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Application of Artificial Intelligence to Lithium-Ion Battery Research and Development

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Abstract: Lithium-ion batteries (LIBs) have become one of the best solutions to the energy storage issue in modern society. However, the battery materials and device development are both complex, and involve multivariable problems. Traditional trial-and-error approach, which relies on researchers to conduct experiments, has encountered bottlenecks in the improvement of the battery performance. Artificial intelligence (AI) is the most potential technology to deal with this issue due to its powerful high-speed and capabilities of processing massive data. In particular, the capability of machine learning (ML) algorithms in assessing multidimensional data variables and discovering patterns in the sets are expected to assist researchers in discovering patterns and elucidating the mechanisms of material synthesis and device fabrication. This review summarizes various challenges encountered in traditional research methods of LIBs and introduces the applications of AI in battery material research, battery device design and manufacturing, material and device characterizations, and battery cycle life and safety assessment in detail. Most importantly, we present the challenges faced by AI and ML in battery research, and discuss the shortcomings and prospects of their applications. We believe that a closer collaboration among experimentalists, modeling specialists, and AI experts in the future will greatly facilitate AI and ML methods for solving battery and materials problems that are difficult to be solved by traditional methods.

Key words: lithium-ion battery; machine learning; materials characterization; battery manufacture; artificial intelligence

1 Introduction

Our country has proposed the "carbon peaking and carbon neutrality goals" in 2021. Renewable energy will promote the process to achieve the "double carbon" goals. However, the sustainability of these energy resources from such as solar and wind is fluctuating, thus their deployments must be accompanied by energy storage with high efficiency. In all the energy storage techniques, secondary batteries, which can be charged/discharged for thousands of times, are suitable for storage time scale of hours, due to their very high energy efficiency and power-energy flexibility. Among them, lithium-ion batteries (LIBs) are one of the most essential rechargeable batteries that have promoted the popularity of the electric vehicles (EVs) and wide application of portable electronics. Even if the performance of LIBs has been remarkably boosted, the demanding in building advanced EVs and grid-scale energy requires even better performance, including longer cycle life, better durability, safer, and lower cost.

However, the research and development of batteries are typically complex while have multivariable problems, which lead to different performcnces, including

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energy, power, cycle life, and safety, etc. (Figure 1). The conventional methods in the research of developing battery typically rely on the materials-centered trail-and-error methodology. The synthesis of electrode materials, and the manufacture of electrodes, the assembly of test cells, and the performance evaluation are conducted in sequence. Thus, the numbers of possibilities for energy storage materials development could be >10100[1], which is almost impossible for determining electrode materials synthesis or electrode manufacturing parameters. The complexity makes the inverse design tools that enable the battery component property prediction highly desired for a specific property target, battery chemistry, and device structure. Recently, the data in the battery research have exponentially expanded, as BASF claimed a production rate of 70 million data points of battery research every day. Furthermore, tremendous literature data lead to the battery information explosion, and more than 100000 publications, which are still rapidly rising, on LIBs have been published. One researcher would need more than 300 years to understand these papers if he or she could read 300 papers every year.

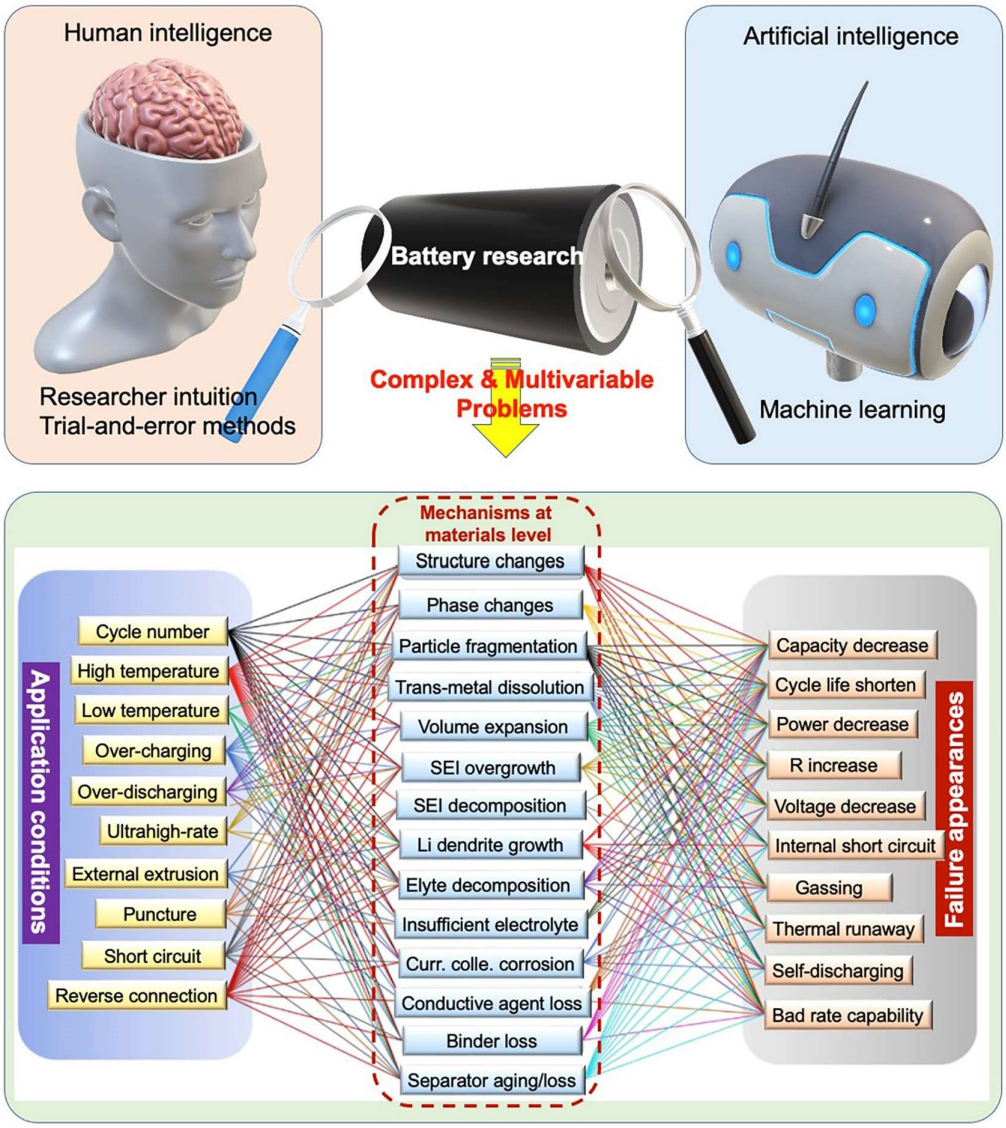

Figure 1 Schematic of the complex while multivariable problems in battery research investigated by human intelligence and artificial intelligence. (color on line)

Therefore, novel tools should be utilized to help battery research. Recently, artificial intelligence (which are typically called AI, whose most useful branch is called machine learning, ML) has exhibited as an effective method that could create a novel paradigm for helping battery research[2], and potentially enabled researchers to conquer the major obstacles on the huge number of variables and big data[3]. Several issues should be addressed firstly, such as the application of standard descriptor in battery research[4]. Furthermore, different battery types generate different challenges and ML methods could be useful in several regions, with one of the typical applications being ML-based imaging analysis for studying cathode cracks or Li dendrite evolution. Other contributions could extend the spatial and time scales of theoretical calculations or other multiscale approaches[5,6].

Recently, hundreds of publications have been focusing on the application of AI in battery research. As several comprehensive reviews have summarized these contributions[7-12], we will not conduct a summary of the published works. Instead, we critically raise the challenges of AI and ML in battery research based on the published results, and discuss the shortcomings and perspectives of their applications. We first give a short description for AI and ML, then the applications of them are discussed following the sequence of materials research, device manufacture, characterization, and cell health estimation.

2 Backgrounds of AI and ML

AI has been widely applied in internet search engines and digital social networks, in gaming such as Deep Blue and AlphaGo, and autonomous driving[13,14]. Researchers have also used AI to boost the research on materials and pharmaceuticals[13,14]. Currently, the advantage of AI mainly benefits from the state-of-art ML algorithms, which allows it to extract underlying information from exiting data. This ability is about to make great contribution in the battery research. The ML algorithms are very good at assessing multidimensional data variables, and discovering patterns in the sets, thus helping researchers clarifying possible mechanisms[15-17]. This methodology is powerful and essential to material development and device structure designing. Both typical issues require the researchers to consider multiple variables in searching for new generations of the batteries. And AI happens to be good at handling these issues.

The effectiveness of ML is mainly determined by the quality and quantity of data, as well as its veracity. Thus, the prerequisite for an effective ML application is to generate an acceptable data set[10]. These data are then used to "train" the algorithm. Usually, only part of the data should be used to train the algorithm, and the predictive capability of the model is evaluated by comparing values that are not used for training model and the data predicted. The aim of the comparison step is evolution, which is usually called a "test". If the trained model is tested as a trustable model, it can further be used for estimation or verification of data.

ML models are usually classified as supervised, unsupervised, or semisupervised methods[18,19]. The major difference between them is whether there is a predetermining step. If it is, that is the supervised method, while unsupervised when it is not. The latter can identify patterns from big data directly. It should be noted that for the supervised method, researchers should distinguish the regression type and classification type. While the semisupervised method, which combines the characteristics of supervised and unsupervised methods together, deals with data of both unlabeled and labeled. We note that classical ML models show effectiveness for discovering patterns from big data; however, they cannot give interpretations of these patterns. Recently, ML methods with physical property directed methods could be developed to find partial differential equations[20-22].

Data quality and quantity are critical to developing reliable ML models. Insufficient or bad data (such as data with errors) sets can generate bad predictions, and thus misleading the following interpretation. For building representative data sets, reasonable experimental design and conducting are both highly desired to enhance the effectiveness of data and the results[23-25]. Also, ML algorithms should be designed following

good standards to eliminate bias during data processing.

3 Application of AI in Battery Materials Research

The publications of battery material development helped by AI are classified into three types: (1) electrode active materials, (2) solid-state electrolytes, and (3) SEI generated from liquid electrolytes. For electrode active materials, AI has been used to dig out valuable properties including capacity retention, discharge capacity, Coulombic efficiency, volume change, and voltage profile. For electrolytes, research is specifically focused on the finding ceramic solid-state electrolytes with high conductivity. A bottleneck issue of applying ML algorithms to materials research is the definition of effective descriptors that can accurately anticipate target properties[26]. Several categories of descriptors have been reported recently[27-32]. However, building universal and powerful tools that are effective for all performances remains unsolved[32].

Until now, atomic-scale models based on statistical physics principles provide us powerful tools to investigate the microscopic mechanisms underlying the macroscopic performance of battery materials. For example, first-principles molecular dynamics (MD) simulations can reveal the kinetic processes of Li intercalation/deintercalation and transport in electrode or electrolyte materials, based on an accurate force field which quantum-mechanically describes the interactions between various atoms in the simulation cells. However, if we aim to study complicated electrochemical environment in battery systems (e.g., the solid electrolyte interphase films on top of electrodes or the phase transition of battery cathode materials, etc.), the highly expensive computational cost of first-principles calculations will limit our molecular simulations in both of the spatial and temporal scales, making it impossible to construct practical atomic-scale models to investigate the key scientific problems relevant to battery performance[33].

The recent development of machine-learning (ML) force field[34-36] offers a great opportunity to resolve the trade-off between the accuracy and cost of molecular simulations. With the first-principles potential energy surface as the input data, we can train a neural network to obtain a ML force field which maps configurations of our interested systems to the corresponding energies and forces. When this ML force field is applied in MD simulations, the accuracy of this atomic interaction description is within the quantum mechanics level as the neural network is trained by first-principles data. More importantly, since the configuration-energy-force mapping is constructed via the neural network, typical self-consistent-field loops (and expensive diagonalization of Hamiltonian matrices) in first-principals calculations are completely skipped, thus leading to a huge improvement in computational efficiency. Assisted by the artificial intelligence (AI) technology, we therefore can obtain a potential energy surface with the advantages of both a high accuracy and a relatively low computational cost, bringing us hope to tackle some more complicated electrochemical problems in battery materials.

Methods capable of dealing with larger systems and longer timescales while keeping the accuracy are required to be developed. With the help of it, the most critical processes in LIBs, such as the SEI generation and changing (Figure 2), ionic transportation in porous electrodes, could be addressed. Jørgensen et al. reported a ML model[37], realizing both the accurate (QM accuracy) and fast prediction. The tool has been verified for a nano metal clusters (NMC) cathode as well as liquid electrolyte (EC).

Recently, the computational high throughput (HT) of screening battery materials is hot, but the speed of validation is becoming the bottleneck. HT synthesis methods, which can generate big experimental result data, are proposed. The results could be automatically analyzed and the relationships between the performances and synthesis parameters could be clarified. This HT synthesis can be enabled by robotic technologies in the future[38,39]. Further studies and demonstrations are on the way, and one of the hardest issues could be the long-term HT synthesis of battery materials realized by machines. Li et al. combined ML and HT computation to study SEI[40]. Results show that

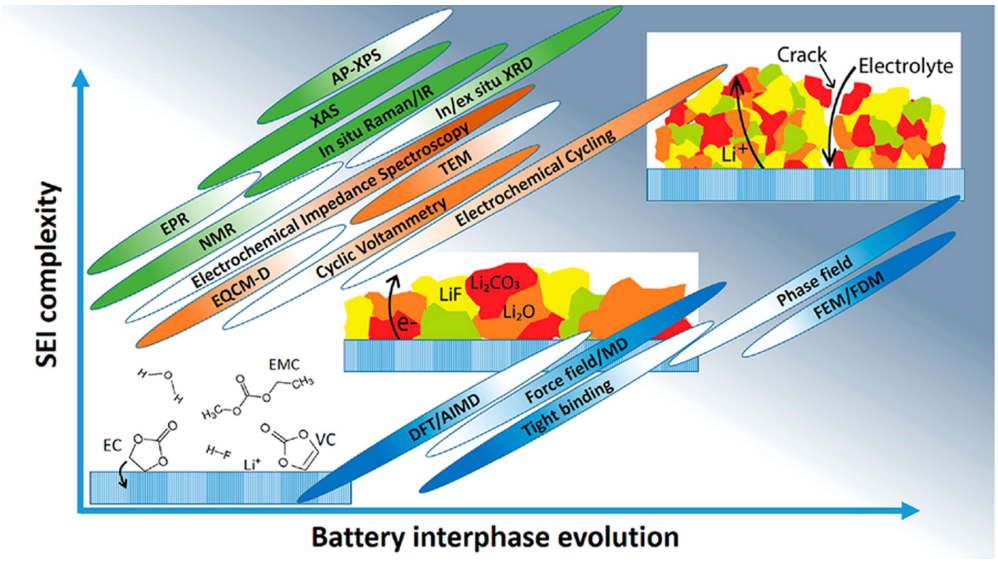

Figure 2 The complexity of a typical battery SEI evolution, from the molecular-scale to macroscale. Investigating the SEI properties needs the combination of a range of simulation (blue), electrochemical (orange), and characterization (green) methods[37]. Figure reproduced with permission from ref 37. Copyright 2019 Elsevier. (color on line)

the effect of mechanical constriction on SEI stabilization is nonlinear. Furthermore, the SEI decomposition predicated by ML is experimentally demonstrated.

Another AI based tool that is powerful for materials development is literature data (text or called natural language) mining. Based on the data from thousands of journal articles on metal oxides and sulfides [41], Ceder et al. clarified the raw data (labeled by the neutral network, NN), extracted main information, and obtained the relationships between composition and synthesis temperature of the metal oxides. From 27 synthesis variables of 22,065 journal articles, they exhibited that the concentration of NaOH precursor is a critical parameter for titania nanotube preparation. The authors also pointed out that the lack of standard test prevents the effective text mining (TM). Furthermore, the disregard for bad data, which would indeed constitute valuable data, could be a huge limitation for the development of text mining.

Other main challenges include universal materials descriptors, data scarcity, immature representation (where AI methods incorporated with physical laws are needed), and lack of standardization. For the last one, the combination of standardized theoretical calculation and experimental result data could be helpful to determine the suitable ML strategy for a special mission, and thus researchers could be able to build novel methods based on established approaches.

4 Applications of AI on Battery Device Design and Manufacture

Battery electrode preparation and device building are new applications of ML methods. These processes rely on very complex multivariable steps, with the parameters including chemical properties of active materials, electrode structure, slurry components, electrolytes, powders premixing time, slurry mixing speed, machinery structures, etc. Furthermore, preparation optimization is complex, and manufacturers fall short of physical fundamental knowledge and the interconnections among parameters. Thus, ML methods are potentially suitable to optimize and boost the electrode and device preparations[43,44]. Turetskyy et al. used a data-driven method to automatically collect production line data, and successfully made use of these data by ML methods for production optimization (Figures 3)[45].

In Cunha et al.'s work[46], three ML methods for estimation of electrode properties based on preparation parameters are compared. The impacts of the parame-

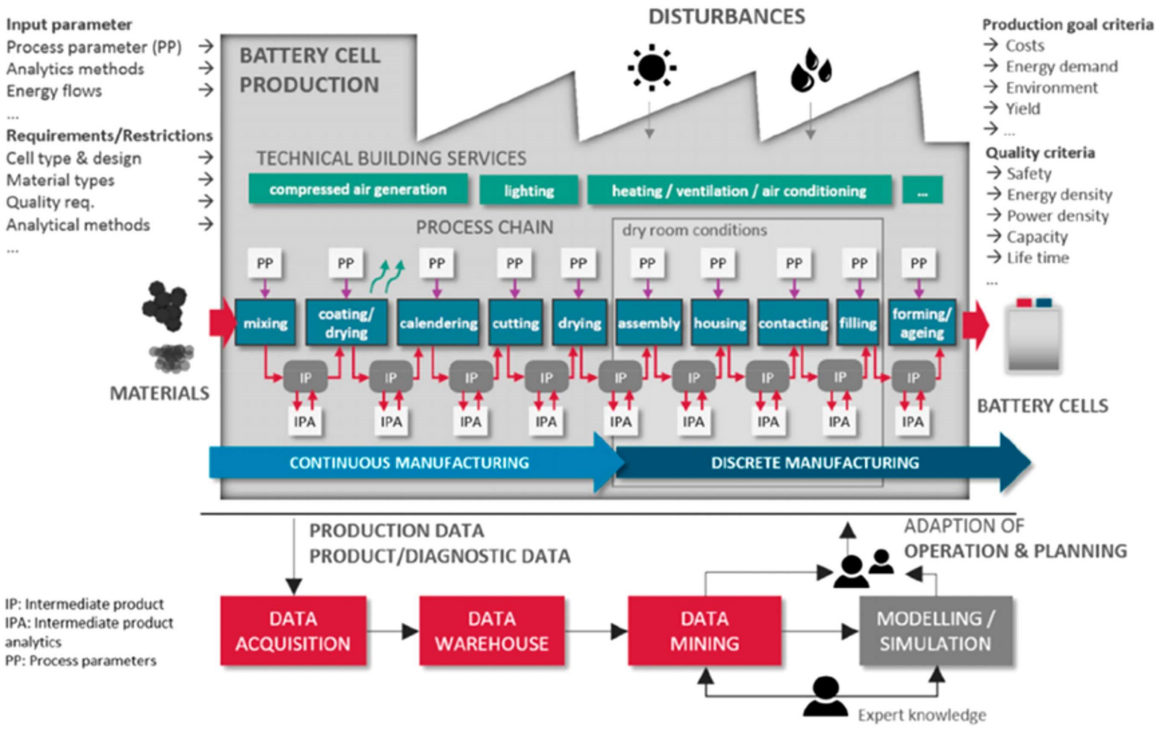

Figure 3 Schematic of a LIB manufacturing chain utilizing a data-driven method[42]. Figure reproduced with permission from ref 42. Copyright 2020 Wiley. (color on line)

ters such as slurry viscosity and solid content on obtained electrode porosity and mass loading are studied. The so-called SVM ML method with high accuracy enables fast identifying trends based on electrode properties and preparation parameters. Furthermore, this work discovers interesting patterns between electrode properties and the slurry characteristics (Figure 4).

Not only experimental results but also physical calculations can be used to train ML models. Duquesnoy et al. built a big database from calculated electrode structures (Figure 5)[5]. Macroscopic properties such as porosity and thickness are based on experimental results, while theoretical calculations are used to quantify the mesostructure change such as the percentage of active surface and contacts. Step B in Figure 5 mathematically describes the trends by a mesostructure generator, which can build relationships among properties including particle size of electrode materials, mass loading of electrodes, and formation parameters of cells. The next step C further builds the data link between properties of materials and manufacturing parameters. The relationships or patterns obtained are prepared for the researcherers' interpretation, generating insight into further optimization. (Step D in Figure 5).

However, the wide application of this method is hindered by its high computational cost. Optimizations have been conducted recently, and its working principle is shown in Figure 6, which could simultaneously launch and analyze many simulations, and the required parameters for specific goals could be obtained. Another ML approach called particle swarm optimization (PSO) combined with deep neural network (DNN, Figure 6B) can identify the most critical parameters and then further speed up the parametrization. Both PSO and DNN results are utilized by the DNN database for further increase the accuracy during the optimization procedure.

Here, an interesting question could be asked: how can AI assist manufacturing help industry 4.0 even 5.0 development? The term Industry 4.0 is commonly directed to features including interconnectivity between cybernetic and physical domains, decentralized

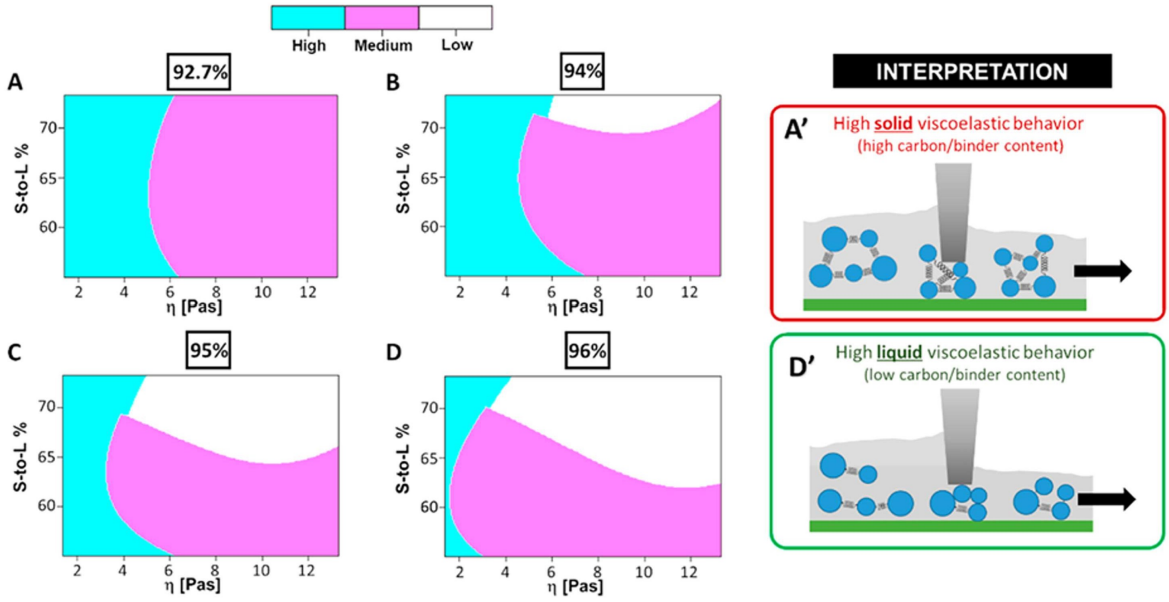

Figure 4 SVM classification in terms of the electrode porosity influenced by the slurry viscosity and solid-to-liquid ratio for different weight contents of NMC active materials: (A) 92.7%, (B) 94%, (C) 95%, and (D) 96%. Panels A′ and D′ exhibit low and high porosity electrodes in Panel A and Panel D, respectively[46]. Figure reproduced with permission from ref 46. Copyright 2020 Wiley. (color on line)

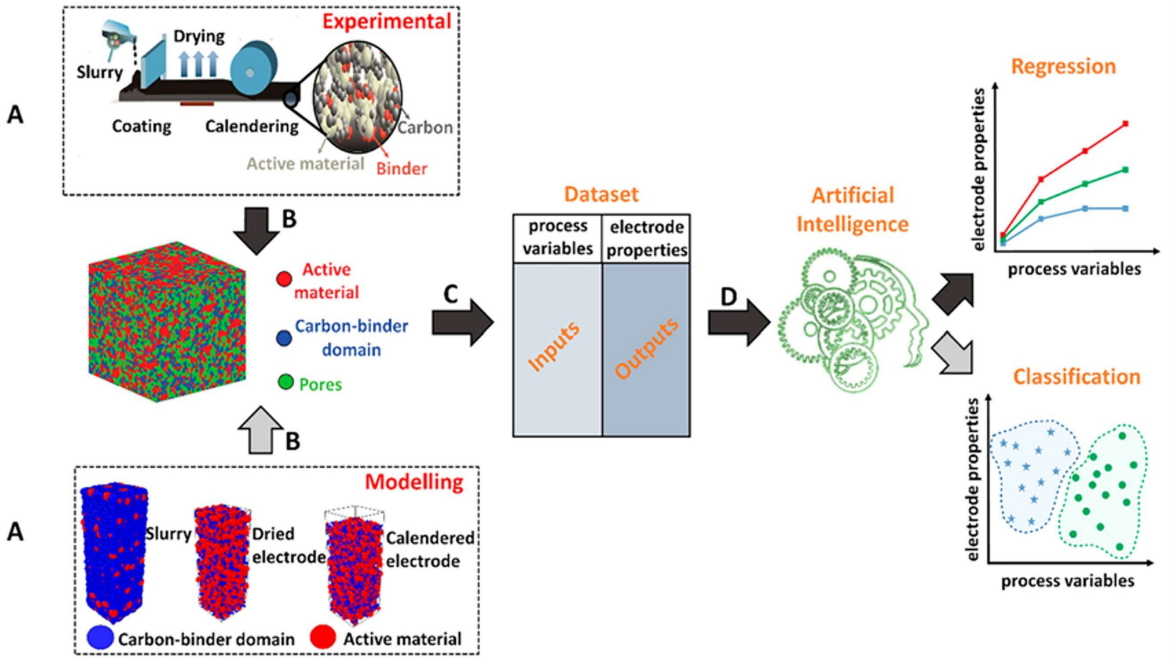

Figure 5 Overall workflow of the hybrid methodology presented in ref 5. Experimental and/or physics-based modeling results capturing the impact of manufacturing parameters on electrode mesostructure properties (A) are embedded in a D-DEMG algorithm (B) that generates electrode mesostructure associated with specific manufacturing conditions. These mesostructures are analyzed, building the data set (C) that is used to train and validate ML algorithms. This allows describing mathematically the correlations between electrode properties and process variables as manufacturing conditions (D). Dark gray arrows represent the steps considered along the case study presented in ref 5, while light gray ones indicate future perspectives of this methodology. Figure reproduced with permission from ref 5. Copyright 2020 Elsevier. (color on line)

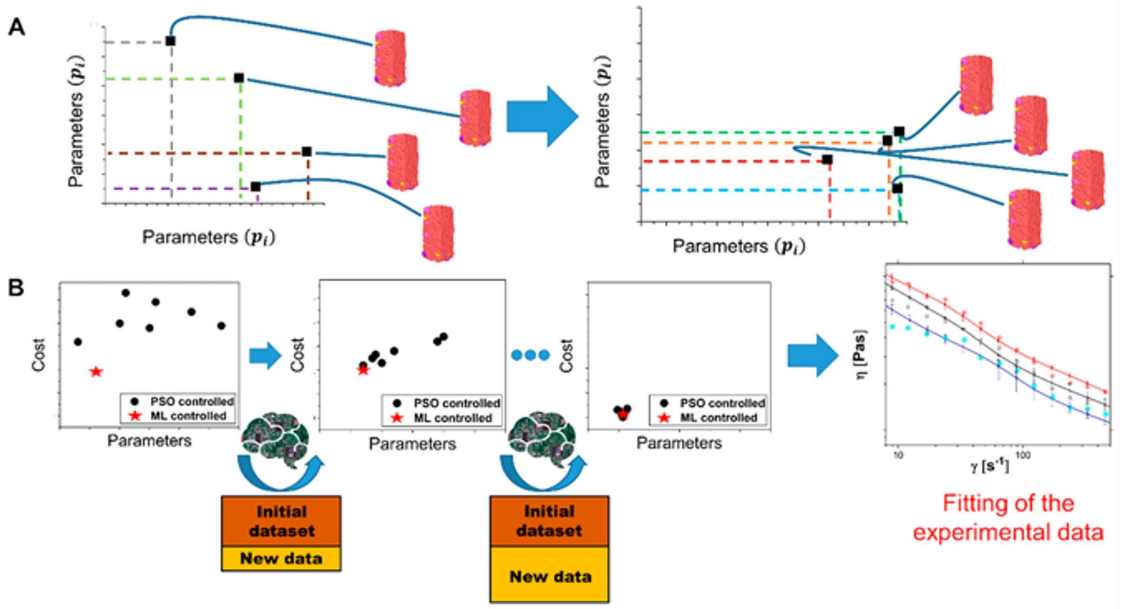

Figure 6 (A) Schematic of the particle swarm optimization algorithm developed by Lombardo et al. Left: the initial guesses of the PSO algorithm in terms of FF parameter values for the coarse-grained molecular dynamics (CGMD) simulations (linked to their associated 3D slurry structures)[47]. Right: the PSO algorithm converged to the FF parameter values needed to match the targeted experimental results. For each set of FF parameter values, a schematic of the associated slurry 3D structure is reported as well. Eight CGMD simulations are launched in parallel for each iteration. (B) PSO merged with a DNN algorithm to speed up the algorithm convergence. For each iteration, dots represent FF parameter values tested by the PSO, while the star indicates the ones predicted by the DNN. All the results of each iteration are added to the data set in order to improve the DNN accuracy. At the end right, a comparison of experimental (line) and simulated (dots) results is reported. Figure adapted with permission from ref 47. Copyright 2020 Wiley. (color on line)

decisions, as well as robot-human collaboration[48]. To reach this goal, industries should collaborate with academic for overcoming the following challenges: (1) the ability of *in-situ* testing in the whole manufacturing chain, (2) enabling the interaction between digital tools and industrial environment, (3) comprehensive network among operators, machines, and digital management systems, and (4) the computational power for handling these data. Thus, the advances in sensors[46], the infrastructures connecting digital/physical worlds, and the ability of accurately estimation of battery health (could be helped by digital twins) are essential aspects and large research efforts are required.

5 Applications of AI on Materials and Device Characterization

For battery materials research, characterization data from spectroscopic techniques (X-ray Absorption Spectroscopy, XAS), diffraction pattern techniques, and Scanning Electron Microscopy (SEM)/Transmission Electron Microscopy (TEM) are the most widely applied for ML training. On the other hand, the amount of characterization data in recent years is several orders larger than that of 20 years ago, which is attributed to the fast growth of instrumental characterization speed. Ceder et al. reported a probabilistic ML method to analyze multiphase compounds by X-Ray Diffraction (XRD) data[50]. The ML model was trained by 140 phases from chemicals formed by Li/Mn/Ti/O/F elements, including some important electrode materials. Both the simulated patterns and experimental patterns are used to test the obtained model and achieve high accuracy (92% ~ 94%) of phase identification. This case indicates that the rapid phase identification ability can potentially support HT experiments and realize the Rietveld analyses.

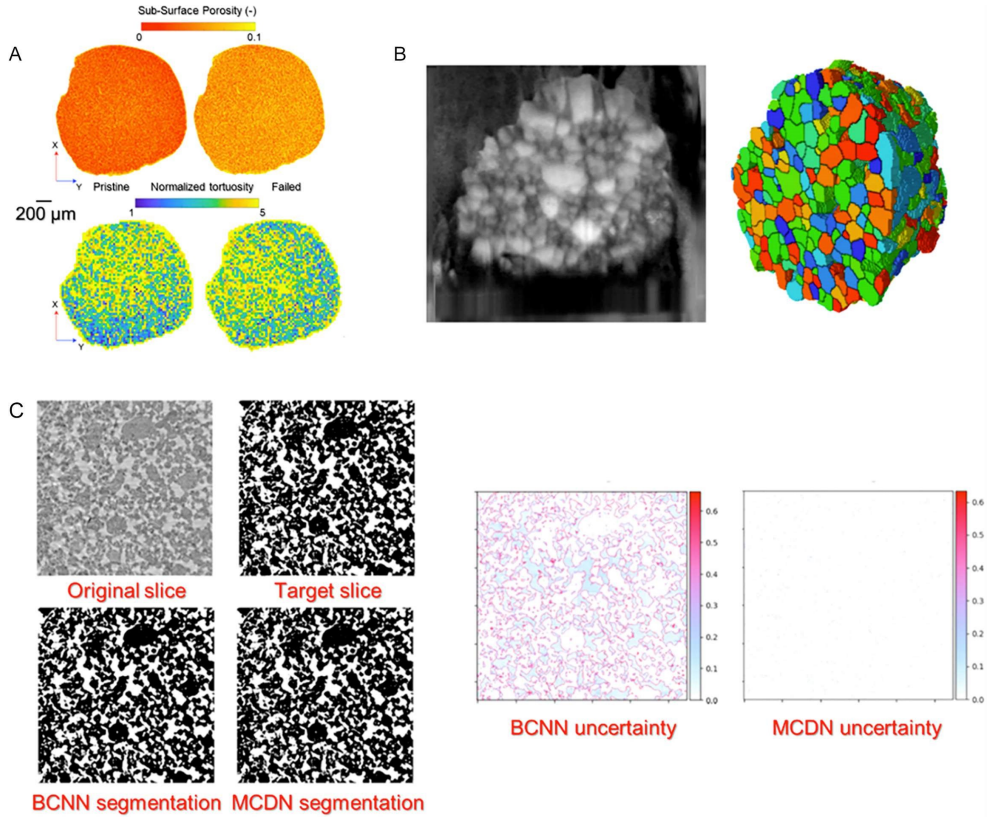

Figure 7 (A) Subsurface porosity map measured through the depth of the sample for the pristine and the failed electrolyte pellet[52]. (B) Cross section through the EBSD image of NMC depicting grain boundaries using FIB-EBSD. Segmentation result of the watershed algorithm in which each region is colored individually after removing regions outside of the considered NMC particle[53]. (C) Results on the graphite electrode with a map of Bayesian convolutional neural network (CNN) uncertainty, which is focused on the light gray edges of the material in the original slice, while the Monte Carlo dropout network uncertainty is pixelated[54]. (A) Figure adapted with permission from ref 52. Copyright 2020 American Chemical Society. (B) Figure adapted with permission from ref 53. Copyright 2021 Elsevier. (C) Figure reproduced with the authors' permission from ref 54. (color on line)

The hierarchical architecture electrodes are critical for the performance of LIBs, as the microstructure affects the ionic and electronic transport properties, and the interface-related the electrochemical kinetics. Thus, a profound insight into the relationship between electrode microstructures and electrochemical properties is crucial. X-ray tomography provides information about microstructural properties, while Raman and XAS could also generate useful data on the microstructures especially the electrodes inhomogeneities. ML is powerful for tomography data analysis. Various ML approaches are reported to be useful in enhancing the tomographic reconstruction ability during 3D imaging[51]. With the help of image segmentation, Dixit et al. quantitatively revealed the morphology evolution of the Li/solid state electrolyte interface during the Li metal plating/striping process[52], identifying the mechanism for electrode degradation (Figure 7A). The segmentation of NMC particles is exhibited by Furat et al. (Figure 7B)[53]. ML also enhances the ability of labeling various particles and even quantitatively describes the inhomogeneity of electrodes. Furthermore, the segmented data can be an input for building connection with electrochemical properties for optimizing electrodes (Figure 7C)[54].

The porosity and inhomogeneity of electrodes are critical for battery performance as they not only affect the transportation of electrolyte ions during charging/discharging, but also the degradation of electrodes in long-term. While the accurate description of

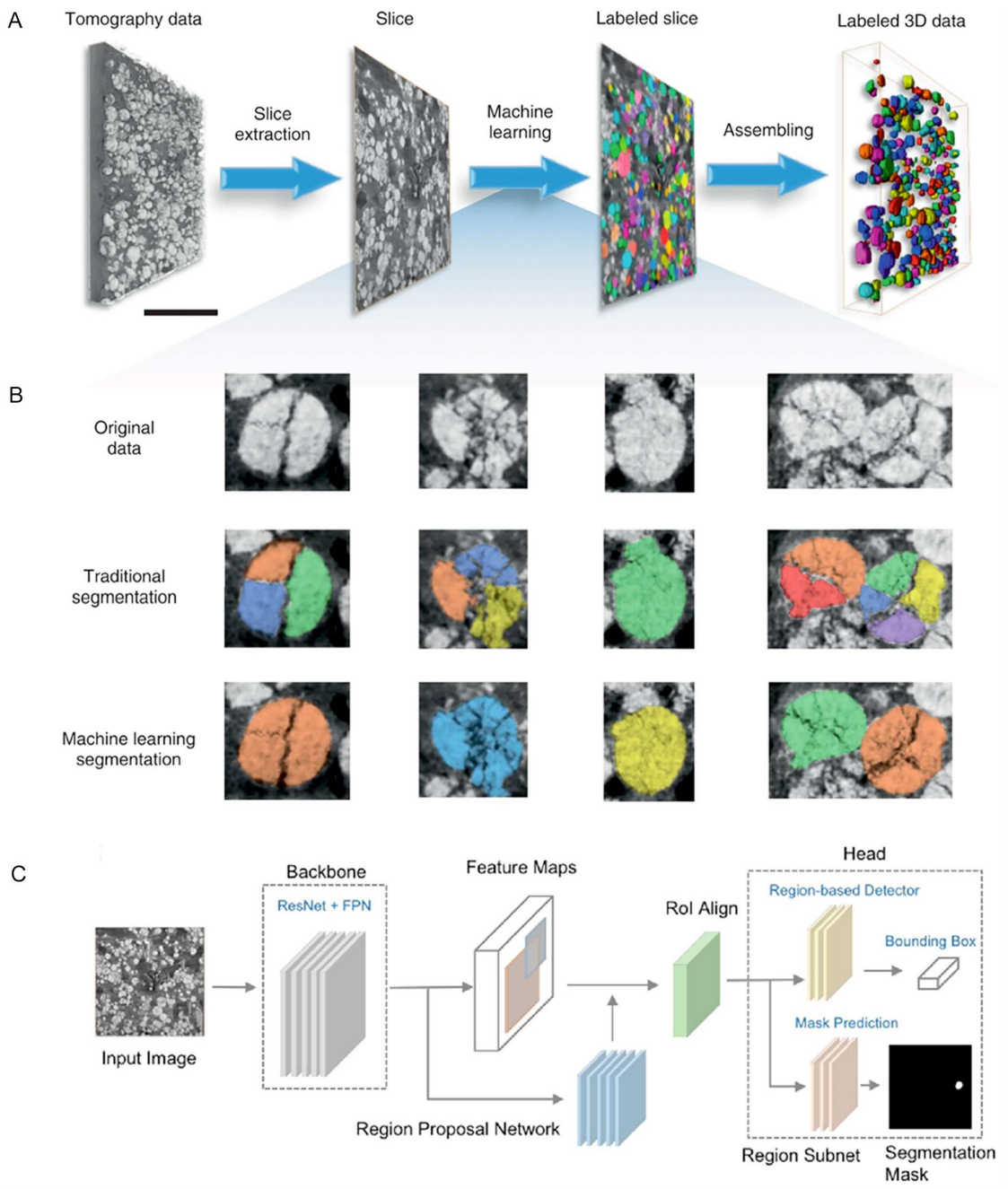

Figure 8 Over 650 unique particles of different sizes, shapes, positions, and degrees of cracking were successfully identified and automatically isolated from the imaging data in an automatic manner. (A) Workflow of the ML-based segmentation. (B) Comparison of conventional segmentation results and the machine- learning-assisted segmentation results for a few representative particles. Different colors denote different particle labels. (C) Schematic illustration of the herein developed ML model based on the Mask R-CNN for particle identification and segmentation. The scale bar in part A is 50 μm[55]. Figures reproduced with permission from ref 55. Copyright 2020 Springer. (color on line)

these inhomogeneities is very challenging. ML methods could effectively accomplish this kind of works through various strategies (Figure 8), and the description is unbiased[55].

Huang et al. combined X-ray nano-CT and ML with STEM and electron energy loss spectroscopy for investigating the structural evolution of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM) at multi-scales upon charging/discharging at

55 ℃ (Figure 9)[56]. Two types of cracks are denoted open and closed cracks. With the helped by ML, researchers found that the high temperature could lead to a remarkably increase of cracks, especially the open cracks, with the capacity rapidly decreasing. The transition metal (TM) ions would migrate into the Li-layer and cause the reduction of TM, thus a rock-salt-like structure could generate and lead to open cracks. In contrary to the mechanism of open cracks, no remarkable structure change is observed for closed cracks, and the reduction of TM is limited[56].

Liu et al. proposed a model to study the evolution of microstructure of electrode materials and the changing of electrochemical activity[57]. Based on X-ray holotomographic data of thousands of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ particles (Figure 10), they claimed that a remarkable inhomogeneity was generated at the beginning, and then this uneven property became weakened subsequently. The method and result can be helpful for better understanding degradation mechanisms of electrodes and further optimizing electrode structure for practical operation.

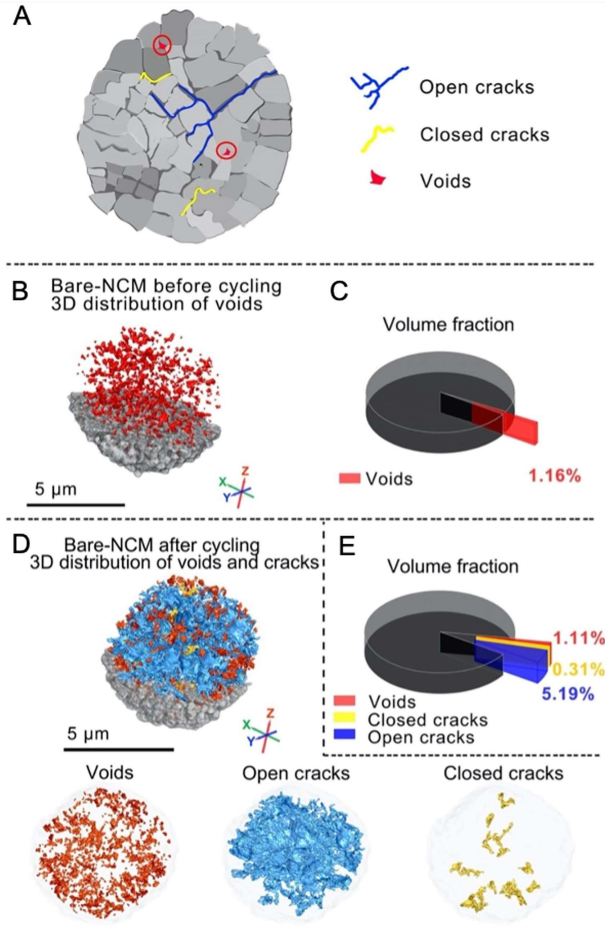

Figure 9 (A) Schematics showing the internal voids, open and closed cracks. (B) Visualization of the 3D void distribution, (C) volume quantification within bare NCM. (D) Visualizations of the 3D cycling-induced void, open crack, and closed crack distributions, and (E) volume quantification. Figures reproduced with permission from ref 56. Copyright 2022 Elsevier Ltd. (color on line)

For ML assisted battery characterization, ML is not only useful for data treatment such as image segmentation and reconstruction[59,60], but also for data fitting and finding correlations between various types of results. The advances in ML-enhanced characterization are not only saving time, but also discriminating various components or phases. What's more, it can support the operando dynamic process study, such as the Li dendrite grown or SEI evolution[61-64]. Thus, ML-enhanced characterization can help accomplish data collection, analysis, and decision-making for multivariable and complex observations, which may revolutionize the state-of-the-art experimental workflow (Figure 11)[65]. With the help of ML, data collection could be done in multiple zones using multiplex sensor and image techniques, which is much more efficient than human eye selection and interpretation.

6 Application of AI on Battery Health Estimation

The prediction of the battery cycle life, performance degradation time, and identification of the cause of aging are crucial for practical applications, such as grid-scale energy storage and EVs. Accurate aging models for predicting remaining life and potential failure under various conditions are very hard to be build but highly desired[7]. Tremendous works were conducted to predict battery degradation from off-line, which is previously collected data, experimental data. In addition, safety is important for practical application of batteries and is one of the major concerns of EVs. The safety concerns of LIB mainly are exothermic side reactions and following thermal runaway. Li et al. developed a safety envelope based

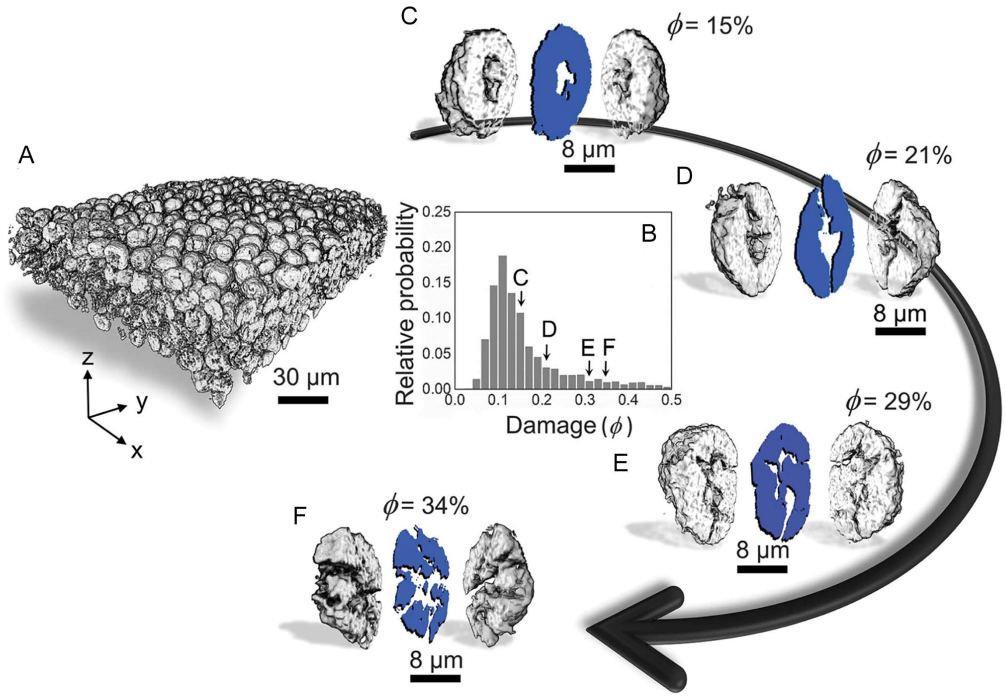

Figure 10 Imaging cathode electrodes with a multilayer of NMC particles using nano-holotomography[57]. (A) Visualization of the composite battery cathode obtained by synchrotron nano-holotomography. Each NMC particle has its own properties in position, particle structure, mesoscale chemistry, and local morphology. (B) Probability distribution of the particle damage level. (C to F) Randomly selected examples of NMC particles with different levels of damage. Figures reproduced with permission from ref 57. Copyright 2022 American Association for the Advancement of Science. (color on line)

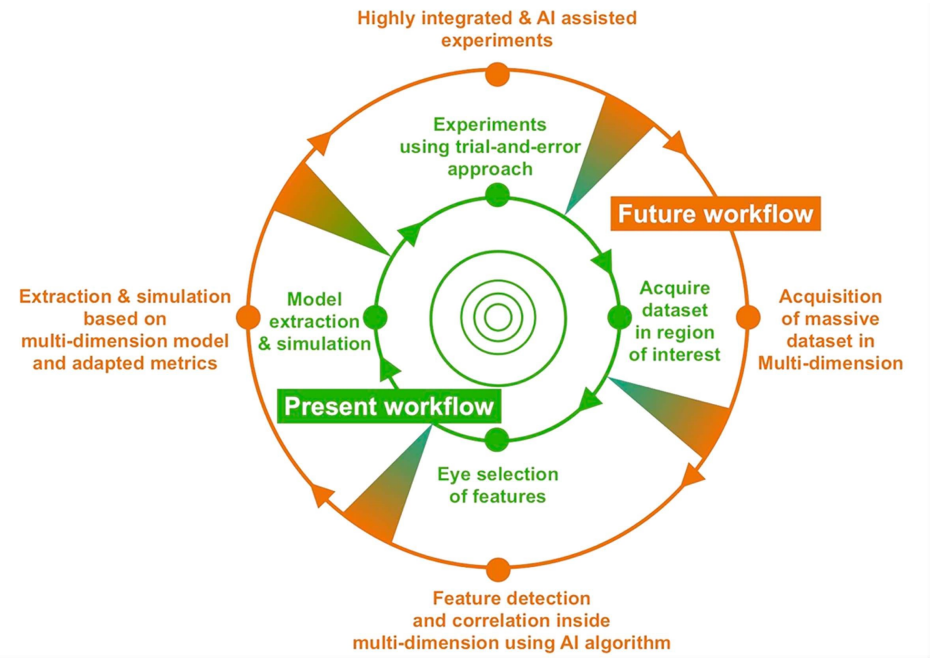

Figure 11 Schematic exhibiting present (green) and future (orange) workflows about conducting experiment, data acquisition, interpretation, and model extraction/simulation[65]. The large and increasing amount of data generated using modern characterization techniques, new generation of detectors, and the emergence of AI/ML methods are likely to transform the way that experiments are performed and data analyzed. Figures reproduced with permission from ref 65. Copyright 2021 American Chemical Society. (color on line)

on ML (Figure 12) and showed reliable calculation for EV applications[66]. Based on a 3D finite element and trained by 2672 simulations, the model can predict fractured geometry and force-displacement data of LIB cells during indentations.

ML has become a powerful tool for reminding useful life (RUL) predictions. Zhu et al. reported a decision tree method based on 138 cells data to estimate the RUL[70], and realized an high accuracy of 95.2% on whether one cell can keep >80% capacity after charging/discharging for 550 cycles. The results could be obtained by the charging/discharging capacity and resistance of the first two cycles. Furthermore, it was claimed that the difference in discharge capacity from the first two cycles was the most critical factor for the estimation of life, and this method is independent of the prior knowledge of degradation mechanisms (Figure 13)[15]. By using the data from the first 100 cycles, researchers could predict cycle life with 9.1% errors, although no significant degradations are observed in these early cycles. Typically, batteries should serve for years, and cycle life test is very time-consuming, thus, this ML method could effectively save time and resources[68,69].

To further decrease the cost and time for battery lifetime optimization[70], Attia et al. proposed a novel ML methodology called closed loop optimization (CLO, Figure 14)[69], to modify batteries for fast-charging applications. They applied an elastic net-based prediction model (as that from Severson's group[15]) to predict RUL by the data of 1 ~ 100 cycles[71]. This method reduces the time cost (from 7700 test hours to 500 hours) compared to the traditional ML-based estimation methods.

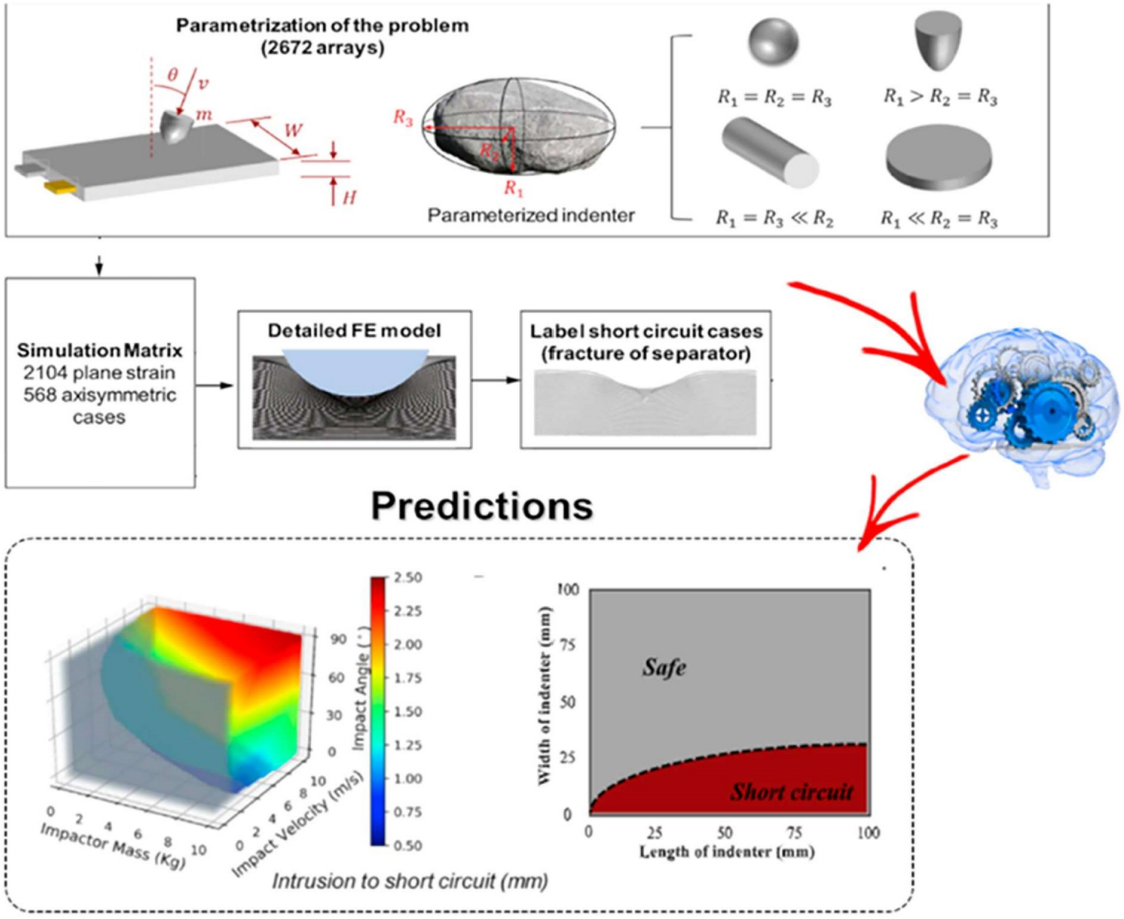

Figure 12 Flow-chart of the data-driven safety envelope using the ML algorithm[66]. Figure adapted with permission from ref 66. Copyright 2019 Elsevier. (color on line)

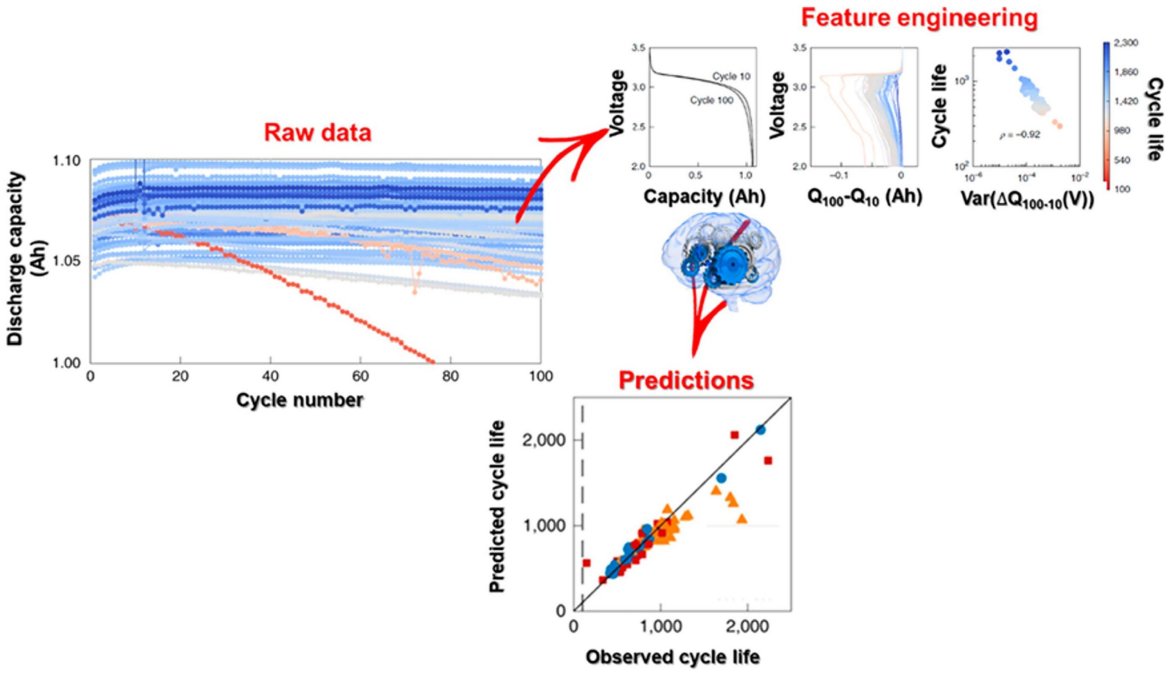

Figure 13 Schematic representation of the approach used by Severson et al. allowing for prediction of battery cycle life from only its first ~100 cycles[15]. Figure adapted with permission from ref 15. Copyright 2019 Springer. (color on line)

Choi's group proposed a ML algorithm for handling multi-channel charging/discharing data, including voltage[72], current, and temperature of a cell for RUL predicting LIB capacity. It is demonstrated that the estimation accuracy could be greatly improved by wider data sources. The framework for the strategy is depicted in Figure 15, where data preprocessing, model training, and life estimation are the main steps. In the data preprocessing, the data is cleaned, and the produced data are clarified for training and testing. In the training stage, a proper model should be selected for training and validation. In the estimation step, the RUL is calculated by data determined in the previous steps.

Besides RUL, performances such as state-of-charge (SOC) and state-of-health (SOH) of LIBs are critical parameters for energy storage and EV applications[73]. Currently, the methods of SOC and SOH estimations could be clarified into data-driven and model-based strategies. The former is mainly based on a specific system, with linear methods including support-vector-based method and probability estimation. While the model-based methods are mainly equivalent circuit and electrochemical models[74,75]. The battery temperature is another critical parameter, and its estimation has also been conducted with the help of various ML methods. Battery temperatures are usually expressed by multiphysics models, especially the electrochemical thermal-neural-network (ETNN) model (Figure 16)[76].

Recently, real-time RUL and failure prediction are demonstrated[77], in which Chen et al. reported an end-to-end ML method by automatic unsupervised extraction of various physical parameters that affect the performance. Then the extracted features were applied to generate a classifier, with a accuracy of 80% for battery classification at an early stage. Furthermore, this model can automatically monitor and waring the LIB safety and determining which battery potentially fails. For better ML method development with higher accuracy and shorter simulation time, researchers should focus on reducing the input data to only several critical features. However, the lengthy training process is typically unavoidable and should be addressed. Furthermore, these models are still for short of physical insight and their application is

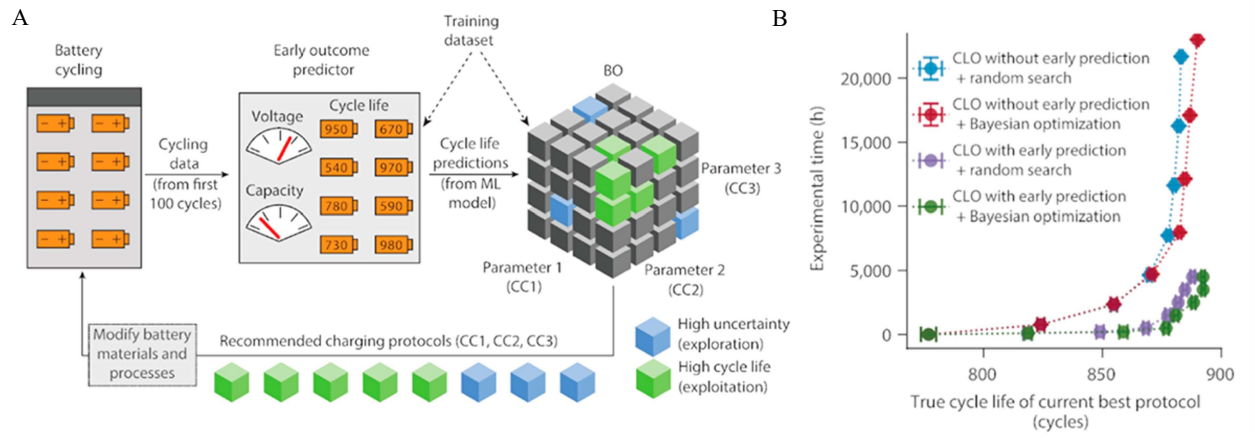

Figure 14 (A) Schematic of the CLO system developed by Attia et al[69].(B) Example of the result showing the optimization time needed for different CLO protocols. Figure reproduced with permission from ref 69. Copyright 2020 Nature Publishing Group. (color on line)

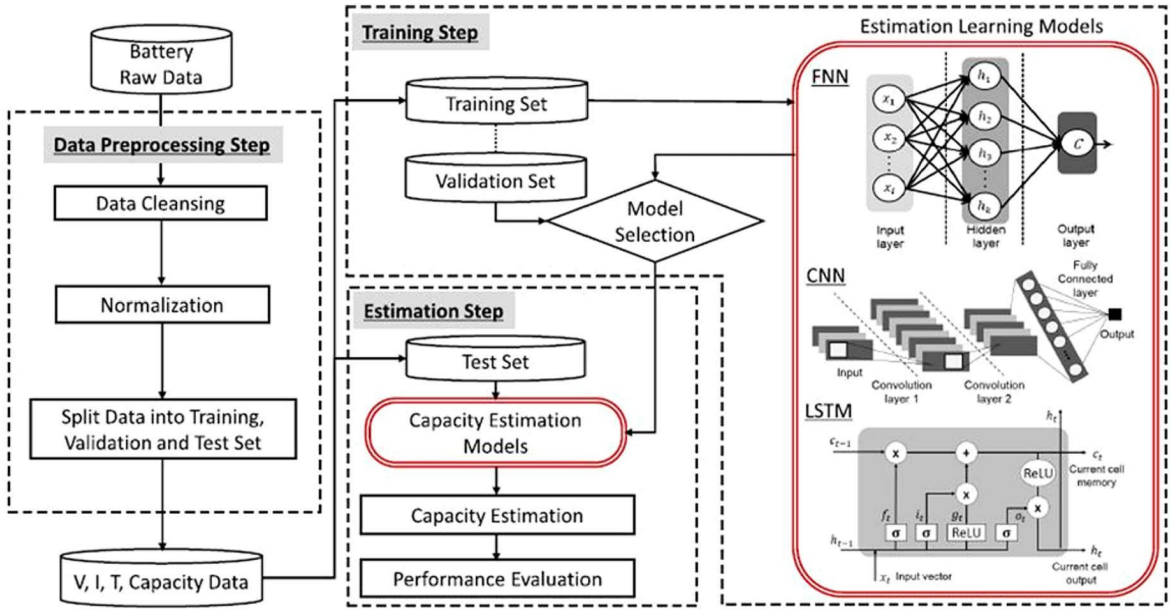

Figure 15 Overall framework of the proposed capacity estimation by Choi et al[72]. Figure reproduced with permission from ref 72. Copyright 2019 IEEE. (color on line)

hampered. Combining different models, such as physical and data driven models, methods potentially can overcome these drawbacks.

Secondary battery recycling is critical for resources reuse and global sustainability. Typically, a retired EV pack of the battery cannot be reused as the consistency of single devices in the pack are very poor. ML method could help judge the status of cells and enable the reuse of them. Recently Zhou et al. exhibited a screening approach, in which only the resistance and capacity should be measured, for used cell selection[78]. The multivariable model was trained to screen the used cells and the cells were clarified into four classes accurately (> 96%), demonstrating a fast and more powerful tool than the traditional manual classification (Figure 17).

The complexity of battery devices makes the control of real battery packs and systems challenging.

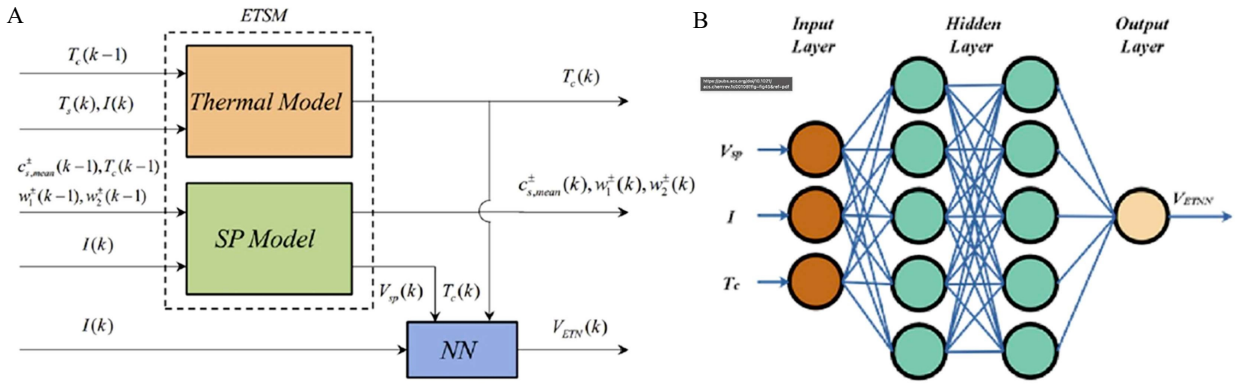

Figure 16 (A) Electrochemical thermal NN (ETNN) model structure and (B) NN detail by Feng et al. Figure reproduced with permission from ref 76. Copyright 2020 Elsevier. (color on line)

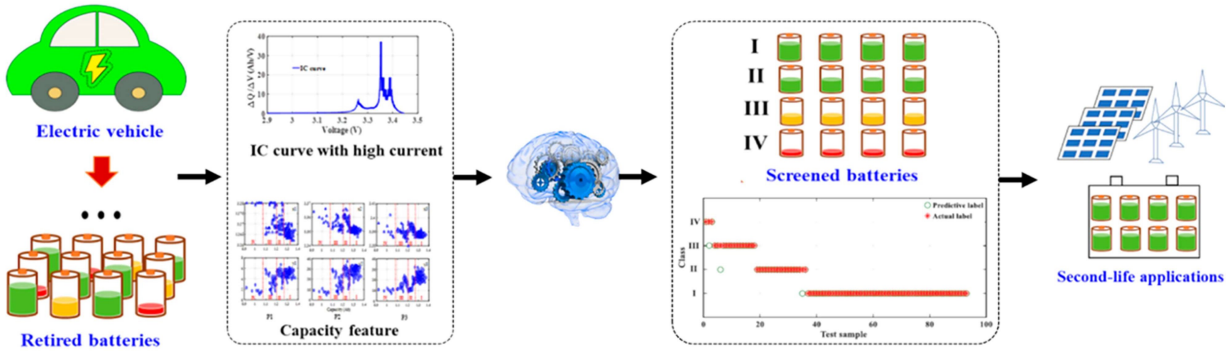

Figure 17 Schematic representation of how the SVM-based approach proposed by Zhou et al. could assist the second life of EV batteries for stationary applications[78]. Figure adapted with permission from ref 78. Copyright 2020 Elsevier. (color on line)

Thanks to the development of ML tools and a recent understanding of degradation mechanisms, a digital twin of battery could be developed by the combination of these advances and modeling tools. Digital twins enable a cyber-physical close interaction and then a better control of the battery system for a longer lifetime (Figure 18), and big challenges exist and require settlement. These challenges include the building of transferrable methods, nanoscale effects considered multiscale physics models, advanced sensor technologies, and physical insights involved in models[79].

In addition to work on the bulk-phase battery materials, the ML-assisted MD simulations also can be applied in a surface or an interfacial system, which actually is the most complicated and important environment in a battery cell, and largely determines the battery performance, cyclic life, and safety. Jiao et al. recently conducted DPMD simulations[80] revealing the self-healing mechanism in the Li deposition process at the Li-metal anode surface and provided insights for suppressing the Li dendrite formation by generating a homogeneous surface.

Given the above examples of successful applications of ML-assisted simulations in the battery research, we can see that the most exciting opportunity lies in the great expansion of the temporal and spatial scales of physical models based on statistical mechanics principles and quantum-mechanical accuracy (for describing the atomic interaction). As the first-principles-level potential energy surface becomes computational affordable with the help of AI technologies, the materials simulation community now can pursue for a more ambitious goal to perform

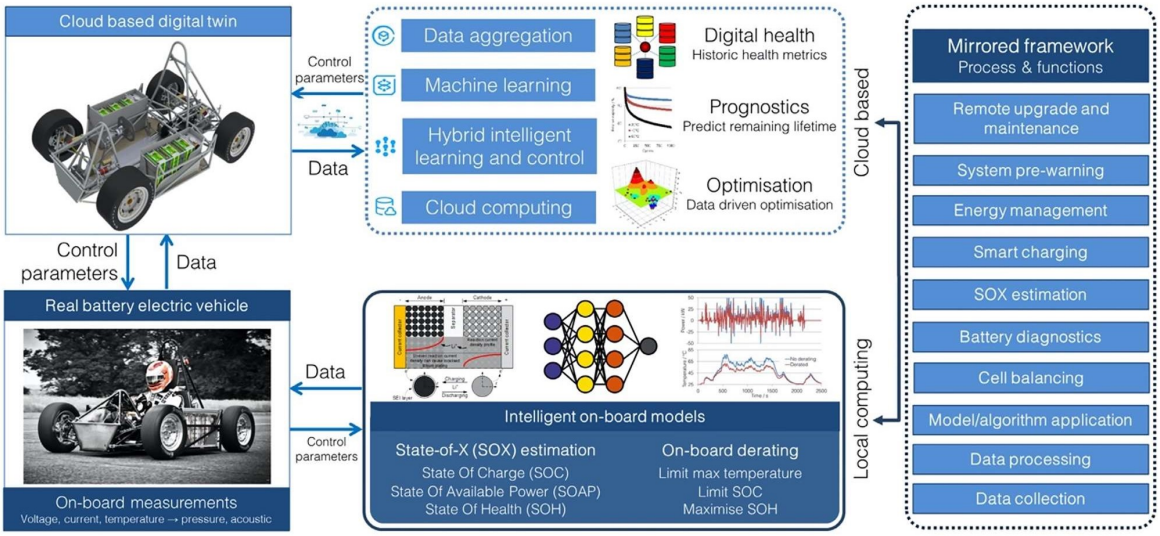

Figure 18 Cyber-physical elements of a battery digital twin[79]. Figure adapted with permission from ref 79. Copyright 1969 Elsevier. (color on line)

multi-scale modeling to tackle down some highly challenging problems in the Li-ion battery science, for example, the formation mechanisms of multi-component heterogeneous electrode-electrolyte interphases, and its effect on the Li transport and Li dendrite growth, phase transitions in the Li-Si alloy and the accompanied cracking issues, and so on. Our ultimate goal is to find or construct "universal" descriptors to predict battery performance or cyclic life based on a realistic physical model. The computational studies with ML force fields + exact statistical physics model not only will provide us reasonable and explainable descriptor systems for predictions, but also will help us better understand the underlying chemical and physical processes governing the battery operation, and guide the community in the battery materials screening or design.

7 Summary and Perspectives

AI (ML) could help dealing with the big data difficulties of battery research caused by a large amount of raw battery data. Whether ML methods are used for boosting materials discovery, device manufacture optimization, smart characterization or cell health estimation, the contribution merits of ML could be divided into two categories, i.e., data/text mining (TM, like the natural language minding by IT corporations) or image processing (like the face recognition). Both methodologies of raw data collecting, and ML algorithms require evolution to better solve the complex while multivariable problems in battery research.

Although TM could be one of the most effective candidates to analyze tremendous battery literatures, the literature text (~ 80%) is unstructured, which makes them hard to be handled by TM methods. Nonconventional retrieval strategy, which is mainly composed of collecting unstructured raw data, cleaning the data collected, structured data converting, and useful information generation, is demonstrated useful for TM of various unstructured data. However, most of these contributions are not from battery research medicine development. Thus, more efforts of TM should be adopted by the battery community, then potentially contribute critical insights for battery research.

Lack of standards is another challenge for TM[81]. Battery test standardization is as crucial as ML algorithms for addressing challenges in battery research. Specifically, for practical battery use, temperature typically fluctuate within a wide range, which is totally different from that in temperature-controlled experiment chambers. Thus, it is obvious that a deep collaboration between battery researchers from academic

and industry is necessary for data standardization.

Another shortcoming of ML method is the lack of physical insight of the pattern obtained. More physical and electrochemical laws should be considered for ML-boosted theoretical calculation. Especially, with the power of supercapacitors, multiscale system could be simultaneously conducted in one project, and then the coupling of multi-parameters, including the properties of the interface, the component of the electrolyte, and the crystal lattice data of the active materials, could be decoupled, ensuring a deep investigation of the dynamic reaction mechanisms in batteries, which is very hard to be accomplished by experimental efforts.

In summary, the ML is becoming a standard tool of battery research to add a new dimension in addition to the conventional materials fabrication, characterization, evaluation, and modeling. However, several challenges have not been addressed and this situation hampers the application of AI in battery development. Closer collaboration between experimentalists, modeling specialists, and AI experts in the future will greatly facilitate AI and ML methods for solving battery and materials problems that are difficult to be solved by traditional methods. Soon, it is anticipated that ML can widely help researchers deal with mega data analyzing missions, while researchers could focus on deciphering patterns discovered by AI. In this regard, we hope this contribution can shed light on the exciting opportunities of employing ML for materials-related problems difficult to be tackled through traditional means.

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人工智能在锂离子电池研发中的应用

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摘要: 锂离子电池已成为解决现代社会储能问题的最佳解决方案之一。然而，电池材料和器件开发都是复杂的多变量问题，传统的依赖研究人员进行实验的试错法在电池性能提升方面遇到了瓶颈。人工智能（AI）具有强大的高速、海量数据处理能力，是上述突破研究瓶颈的最具潜力的技术。其中，机器学习 (ML) 算法在评估多维数据变量和集合之间的组合关联方面的独特优势有望帮助研究人员发现不同因素之间的相互作用规律并阐明材料合成和设备制造的机制。本综述总结了锂离子电池传统研究方法遇到的各种挑战，并详细介绍了人工智能在电池材料研究、电池器件设计与制造、材料与器件表征、电池循环寿命与安全性评估等方面的应用。最重要的是，我们介绍了 AI 和 ML 在电池研究中面临的挑战，并讨论了它们应用的缺点和前景。我们相信，未来实验科学家、数学建模专家和 AI 专家之间更紧密的合作将极大地促进 AI 和 ML 方法用以解决传统方法难以克服的电池和材料问题。

关键词: 锂离子电池; 机器学习; 材料表征; 电池制造; 人工智能