Enabling battery digital twins at the industrial scale

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Summary

Digital twins are cyber-physical systems that fuse real-time sensor data with models to make accurate asset-specific predictions and optimal decisions. For batteries, this concept has been applied across length scales, from materials to systems. However, a holistic approach with a strong conceptual and mathematical framework is needed for battery digital twins to achieve their full potential at the industrial scale. Developing a standardized and transparent approach for data sharing between stakeholders that respect confidentiality is essential. Industrial battery digital twins also need principled methods to quantify and propagate uncertainty from sensors and models to predictions. Ensuring retention of physical understanding is important for the identification of "stiff" parameters, which require careful measurement. Combined with uncertainty analysis, this can unlock optimal data-driven sensor selection and placement and improved root-cause analysis. However, better physical modelling and sensing approaches for battery manufacturing and thermal runaway are needed. Furthermore, immutability of data is also necessary for industrial uptake, with digital ledger technology providing new avenues of research. We believe that digital twins could be transformative for the current lithium-ion battery technologies and also as an enabler for emerging new battery technologies, optimizing lifetime and value through asset-specific control.

Keywords: digital twin, cyber-physical system, lithium-ion, battery, model, data

Introduction – What are digital twins?

The aim of a digital twin is to make intelligent, data-driven, asset-specific decisions that improve performance. To achieve this, real-time sensor data and physically relevant models need to be combined within a computationally efficient framework.

Initially known as "mirrored models", digital twins were introduced in the early 2000s by Grieves[1] for product life cycle management. NASA embraced the concept in the early 2010s[2] and used digital twins as a means of monitoring and extending the lifetime of their vehicles. They describe a digital twin as a multi-physics and multi-scale probabilistic simulation that uses a combination of physical models, sensor data and fleet history to mirror the life of a physical vehicle[3].

Today, the core aim of a digital twin remains to connect a physical asset with a (near) real-time model that accurately reflects real behavior. Yet, despite many reviews of these

cyber-physical systems[2,4-6], the definition remains inconsistent, with several meta-reviews solely devoted to compiling and comparing definitions[5,7-10]. An interesting meta-review summarizing the different definitions was published by Kuehner *et al.*[8], who showcased four prevailing elements: virtual representation, bidirectional connection, simulation, and connection across lifecycle phases. Further high-level description of the concept can be found in other references[11-13].

The first mention of the digital twin concept for batteries can be traced to Peng *et al.*[14] in 2019 who created a digital twin for degradation assessment in spacecraft lithium-ion battery packs. More studies followed in subsequent years[15-31], covering various length scales and applications. However, whilst there is a growing interest in the battery digital twin concept, we agree with Niederer *et al.*[32] that these efforts need to transition from current one-off artisanal implementations to scalable industrial deployments. A robust conceptual and mathematical framework across battery stakeholders is essential to enable this transition. A notable example of what can be achieved was presented by Kapteyn *et al.*[33] who proposed the use of a probabilistic graphical model framework leveraging Bayesian statistics, uncertainty quantification, dynamical systems and control theory.

Today, a cynical view might be that a digital twin is just a rebranding of the idea of a model, however we suggest that digital twins bring additional value by capturing high-fidelity operational behaviour that enables optimal asset-specific decisions. A holistic approach, integrating data streams from mining to recycling, could enable rapid and reliable root cause analysis of battery failure which remains a key challenge. Essential elements of digital twins therefore include computationally efficient physical modelling, real-time data collection of key quantities of interest, robust and fast data assimilation techniques, and a stochastic optimization framework for intelligent decision-making (Figure 1). In the transition to industrial uptake, we also highlight the need for credible data and the emerging opportunity of immutable data via digital ledger technologies.

Visions of the battery digital twin concept from Wu *et al.*[16] and Yang *et al.*[34] provide a broad conceptual foundation, however in this perspective we tackle some of the key challenges hindering robust and industrial deployment. Finally, we argue that this approach should be applied not just to current lithium-ion battery technologies, but could be a transformative enabler for future battery chemistries such as lithium-metal and lithium-sulfur, where asset-specific decision-making is seldom considered in early-stage deployments, hindering commercialisation efforts.

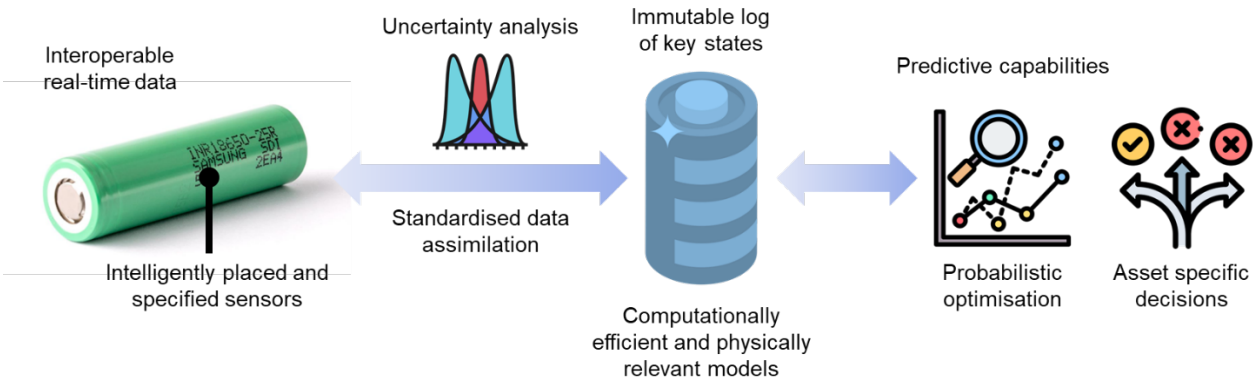

Figure 1 – Core elements of a robust battery digital twin framework

Hierarchy of battery digital twins

An industrial battery digital twin requires physical insight in order to achieve accurate state predictions (charge, energy, power, health, or safety). Data describing these states is collected by many stakeholders across the lifecycle, but often not shared, resulting in repeated experiments and loss of key physical information. Digital twins could be the needed unifying approach. While terminology can change, there are different types of digital twin depending on the level of abstraction[13]. For batteries, digital twins can be separated into component, device, and system twins, Figure 2, that describe the multi-length scale phenomena from microns to meters.

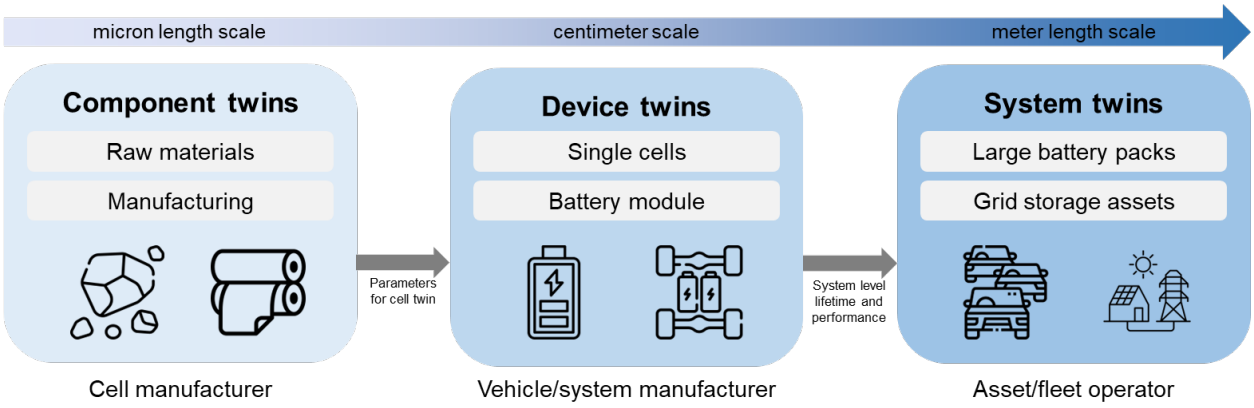

Figure 2 – Multi-length scale battery digital twins

Component twins – For battery component twins, the vision is to track properties and behaviors of individual cells and their constituent materials through the production process and relate performance to manufacturing conditions[29,35]. Notable efforts at this small length scale include Zanotto *et al.*[36] who provided an exhaustive description of data specifications for battery manufacturing digitalization. They highlight the need for a global overview of the links between experimental data and computing approaches. Here, there exist opportunities to fuse sensor data from raw materials extraction and manufacturing processes with higher length scale models similar to what was proposed by Yang et al.[34]. Yet, whilst battery production lines are becoming increasingly instrumented, physically

meaningful models of the manufacturing process and approaches that fuse these with *operando* usage data are extremely lacking, limiting the ability to make optimal decisions that are physically informed.

Furthermore, many high-fidelity characterization techniques used for probing the structure-function relationships in electrodes are often destructive or use small volumes of interest; limiting their applicability to digital twins. However, recent advances in the fusion of multi-modal characterization techniques with machine learning (ML) techniques have the potential to bridge the gap, as highlighted by Finegan *et al.*[37] A notable example is the work by Dahari *et al*[38], where they fused 2D and 3D microstructural datasets which have complimentary resolutions and field of views, with generative adversarial networks to achieve "super-resolution" and dimensional expansion, towards device level simulations.

Device twins – A device is composed of different components working together, and a device digital twin enables the study of how components interact with each other[13]. For batteries, this category encompasses single cells and modules. A notable opportunity here is to inform the initial parameterization of models directly from the manufacturing process, rather than the conventional approach using cell teardowns by third parties. If this is achieved, cell-to-cell variability effects could be better quantified, and their root causes understood. For instance, active material particle size distributions or in-line electrode thickness measurements could directly be fed into continuum-level device models. However, for robust adoption of this approach, careful estimation techniques for the key manufacturing parameters both in the factory and in the end-use application need to be considered, because certain properties, such as porosity, vary though the lifecycle of a cell.

System twins – A system is composed of multiple devices that combine to form a functioning whole. An example is a multi-module battery pack with control and monitoring of each single cell or module individually[28]. This category also includes battery management systems that gather data from multiple components[14-16,19-21,25,26]. At the highest level of magnification, this level includes systems that work together to create an entire network or a single asset (e.g., a large grid battery) from tens to thousands of individual cells. This also applies to a fleet of grid-scale batteries or electric vehicles, where system operators give specific attention to lifetime optimization. An opportunity that arises with a system of battery digital twins is that data can be pooled together to increase the predictive capabilities of a single asset and reduce uncertainty. Furthermore, interactions of the system twin with other non-battery digital twins might be considered, but this would require a unified standard for information transfer across all digital twin applications (not just batteries) which does not yet exist.

Integration across scales

Ideally, digital twins would encompass all aspects of components, devices, and systems, over all the various use phases of a battery[35]. Figure 3 highlights these main lifecycle phases, spanning manufacturing, operation (divided into 'devices' and 'systems') and recycling. This figure illustrates key points where data can be collected to feed into a digital twin. Broad data collection throughout life could enable discovery of the relationship between long-term performance (including end-of-life) and early-stage design and manufacturing choices, enhancing research and battery design efforts as well as being

an effective communication interface between scales. However, we recognize that within the battery field, protection of proprietary information is, and will continue to be, crucial. However, we argue that this can be achieved by careful consideration and integration of stakeholder-relevant viewpoints in digital twins to capture key physical aspects without revealing sensitive information. Notably, the big picture view of a battery digital twin presented in Figure 3 does not have to be developed or operated by a single stakeholder. Instead, the development could be shared between academia, manufacturers, OEMs, and asset operators; digital twins should allow interoperability of data standards across many stakeholders, which is critical.

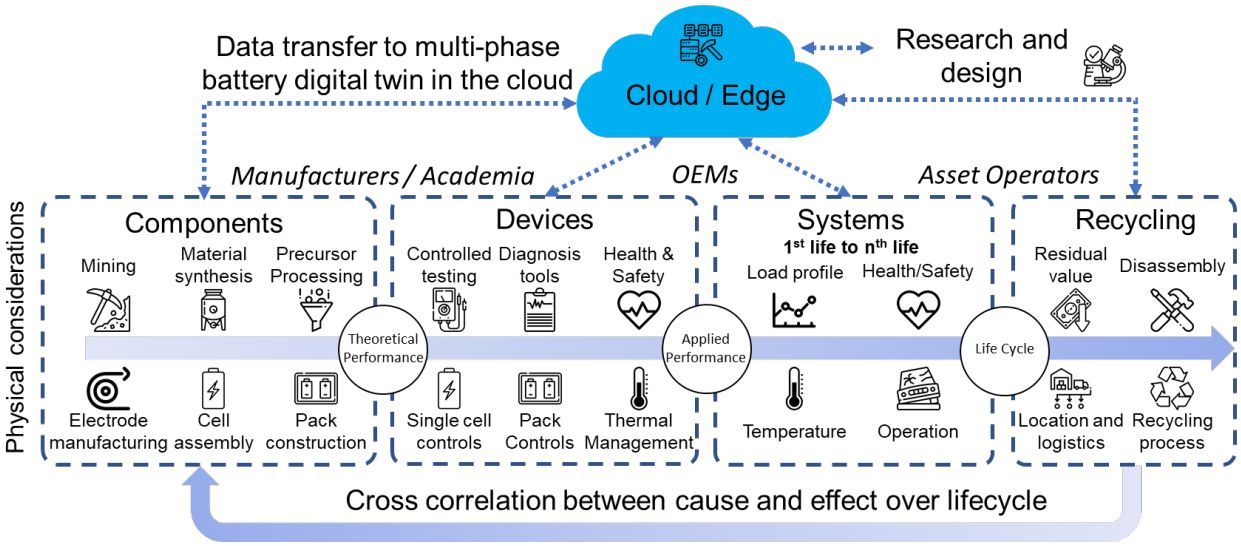

Figure 3 – Lifecycle considerations of a lithium-ion battery and opportunities for data collection towards an integrated battery digital twin

This inter-scale communication concept is represented in Figure 3 via the circles linking the different boxes. At the interface between the components and devices levels, it is important to have access to the theoretical performance of the cells or packs under different conditions, but there is no need to have full access to all details on the manufacturing process. An example of this connection, already well accepted, is the use of degradation modes[39,40] for diagnosis of health instead of the actual degradation mechanisms. Degradation modes refer to the impact on cells, such as lost active material or lost lithium inventory, but without having to relate to specific underlying mechanisms, such as mechanical cracking or binder decomposition. At the interface between the device and system levels, it is essential to understand the aspects that impact overall pack/cell performance and degradation (e.g., path dependence[41]) in order to enable long and safe operation of deployed systems. A digital twin should combine data from different sources and take advantage of initiatives like the battery data genome[42] to benchmark performance with known open datasets. At the interface between systems and recycling, digital twins must help in assessing state-of-health and state-of-safety without requiring a cost- and time-consuming deep dive into cells' electrochemical properties.

On the latter point, cross-correlating late-life rapidly changing behaviour such as thermal runaway failure and knee point capacity fade[43] against early-stage effects such as material impurities or manufacturing defects will be key. Here, we envisage increased

digitalization of the entire battery supply/usage chain as being a key enabler to provide new data streams, however suitable data-driven approaches for feature extraction, clustering and optimization are also needed. In recent years, a plethora of ML/artificial intelligence techniques have been applied to estimate behaviours such as capacity fade, however we argue that the battery community is still very much limited by the massive lack of available data, particularly from real-world performance conditions, despite the emergence of synthetic data[44]. In addition, explainable artificial intelligence approaches increasingly need to be exploited to ensure that physical insights are sought from data, as championed in other fields[45,46].

Scalable and principled assimilation of data and models

The choice of modelling approach for a battery digital twin is important, and to-date, empirical, semi-empirical, data-driven and physics-based models have been explored[47]. Of these, we see a hybrid approach of physics-based and data-driven methods being the most suitable for accurate and consistent predictions that can assimilate significant amounts of data because it offers a balance between flexibility and transparency. The large number of parameters involved in physics-based models (such as continuum models based on porous electrode theory) makes parameter estimation ill-posed, especially in the context of *operando* parameterization. On the other hand, pure data-driven approaches are promising—and research using these has exploded in recent years—, but it is too easy for researchers to fall into a trap of incremental changes without insight: for example, downloading a known (but limited) open dataset and trying some new feature or black-box ML technique, then using an over-simple metric such as root-mean-square error (RMSE) to claim improvement. Often this will also be a 'sledgehammer to crack a nut', for example a complex deep learning algorithm to solve what could be a simple linear regression problem.

This reduction in the signal-to-noise ratio of the literature unfortunately pulls focus away from the fact that firstly, most openly available datasets are severely limited in both the number of cells tested and the time they are tested for, and secondly, what one ought to strive for is *understanding of the physical mechanisms* that impact performance. There is thirdly the critical issue that proper statistics should be used to compare performance of data-driven models—for example by asking questions such as "what is the probability that this 0.1% RMSE improvement could have been caused by random chance". We implore the community to think about getting better data—more representative of real conditions, and across more cells and longer time periods—and aiming for methods that exploit the flexibility of data-driven approaches but do not ignore known physics. Besides the already mentioned synthetic datasets[44,48], two promising routes are, firstly, parameter estimation for continuum models using Bayesian techniques that give insight into parameter identifiability[49-51] and secondly, the use of ML tools to choose or fit functions within parametric models[52]. While all the possible degradation pathways can be computed from the evolution of the degradation modes[40,44], the method does not allow forecasting of the relationships between usage and degradation, especially at the mechanism level. Since no physics-based model currently captures all battery degradation mechanisms either, there is an opportunity for hybrid physics/data driven approaches to learn relationships not captured by the different models. An excellent overview of a number of

different ways of combining physics-based and data-driven approaches was given by Aykol *et al.*[53].

The ill-posed nature of *operando* real-world parameterization of physics-based models is also commonplace in other field such as computational biology. Here, notable work from Gutenkunst *et al.*[54] highlights challenges with model parameterization, but note that fitting can still result in accurate predictions despite some parameters being very poorly constrained (i.e., not affecting the measured data). From this, they suggest the notation of “sloppy” parameters, with model outputs effectively being dictated by only a few “stiff" parameters. In a similar vein, control engineers have long understood the concepts of observability and identifiability of states and parameters from measured data[55-57] and have many mathematical and software tools available to analyse these, such as the STRIKE-GOLDD toolbox[58]. Unfortunately, these critical issues have been largely ignored by the growing battery modelling community who need to highlight more clearly the key “stiff” parameters in their models, ensure these are measured to a sufficient accuracy, and understand the uncertainties of parameters and how they propagate to model predictions. All these challenges become even more acute as one scales to larger models such as are being proposed for some digital twins[59].

In parallel, optimal sensing and data collection strategies are needed. Current approaches often fall into the artisanal category, with often suboptimal placement and selection of sensors. A review by Liu et al.[60] and a perspective by Yang et al[34]. showcased characterization and modelling tools from materials to packs. While all these sensing approaches have value, the community also needs to consider what are the key states to measure, the practicalities of measurement, and the required frequency of measurement.

An example of this is the internal temperature of a battery, which is often inaccessible but important for determining thermal cut-off limits. To address this, ‘virtual sensors’ are being developed to estimate inaccessible states, based on accessible measurements and modelling. For instance, Richardson et al.[61] proposed a battery internal temperature estimation approach using impedance measurements. Another key state that is difficult to measure is negative electrode potential vs. Li/Li^+, which is important for the development of fast charging schemes that account for lithium plating. Here, the most common approaches include the use of physics-based pseudo-2D models that estimate negative electrode potential, however more recent work has shown the possibility of using other modeling approaches[31] as well as data-driven methods[62]. Furthermore, heterogeneous degradation[63] can cause low-order model predictions to deviate over lifetime, motivating some interest in higher fidelity models, however computational efficiency remains a barrier to uptake, and reduced order modelling efforts are also needed.

Finally, understanding how sensor noise propagates through models to estimated states and thus the prediction accuracy is needed, with this information then being used to better inform the selection and placement of sensors. Approaches for industrial battery digital twins should be considered with a probabilistic lens, rather than deterministically.

Future directions for battery digital twins

With battery digital twins still in their relative infancy, the work done to date has mostly focused on tracking and estimating states relating to electrochemical behaviour and cell degradation. However, on top of multi-scale communication features mentioned above and the need for more robust frameworks, a major facet which will need consideration in future battery digital twins is safety, where ideally, the digital twin is able to track and predict rapid failure. Whilst research in battery safety modelling has progressed, the tightly coupled relationship between mechanical, electrical, thermal and electrochemical considerations leads to highly variable behavior as reviewed by Deng et al.[64]. Better understanding of degradation and its impact on safety is therefore needed in addition to datasets which allow researchers to validate their models. This issue was highlighted by Finegan et al.[65] who also provided perspectives on combined data-driven and physics approaches to reliably recreate failure scenarios and gain better insights into failure modes.

Beyond the use cases for digital twins in first-life applications, there are emerging opportunities driven by challenges in second-life battery grading and end-of-life traceability. An interesting approach to address the issue of traceability and trustworthiness of usage data is the application of digital ledger technology, with blockchain being one specific form of this, using cryptography to control new data entries. Here a blockchain is a decentralized ledger shared amongst a network of computers and is able to track ownership. Junior et al.[66] reviewed how this can be applied to the battery supply chain by identifying challenges around the development of new unique identifiers for the different parts of the battery manufacturing and use phase, towards creating an immutable database. The issue of how best to link physical and digital assets in a trustworthy way remains an open question. A notable effort towards a realistic implementation is that of the mobility open blockchain initiative (MOBI) battery initiative[67]. Designed to aid regulatory agencies such as the EU Battery Directive to improve battery cycle life and stimulate circular economy business models, MOBI released, in 2018, the VID standard (a vehicle's self-sovereign digital twin), which allows vehicles to be anchored on a blockchain. Moving forward, there is also work towards developing standards around state-of-health tracking within a battery passport framework, and digital twin approaches are likely to have a role to play here.

In this regard, proposed EU legislation is moving towards mandatory labelling of batteries, with QR codes which present information on carbon footprint, capacity, durability and chemical composition[68]. As more information is being provided, and critical economic decisions being made based on this, it is therefore increasingly key to ensure immutability of the information. Here, the field of physical unclonable functions (PUFs) has significant potential. PUFs exploit inherent randomness introduced in the manufacturing to provide a unique physical "fingerprint" of a device. Gao et al.[69] summarized recent advances in PUFs which exploit optical, circuit time-delay and volatile/non-volatile memory characteristic effects as well as providing examples of applications. To our knowledge, this has not yet been applied in the field of batteries and could be an approach to address the immutable digital-to-physical coupling of digital twins.

With such a large focus on the assimilation of data in battery digital twins, the temptation is to collect as much data as possible. However, this can rapidly result in very large time-

series datasets from millions to billions of cells, which will lead to insurmountable storage and processing costs. Thus, looking forward, approaches that distil the core underpinning insights in a data-efficient manner will be critical for a practical digital twin.

Finally, next generation battery chemistries such as lithium-metal, lithium-sulfur and sodium-ion batteries have the significant potential, however their commercial uptake has been limited in part due to poor lifetime, uncertain performance and a lack of engineering-focused modelling tools. Improvements in the core chemistry are still needed, however we argue that a battery digital twin approach applied to these emerging chemistries could also have a significant role to play to accelerate their deployment. For instance, the stability of the lithium-metal plating/stripping is a key factor dictating the lifetime of lithium-metal based batteries. More intelligent and health aware regulation of the applied current in these cases can significantly influence the performance, yet better models of this process are needed. Similarity, within the family of lithium-sulfur batteries, understanding the polysulfide shuttle reaction is needed, as well as models which describe this, but which are observable with real-world *operando* techniques. As such, materials chemists and control engineers need to more closely work together to translate state-of-the-art understanding of chemical physics into applicable mathematical descriptions which enable parameterization and controllability.

Conclusions and recommendations

Digital twins fuse (near) real-time sensor data with models towards making asset-specific optimal decisions, with this concept now applied across the battery lifecycle; from manufacturing to recycling. However, these are largely isolated efforts, with artisanal implementations and we argue that a holistic approach with a robust conceptual and mathematical framework is needed to unlock the full potential and enable industrial uptake. However, we acknowledge that barriers to this include commercial sensitivities around the information, but argue that a battery digital twin can act as an effective communication vehicle or proxy between stakeholders; providing only the required information in a transparent way.

In this respect, we make the following conceptual recommendations to the battery community in order to enable battery digital twins at the industrial scale:

- Stakeholders across the battery supply chain need to come together to create a unifying and interoperable framework with agreed standards that respects individual stakeholders' intellectual property.
- Conceptually, the community should approach industrial battery digital twins from a probabilistic lens rather than deterministically.
- Frameworks are needed to describe how uncertainty propagates through a battery digital twin, fusing physics-based models for the identification of "stiff" critical parameters, with understanding of how sensor noise impacts predictions.
- Data-driven approaches for optimal sensor selection and placement are needed, with data acquisition strategies that avoid over sampling of data without loss in accuracy in state-estimation.
- The best aspects of physics-based and data-driven modelling approaches should be combined to give models that are accurate and computationally efficient, but with explainable predictions.

- The development of physically meaningful models and data assimilation approaches for the battery manufacturing process which enable accurate prediction and optimization should be prioritized.
- Authors should move away from static and basic cell datasheets in favor of a robust battery digital twin.
- Focus on real-world detectability and predictability of thermal runaway events should be increased through improved physical models, which capture the influence of degradation, and early-stage detection approaches.
- Early adoption of a battery digital twin framework for new battery chemistries should be encouraged, with closer co-operation between material chemists, modellers and control engineers.

As battery digital twins become increasing useful, so does the importance of ensuring that the data provided to and by them is trustworthy, since economic decisions will be increasingly based on it. Here, opportunities within the field of digital ledger technology have the potential to enhance the trustworthiness of the data; from ensuring raw materials are sourced ethically, to reliable lifetime data for accurate calculation of remaining asset value. Furthermore, providing an immutable cyber-physical link will be critical with approaches such as physical unclonable functions providing an interesting potential solution for physically defined digital fingerprints.

Thus, with a combined effort across the battery supply chain, battery digital twins have the potential to significantly accelerate the pace of development, improve understanding of root-causes of failure, whilst reducing cost and enhancing battery lifetime.

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