-learning-assisted binary descriptor (BD), integrating a band match index and a lattice mismatch index, to capture both electronic coupling and structural lattice effects. This descriptor quantitatively deciphers how d-p and s-p orbital hybridizations, together with lattice strain, govern the catalytic kinetics of lithium polysulfide conversion. Guided by this framework, NiSe₂ was identified as an optimal catalyst, delivering 402 Wh kg⁻¹ energy density and stable operation under high sulfur loading and lean-electrolyte conditions. Beyond its empirical performance, the study establishes a transferable paradigm for rational catalyst design in multi-electron redox systems, demonstrating the synergy between data-driven modeling and physicochemical insights.

For lithium-metal batteries (LMBs) and solid-state batteries (SSBs), whose performance is limited by dendrite growth and interfacial impedance evolution, respectively. Physics-informed AI coupled with digital-twin-based modeling provides a promising route for predictive failure analysis. In LMBs, Piao *et al.* [154] developed a machine-learning-enabled pre-mortem framework that identifies failure pathways directly from the first two electrochemical cycles, representing less than 2% of the battery lifetime. Using a dataset spanning four years, 18,000 cycles, and 12 million data points, the model achieves classification accuracy up to 0.98, distinguishing kinetic, reversible, and co-degradation failures. The approach reveals that initial electrochemical curve “fingerprints” encode critical SEI and lithium microstructural features, which govern long-term kinetics and reversibility. Conceptually, this work transforms failure analysis from post-mortem diagnostics to pre-mortem prediction, offering a new paradigm for rapid reliability assessment and elec-

Table 4 Comparison of mainstream AI models for scientific and industrial applications and their potential applications in LIBs research

Model category	Core algorithm	Inference paradigm	Distinctive features	Representative applications	Data requirement	Potential applications in LIBs
Transformer	<ul style="list-style-type: none"> Self-attention, feedforward networks (FFN) 	<ul style="list-style-type: none"> Parallel processing, autoregressive inference 	<ul style="list-style-type: none"> Encoder-decoder structure, strong long-range dependency modeling, high computational cost 	<ul style="list-style-type: none"> Natural language processing (NLP), vision transformers (ViT), multimodal learning 	<ul style="list-style-type: none"> Requires large-scale datasets, applicable to diverse modalities (text, image, audio) 	<ul style="list-style-type: none"> Process sequential relationships in complex battery data, enhance predictive modeling for material properties, degradation patterns, and optimization strategies
BERT	<ul style="list-style-type: none"> Pretraining-finetuning, masked language model (MLM) 	<ul style="list-style-type: none"> Context-aware masked token prediction 	<ul style="list-style-type: none"> Encoder-only architecture, bidirectional contextual understanding, optimized for text comprehension 	<ul style="list-style-type: none"> Machine reading comprehension, sentiment analysis, named entity recognition 	<ul style="list-style-type: none"> Trained on arge-scale unsupervised text corpora, requires task-specific finetuning 	<ul style="list-style-type: none"> Extract key information from scientific literature, patents, and technical documents to assist in material discovery, process optimization, and R&D decision-making
GPT series	<ul style="list-style-type: none"> Autoregressive language modeling, transformer decoder 	<ul style="list-style-type: none"> Token-by-token generation, probabilistic sampling 	<ul style="list-style-type: none"> Decoder-only model, strong generative capability, constrained by prior context 	<ul style="list-style-type: none"> Text generation (ChatGPT), conversational AI, code synthesis, creative content generation 	<ul style="list-style-type: none"> Pretrained on vast web-scale text, fine-tuning enhances controllability and factual accuracy 	<ul style="list-style-type: none"> Generate structured technical reports, automate experimental documentation, suggest optimized experimental designs, and support AI-driven material screening
T5	<ul style="list-style-type: none"> Text-to-text, sequence-to-sequence (Seq2Seq) 	<ul style="list-style-type: none"> Converts all NLP tasks into text generation 	<ul style="list-style-type: none"> Full encoder-decoder framework, reformulates NLP tasks into a unified text generation problem 	<ul style="list-style-type: none"> Machine translation, text summarization, knowledge extraction, question answering 	<ul style="list-style-type: none"> Span-corruption-based pretraining, adaptable to diverse text-based applications 	<ul style="list-style-type: none"> Standardize battery simulation and experimental data formats, improve data interoperability, and enhance analysis consistency across different datasets
Hybrid models	<ul style="list-style-type: none"> Transformer + CNN/RNN/GNN (multimodal Fusion) 	<ul style="list-style-type: none"> Task-adaptive, hierarchical reasoning 	<ul style="list-style-type: none"> Integrates multiple architectures, enhances multimodal representation learning, improves computational efficiency 	<ul style="list-style-type: none"> Speech recognition (Whisper), video analysis, multimodal information retrieval 	<ul style="list-style-type: none"> Requires cross-domain labeled datasets, optimized for heterogeneous data fusion 	<ul style="list-style-type: none"> Integrate multimodal data (e.g., material composition, electrochemical performance, and manufacturing parameters) to optimize battery design and performance prediction
Diffusion models	<ul style="list-style-type: none"> Variational inference, Markov process 	<ul style="list-style-type: none"> Iterative denoising-based generative modeling 	<ul style="list-style-type: none"> Learns data distribution via noise transformation, generates high-fidelity synthetic outputs 	<ul style="list-style-type: none"> Image and video generation (stable diffusion, midjourney), 3D modeling, medical image synthesis 	<ul style="list-style-type: none"> Computationally intensive, requires extensive high-quality labeled data 	<ul style="list-style-type: none"> Generate novel battery material structures, enhance simulation data diversity, predict molecular configurations, and improve experimental efficiency by reducing trial-and-error cycles

trolyte design in next-generation LMBs. In SSBs, phase-field simulations of solid electrolyte-electrode interfaces can be embedded in the digital twin to predict ion transport pathways and optimize interfacial contact morphology [155,156].

Beyond lithium systems, the framework can be extended to sodium-ion (Na-ion) and multivalent (Mg^{2+} , Ca^{2+}) batteries by reconstructing the underlying ion-transport and reaction models to reflect their distinct electrochemical behaviors. For instance, substituting Li^+ with Na^+ in DFT simulations of diffusion in hard carbon anodes allows optimization of interlayer spacing [157], while for multivalent systems, multi-electron transfer and interface stability can be captured through enhanced reactive force fields and continuum models.

Furthermore, the architecture naturally expands toward other types of electrochemical devices, such as various fuel cells, and MOF-based electrochemical devices, bridging the frontier between neuromodulation and energy storage. The study also highlights a cross-scale regulatory mechanism inspired by “MOF neurons”, offering new insights into dynamic interfacial control. The “MOF neuron” concept [158] demonstrates the feasibility of integrating ionic transport with neuromorphic control, pointing to an emerging class of intelligent energy-sensing systems that transcend the conventional paradigm of passive energy supply.

Collectively, these extensions exemplify the framework’s universality and scalability, guided by three core principles: (1) model modularization, enabling structural flexibility across chemistries; (2) AI algorithm transferability, ensuring efficient adaptation with minimal retraining; and (3) digital-twin lifecycle coupling, maintaining coherence from materials discovery to recycling. Together, these capabilities establish a unified foundation for the intelligent design, operation, and evolution of beyond-lithium energy systems.

AI-driven sustainability and the future of LIBs

AI’s impact extends beyond performance optimization to sustainability and lifecycle management. Digital twin technology, in conjunction with cloud-based BMS and edge computing, is set to revolutionize real-time monitoring, predictive maintenance, and lifecycle optimization. By integrating lab research with industrial data, digital twins will enhance safety, reliability, and performance longevity.

As the world moves toward carbon neutrality and circular economies, AI-driven intelligent lifecycle management will improve recyclability, promote second-life applications, and streamline sustainable resource utilization. The Battery Passport initiative will enhance transparency in carbon footprint tracking, material provenance, and recycling, reinforcing global commitments to greenhouse gas reduction.

Despite significant progress, AI-driven battery lifecycle management faces critical challenges in data quality, model interpretability, computational efficiency, and cross-sector integration. For emerging chemistries such as solid-state and lithium-sulfur batteries, limited and heterogeneous data constrain model training. Active learning and physics-based data augmentation can improve robustness and transferability.

Computational demands and model opacity remain bottlenecks. PINNs and digital-twin architectures require substantial resources, motivating edge-AI deployment and model compression for real-time operation. Explainable AI frameworks that link latent representations to physically meaningful parameters are essential to ensure transparency and trust.

Cross-stakeholder data silos further impede progress. Open and standardized platforms can promote interoperability and collaboration. Integrating accessible data infrastructures, efficient AI frameworks, and policy-aligned standards is pivotal to scaling AI-enabled battery management from research to industrial

practice.

With the rapid electrification of global energy systems and increasing integration of renewable energy, the LIB industry is positioned to become a multi-trillion-dollar sector, driving the clean energy transition. The convergence of standardization, digitization, modularization, and AI-driven intelligence will not only accelerate technological breakthroughs but also unlock significant economic growth. By embracing these innovations, the battery industry can enhance energy security, expedite carbon neutrality, and pave the way for a smarter, more sustainable future.

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Author contributions

Y.L. conceptualized and coordinated the review and wrote part of the article. S.Y., X.D. and X.W. designed the manuscript structure, conducted the literature review, wrote the article, integrated contributions from the team, and refined the content. Z.Q. systematically identified and organized the relevant references. J.X. and M.S.W. provided expert critique on the entire manuscript and overall narrative from an academic perspective. Y.Z. offered professional guidance from an industrial perspective, particularly on the practical applications of the reviewed technologies. Y.L. integrated perspectives from multiple disciplines to ensure a comprehensive and multidisciplinary approach. All authors contributed to revisions and approved the final manuscript.

Conflict of interest

The authors declare no conflict of interest.

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