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Understanding end-user requirements is pivotal in battery research. Notably, battery experiments conducted in academic laboratories frequently operate under conditions and parameters that diverge substantially from those encountered by EVs²⁰. The pitfalls associated with the creation of real-life experimental conditions can hinder the scaling-up and manufacturing of batteries, as well as impede the seamless transfer of technology to industry. This section delves into some of the bottlenecks inherent in existing methodologies.

A critical challenge in meeting industry demands lies in the scarcity of high-accuracy and economically viable battery models, which are essential for optimizing performance, ensuring safety, and facilitating diagnosis. Existing LIB models fall broadly into two categories: physics-based and machine-learning models. Physics-based models, classified as white-box models, intricately capture the dynamics of physical processes and are commonly formulated through partial differential equations (PDEs) or ordinary differential equations. This category can be further divided into electrochemical models and equivalent circuit models (ECMs)²¹.

In contrast, machine learning operates as a black-box model that typically lacks the incorporation of physically meaningful information, thereby constraining its utility for accurate physical state estimation. As previously highlighted, machine learning necessitates substantial and high-quality data for effective training and validation and operates independently of the laws of physics, which occasionally yields solutions that are physically impractical. Nonetheless, the advantage of machine learning over physics-based models lies in its ability to discern patterns within measured data, particularly in cases where the underlying physical laws are not well understood²⁵.

As shown in Table 1, the comparison of pure physics-based and machine-learning models is demonstrated. As evident, physics-based models require lower data requirements and have better extrapolation and interpretation but higher computation costs. On the contrary, machine learning enables lower computation costs but higher data requirements and worse extrapolation and interpretation. Based on the comparison, we are motivated to explore the prospects of combining physics and machine learning to compensate for their respective weaknesses and, at the same time, accommodate the strengths of each approach.

The integration of physics and machine learning proves advantageous for battery management due to the essential roles played by both disciplines. Managing batteries poses a real engineering challenge, requiring consideration of multiple factors simultaneously, including accuracy, robustness, computation cost, deployment cost, and more. Consequently, it becomes imperative to leverage available information in an

optimized manner to address this multifaceted problem effectively²⁶.

Limitations of pure physics-based models and machine learning models.

In 2021, Karniadakis et al.³⁸ introduced the innovative approach of crafting machine learning algorithms that incorporate physical information, aiming to mitigate the arduous task of training networks with vast amounts of data. This methodology capitalizes on leveraging the insights offered by physical laws, advocating for the integration of physical models into machine learning frameworks. Notably, this approach is applicable even in scenarios involving partially understood and uncertain systems, demonstrating scalability to address large-scale problems. In practical terms, where retrieving and cataloging data from experiments or real-life operations incurs substantial costs, conventional machine learning becomes a less favorable option for performance modeling.

a General integration framework; b representative examples of internal integration; c representative examples of external integration.

Effective battery health management, encompassing diagnosis, prognosis, and optimization, is paramount for enhancing efficiency and reliability throughout the battery's entire life cycle⁴⁹. Real-time improvement in battery health management is achievable by harnessing the potential of both physics and machine learning. In Table 2, we present a comprehensive summary of representative papers focusing on battery health management based on the integration of physics and machine learning. This table provides classification and detailed insights into the strategies employed to seamlessly integrate physics and machine learning for superior battery health management.

In LIBs, a critical safety concern is thermal runaway⁶⁸. This hazardous event arises from internal short circuits, resulting in an uncontrollable increase in cell temperature, potentially leading to combustion. The irreversible phenomenon of battery explosion poses a profound safety risk in industrial applications. Finegan et al.⁶⁹ present a comprehensive set of perspectives on the integration of physics and machine learning for predicting battery safety. In this context, we provide a summary of representative papers that have successfully integrated physics and machine learning for battery safety management in Table 3.

Based on our systematic survey and analyses of the existing challenges on battery health and safety, we identify the following perspectives of research in battery technology through the synergy of physics and machine learning.

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