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Digitalization of Battery Manufacturing: Current Status, Challenges, and Opportunities

Elixabete Ayerbe,* Maitane Berecibar, Simon Clark, Alejandro A. Franco, and Janna Ruhland

As the world races to respond to the diverse and expanding demands for electrochemical energy storage solutions, lithium-ion batteries (LIBs) remain the most advanced technology in the battery ecosystem. Even as unprecedented demand for state-of-the-art batteries drives gigascale production around the world, there are increasing calls for next-generation batteries that are safer, more affordable, and energy-dense. These trends motivate the intense pursuit of battery manufacturing processes that are cost effective, scalable, and sustainable. The digital transformation of battery manufacturing plants can help meet these needs. This review provides a detailed discussion of the current and near-term developments for the digitalization of the battery cell manufacturing chain and presents future perspectives in this field. Current modelling approaches are reviewed, and a discussion is presented on how these elements can be combined with data acquisition instruments and communication protocols in a framework for building a digital twin of the battery manufacturing chain. The challenges and emerging techniques provided here is expected to give scientists and engineers from both industry and academia a guide toward more intelligent and interconnected battery manufacturing processes in the future.

1. Introduction

With the advent of electromobility, the market for electric vehicle (EV) batteries has seen consistently high growth rates over the past few years, and it is expected to grow further, as it is forecasted by BloombergNEF, which stated that EVs will represent 70 percent of all passenger vehicles by 2040.[1] At the same time, the share of renewable energy sources in the electric

grid are growing, and by 2025 the installed capacity of wind and solar will exceed that of coal, natural gas, and hydropower.[2] The need for grid-scale energy storage to buffer supply from these intermittent sources is motivating the development of "mega-batteries" powering regional electric grids. Regardless of the application, cost-efficient, high-performance and sustainable batteries are essential to meet these demands and to maintain the competitiveness and guarantee the economic viability of these applications (i.e., EVs and grid-scale storage).

Today, lithium-ion batteries (LIBs) are the dominant battery technology and have been widely deployed in portable electronics, EVs, and grid storage due to their enhanced features, such as high energy density, high power density, and long cycle life.[3] Despite this dominance, LIB technology undergoes continuous development to meet the tightening cost and performance requirements from industry. These efforts employ several strategies across the battery value chain, targeting improved materials, cell designs, operational controls, manufacturing processes, and recycling. On one hand, the research on LIB materials has scored tremendous achievements and many innovative materials have been adopted by the industry.[4–8] On the other, the LIB technology does have some fundamental limitations for which alternative battery

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technologies beyond the LIBs are also in development.[9] In any case, to meet battery performance, cost and sustainability targets, several improvements on both materials and cell manufacturing are needed. The latter, the research on LIB manufacturing process, has received less attention[10–12] and this leaves a potential opportunity to improve the cell manufacturing process, making it more efficient, more cost effective, and more sustainable.

Furthermore, economies of scales[13,14] enables to reduce battery manufacturing costs, and to gain an advantage over the competition. Although the gigascale production of LIBs has succeeded in reducing costs, they present a variety of challenges for maintaining operational and quality standards. In addition to the logistical challenges that involves moving such vast amounts of material in a reliable way, it is well-established that LIB cell performance (i.e., energy density and cycle-life) is sensitive to variations in the manufacturing process. Thus, due to numerous consecutive process steps that make up the battery manufacturing chain and the interaction of these steps and the high number of individual process parameters, an optimization going beyond traditional trial-and-error approach is crucially needed. And here is where digitalization-based automation can play a capital role.[15,16] Virtual replicas of the actual manufacturing process can help to shorten time-to-market, leading to a greater profitability by reducing expenses for cell prototyping and optimization. Even more, virtual developments can reduce the expense of redesigns and tool changes for problems found during pre-series launch. Eventually, virtual prototyping may completely replace physical prototyping and it is expected that digitalized gigafactory operations can optimize their production in real time, improving productivity, product reliability and quality. In this way, gigascale battery cell production also needs to be occurring within the background of the wider ongoing shift toward the so-called Industry 4.0 paradigm. This provides excellent opportunities for the adoption of digitalization to address the challenges of gigascale battery cell production, not only because it can effectively manage the production logistics (production and distribution efficiency, time-management, energy usage, etc.), but also it can assess and optimize the properties of the resulting battery cells.[17–21]

The process of digitalization, which has been demonstrated with success across many fields,[22–24] is characterized by the transfer of analogue product features into digital values, to enable an electronic and informational transfer, storage, and processing of the data.[25] Despite some of the goals for digitalization of the battery manufacturing process are quite ambitious, the hope is that it can evolve into automated decision-making, near perfect mechanical automation and symbiotic human integration, leading to battery manufacturing facilities that will be completely interconnected and "smart", from raw materials to finished battery cells.

In this review, we first evaluate the current developments and those that are being developing in the framework of the digitalization of LIB manufacturing processes. Then, we summarize the challenges and opportunities of the implementation of these new technologies. And, finally, we provide a summary of future trends on battery manufacturing processes evolving new manufacturing processes and new battery chemistries. Thus, this manuscript highlights the challenges that still need

to be overcome toward the digital transformation of the current LIB manufacturing chain, with the ultimate goal to solve some key issues of LIB manufacturing, but keeping an eye on emerging technologies and disruptive manufacturing processes, which may eventually result in increasing the production efficiency and lowering the cost and energy consumption of the batteries.

2. Current and Near-Future Developments in Digitalization of the LIBs Manufacturing Processes

The battery community continues to make strides toward Industry 4.0 with the aim to achieve smart manufacturing processes with greater intelligence, sustainability, and customization. This approach facilitates the interaction, integration, and fusion between the physical and cyber worlds of manufacturing.[26] Digital Twins (DTs) are attracting growing attention from academic researchers, as well as industrial players in recent years, as a promising means to achieve the cyber-physical fusion of both manufacturing processes and products.[27–30] Through high-fidelity modelling, real-time interaction and data fusion, DTs can reproduce a physical asset or process accurately in the digital world and enable more effective monitoring, optimization, and prediction of the physical counterpart through its lifecycle.[31–34]

Inspired in the work of Bazaz,[35] which presented a five-layer digital model to replicate the physical object as a virtual object and to collect and convert data within a manufacturing plant, the present paper considers hypothetical three-layer DTs that will enable covering all requirements to represent the physical space in the virtual space. The proposed 3-layer structure of the DT of the gigascale LIB manufacturing,[36] which includes the main steps of 1) electrode preparation, 2) cell assembly and 3) activation by formation steps, is depicted in **Figure 1**.

1) *Digital manufacturing framework layer* contains data collected from the physical manufacturing plant and deals with the communication network. The communication between a DT and its counterpart in the physical space relies on bi-directional and real-time data sharing. This framework collects data in real time through cost-effective sensors and stores the data in a Cloud space to promote the remote management of the plant.

2) *Models' layer* describes, provides understanding, and predicts the twin's operation. For this evaluation, we draw a distinction between process and machine models. Process models are used to describe the relationship between the process and structural parameters, while machine models refer to representation of machines and equipment in the manufacturing process chain. In any case, coupling of models across scales is required in the digital twin to analyze the interactions between machining processes and related machine tools.

3) *Standards* layer: the full digital twin vision requires interoperable digital twin definitions and tools. Considerations for digital twin, cybersecurity and interoperability take place in this layer.
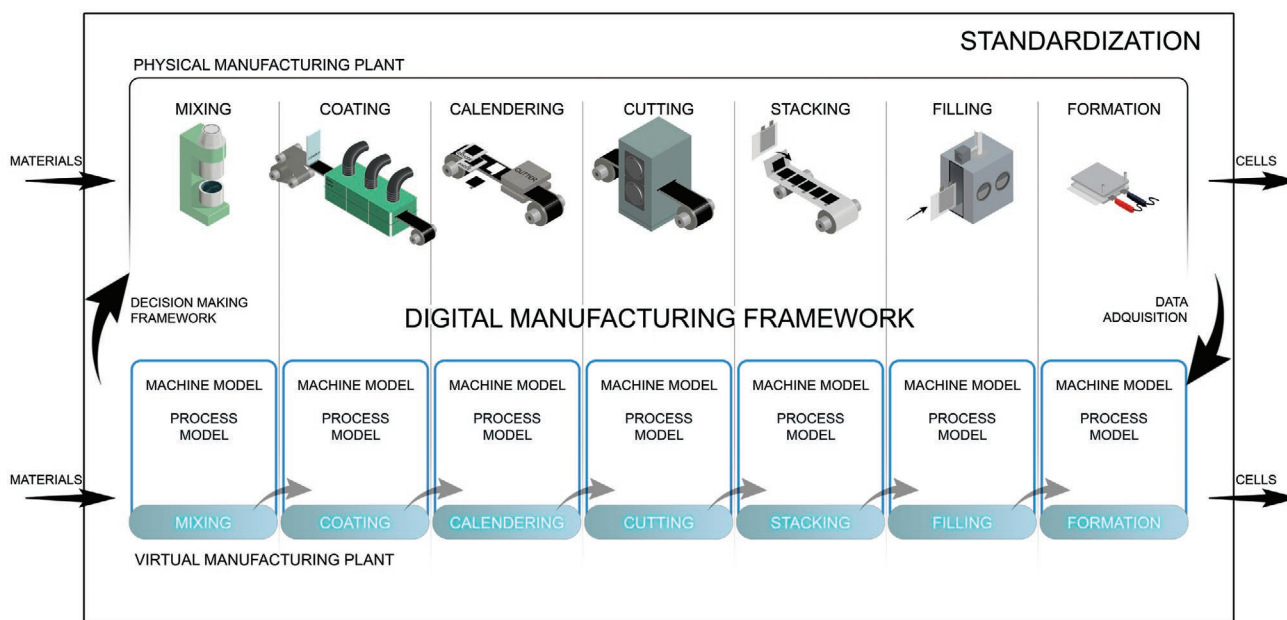
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Figure 1. Overview of the 3-layer structure for the proposed Digital Twin of the LIB manufacturing chain.

Within this Section, we analyze the current developments and those foreseen in a near-future, in the field of digitalization of the LIB cell manufacturing, with special emphasis in each of the layers presented in Figure 1. The enabling technologies and related tools are also discussed in detail.

2.1. Digital Manufacturing Framework

The *digital manufacturing framework* consists of a smart digital infrastructure[37] that deals with the communication network and data processing methods. The communication network is one of the critical factors for enabling the establishment of DTs. State synchronization between a DT and its counterpart in the physical space relies on bi-directional and real-time flow of data.[38] In parallel, sensors are integrated to measure different relevant quantities along the whole manufacturing process, and to generate data that can be stored in a central data warehouse to allow for post-processing of historical information to support process optimization or root cause analysis.

2.1.1. Data Acquisition

Data acquisition represents a crucial aspect of the digitization of production environments.[39] In the field of battery cell manufacturing process, this consists of sequential steps with many interdependencies.[40] A large quantity of data reflecting both the processes and equipment must be collected to guarantee the monitoring of the battery cells, ensuring required quality control, sustainability and cost efficiency. The work developed by Huber et al.[41] goes toward this direction and presents a method for the automated classification of battery separator defects based on the data recorded by a machine vision system.

Data acquisition can be performed manually or through automated workflows. During manual data acquisition, the user uploads data (offline product analytics, production plans, etc.) through for example a web-based user interface. However, manual data acquisition is often too slow and cumbersome to support highly efficient processing. Instead, automated data collection can supply information as soon as it is available and enable workers to promptly intervene on unplanned production downtime, and even take conscious decisions on what to improve. An example of the automatization data extraction in battery manufacturing is the approach described by Thiede et al.[42] that considers over 500 changeable process parameters (e.g., line speed of coating/drying or calendering), and resulting state variables (e.g., power demand), 1029 intermediate product features (e.g., average particle diameter, conductivity, and tortuosity), as well as 65 final product properties (e.g., capacity and inner resistance). In this case, industrial data acquisition systems like the Supervisory Control and Data Acquisition system (SCADA) or Manufacturing Execution System (MES) were used. The data was extracted and transformed into a form that was stored and further processed in a data warehouse.

Contrarily to a database, which only stores the data, the main function of a data warehouse is to gather, merge and store the data in the way that it would be accessible for further usage. Turetskyy et al.[43] outlined a holistic approach to represent the entire production cycle of battery cell manufacturing in a data-driven manner. Furthermore, the authors described the combination of automated and manual data acquisition, as well as merging of data from different sources, of different communicational protocols, and of different formats toward accessibility, convenient data management, and visualization.

In this landscape, the demand of intelligent sensors and sensor systems as the key enabler of enhanced flexibility, adaptability, configurability, and agility in manufacturing processes has been fully recognized, and also confirmed in other

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fields.[44,45] Sensors (e.g., inductive proximity sensors, optical sensors and laser sensors) can provide the actual status of the production phase. However, to the best of the authors' knowledge, in the battery manufacturing field the use of this kind of sensors and their interaction with their environment, is currently mostly limited to safety functions, defect detection, automatic calibration of workpieces or simple measurement methods. Various types of sensors are already used in battery cell manufacturing processes to monitor quality. For example, the coating thickness can be measured at various points in production using appropriate sensors, such as a laser triangulation or inductive measurement.[46] Similarly, in the separation and stack formation steps, camera-based measurement methods are used to measure positioning accuracy.[47,48] However, this could be insufficient, especially for stack assembly, because the position and three-dimensional shape of the individual sheets can change during the stacking process, as well as, during further processing of the stack.

Furthermore, during calendering step, the force on the rollers can be measured as described by Meyer et al.,[49] and in handling tasks with negative pressure, such as stacking, parameters such as the pressure and the air flow rate can be measured as shown in several works.[50,51]

2.1.2. Interoperability and Communication Protocols

Enabling interconnectivity across a diverse set of devices is one of the main requirements to achieve the vision of Industry 4.0.[52] This must be supported by large amounts of data that can be used to inform production decisions.[53] However, one of the main challenges in implementing this solution is establishing interoperability of data among devices. This challenge can be overcome through the acceptance of relevant standards for the exchange of models and cyber-physical assets[54] as well as the development of dedicated data tools for the battery domain.

The Functional Mock-up Interface (FMI)[55] standard has become a preferred approach to support the exchange and co-simulation of models describing the overall behavior of complex systems. The FMI is a free standard that defines a container and an interface to exchange dynamic models using a combination of XML files, binaries, and C code zipped into a single file. FMI was developed with the intention to simplify the creation, storage, exchange, and reuse of dynamic system models of different simulation systems for cyber physical systems, among other applications. Today, FMI is applied for two main purposes: model exchange and co-simulation.

The model is encapsulated as package called a Functional Mock-up Unit (FMU), which describes the model as a system of differential, algebraic and discrete equations with time-, state- and step-events. The FMU can then be distributed as a single zip file.

The definition of standardized FMUs also enables a relatively new simulation paradigm called co-simulation, which targets the joint simulation of loosely coupled stand-alone sub-simulators. In a co-simulation system, the sub-simulators are solved independently of each other, with the exchange of data limited to discrete communication points. Each sub-simulator accepts inputs from other sub-simulators, use a built-in solver routine to advance to the next time step, and output some results. The co-simulation algorithm coordinates the time synchronization and interactions across the sub-simulators. This black-box approach can also allow developers to share their models, while also protecting their knowledge and associated intellectual property rights (IPR).

FMI has been applied to simulate complex physical systems, including multifunctional production engineering applications.[56] First steps have also been taken toward implementing FMI standards for model co-simulation in a multi-scale core model for battery cell production, such as the model described by Schönemann et al..[57,58] This approach, shown in **Figure 2**, proposes a method to analyze LIB production systems based on coupled simulation models, with a focus on the interactions between production units, processes, machines, technical building services, and the building structure. In a case of study for battery electrode production, the method is applied to evaluate the influences of different process configurations on intermediate product characteristics and seasonal effects of energy demand. The case study also investigated how different process routes and parameters in electrode production affect the characteristics of battery slurries and coated electrode metal foils.

To enable this interoperability, standardized interfaces, and protocols for communication between systems are required. The communication needs of a DT can be divided into the following categories:1) communication between the subsystems of a digital twin and 2) communication between a digital twin and its corresponding physical counterpart. For models, the utilization of FMI/FMU standards is a significant development to support the model exchange and co-simulation. However, physical assets that should be incorporated into a digital world of information also require similar standardized interfaces to allow for the implementation of DTs and to ensure cross-platform interoperability. This is the purpose of the Asset Administration Shell.

Within the Industry 4.0 paradigm, an *asset* is defined as anything that requires a connection to the network. The Asset Administration Shell (AAS)[59–61] is a standardized and secure communication interface designed to integrate an asset into a network. It provides an asset with an unambiguous identity such that it can be addressed on the network and regulates access to information about the asset. The AAS forms the digital basis for autonomous systems and AI, and it enables the implementation of digital twins. The AAS comprises a variety of submodels, which describe all the information and functionalities of a given asset. This includes information like the features, characteristics, properties, status, parameters, measurement data, and capabilities of an asset. For developers, a free open-source tool called the AASX Package Editor is available to create and edit Asset Administration Shells for a given use case in XML and JSON formats. The AASX Explorer can be downloaded as compiled software licensed under Eclipse Public License 2.0 (EPL 2.0).

The Open Platform Communications Unified Architecture (OPC UA),[62] created by OPC Foundation, is another example of standardized communication protocols. The OPC UA defines a set of common data description and syntax expression methods; that is, each heterogeneous control system can
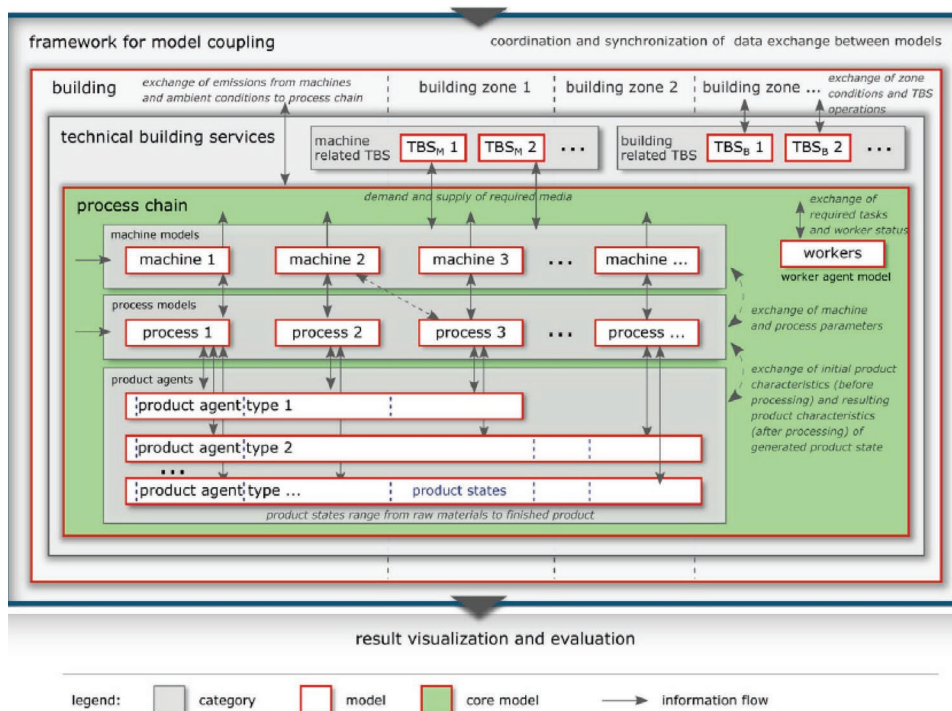
Figure 2. Schematic of a unifying multi-scale core model. Reproduced with permission.[58] Copyright 2021, Springer Nature.

use OPC UA specification to describe its own information, and then through OPC server/client mode, the third-party system can obtain the data of a heterogeneous control system.[63] With respect to the implementation of OPC UA in LIB manufacturing, Han et al.[64] established an information model of the intelligent manufacturing based on the analysis of the architecture, functional categories, and information interaction of the intelligent manufacturing workshop. The approach for implementing data storage and interaction of the information model based on the OPC UA server/client was also discussed. The information model was applied to realize the interconnection and interoperability of production management data, material management data, equipment management data, and quality management data among various levels of the workshop, which verified the feasibility of the proposed information model.

In the area of cross-machine information models, as a basis for the corresponding data-based applications, there are already numerous generic machine models based on OPC UA, which underline the necessity of merging proprietary information models, but require manual identification and linking of the parameters.[65,66] The universal machine technology interface (UMaTI)[67] standardization initiative represents a step in the right direction in this respect, but only covers a fraction of the relevant parameters and does not offer a solution for a large proportion of existing plants and for high-frequency data. With UMaTI, an OPC UA Companion Specification is derived on the basis of certain defined use cases, with the aim of generating a suitable information model as a standardized interface that already exists for machine tools within the framework of a restricted parameter space. There are plans to extend the

parameter space, but no significant efforts exist yet with regard to battery cell manufacturing equipment's. Another example of interface standardization is Packaging Machine Language (PackML),[68] but to the authors' knowledge it has not yet been applied in battery manufacturing field.

Cyber-physical production systems enable an interaction between the physical components and the virtual data layer of a production system, by considering the corresponding technologies for data acquisition, data storage, and data processing in an integrated manner.[69,70] A standardized information model for battery cell production plants still needs to be developed, so that existing models can be applied flexibly and with little effort to real battery cell manufacturing plants.

The need to exchange data across the battery value chain is driving a push for a common Battery Identity Global Passport (BIGP),[71] supported by the Global Battery Alliance (GBA). The proposal calls for the BIGP to be a digital asset that accompanies the battery throughout its lifetime, all the way from manufacturing to recycling. The BIGP should contain descriptions of the key technical data, including battery chemistry and origin, as well as data related to the operational history of the battery such as state of health and chain of custody. This information will be helpful for second-life users who want to evaluate the suitability of a specific battery for their application or recyclers who want to direct cells to the appropriate recycling process, based on their chemistry.

The vision of digitalized battery manufacturing ultimately requires some common machine-readable language for describing battery data, based on a common conceptualization shared by the community. Ontologies are a tool ideally suited to meet this need, and efforts by the battery research and

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development community to develop fully open battery cell and manufacturing ontologies are underway.

2.1.3. Ontologies for Battery Manufacturing

An ontology is a data model that encompasses the knowledge about a topic or domain. It describes a domain as a set of concepts and the relationships between them, and provides a common standardization platform for exchange of data and information processing by humans and machines.[72] Once established in an electronically readable form, the ontology provides a formal categorization scheme to facilitate digitalization of industrial technologies and support the integration of Artificial Intelligence (AI) and Big Data approaches. The uses of ontologies in the digitalization of battery manufacturing mainly include: (i) Defining a standard vocabulary for battery classes and properties to support consistency in digital assets, (ii) Facilitating the development of co-simulation frameworks by defining reason-based interfaces between sub-models;[73] and (iii) Accelerating AI optimization by allowing machine reasoning over large datasets.

Manufacturing is one application area that is embracing the adoption of ontologies for both sharing data between computerized tools and establishing a standard vocabulary for efficient communication.[74] Modern manufacturing is generally reliant on global supply chains, which may include subcontracting, distribution of industrial processes, and collaboration both internally and externally. In the digital age, all these activities must be coordinated by information systems, which may themselves include interfaces to many different software systems. To add an additional layer to the challenge, software and hardware are constantly changing, thus requiring any unifying framework to constantly adapt. Therefore, achieving reliable interoperability of data and software that is resilient to a changing technological environment is essential to the success of manufacturing enterprises today.

Industry 4.0 takes this one step further and envisions fully automated manufacturing environments in which Cyber-Physical Production Systems (CPPS) continuously exchange data among each other, and autonomously adapt themselves to a given task. Ontologies fulfil a unifying role by providing a common, logically consistent vocabulary for describing knowledge in the domain and guiding the development of associated software. However, the successful integration of ontologies into real applications is difficult due to the challenge of developing and maintaining ontologies that are correctly built on established standards, well-documented, and maintained beyond the initial development period. Successful ontologies must stem from a robust and globally relevant top-level ontology that provides reusable modules for shared terminology, definitions, and formalizations. Such a top-level ontology serves as a common basis for derived domain ontologies to describe specific processes or software applications.

To date, there has been relatively little development of ontologies dedicated to batteries and battery manufacturing. There are currently two coupled ontologies in development to meet this need: the Battery Interface Ontology (BattINFO)[75] and the Battery Value Chain Ontology (BVCO).[76] BattINFO is designed to cover all knowledge related to the battery cell itself. This includes descriptions of electrochemistry, battery properties, characterization, observation, and modelling. BattINFO is developed through the European Union project BIG-MAP with the immediate goal of supporting AI-driven discovery of new battery materials. The BVCO describes the processes, materials, and equipment used in the value chain related to battery manufacturing and recycling. BVCO imports BattINFO to provide a single consistent description of a battery cell, and supplements it with knowledge related to battery materials mining and processing, the battery manufacturing process steps, as well as battery second life and recycling processes. Both BattINFO and BVCO use the top-level European Materials and Modelling Ontology (EMMO), which allows them to integrate with other domain ontologies stemming from EMMO. More information on ontologies for battery development, BattINFO, and BVCO is available in a dedicated review paper.[77]

2.1.4. Digitalization Frameworks and APIs

Initiatives for the development of multi-scale frameworks and application programming interfaces (APIs) for battery digitalization are currently the focus of intense interest from both industry and academia. A variety of approaches are in development to address the challenges of storing, processing, and utilizing large volumes of heterogeneous battery data. Some common aspects include battery data collection, storage, processing, and integration into model-based workflows.

Frameworks for the digitalization of battery manufacturing and data management are in development by both diversified engineering companies,[78] as well as start-ups. Recent commercial solutions for battery data management and analytics have been developed by battery technology companies and research spin-offs like, Voltaiq,[79] Energsoft,[80] Astrolabe Analytics,[81] and Batalyse.[82]

Typical commercial solutions focus on implementing workflows to gather battery data from different characterization equipment, which may have different standards and formats for storing data depending on the manufacturer. This data is then parsed and stored into a semantic query language (SQL), or similar database to support semantic querying of large datasets. Featurizers are often included to extract out relevant indicators of battery performance from the dataset and may be combined with ML-driven analytics or physics-based models.

The research battery data community is creating similar frameworks to support digitalization of battery discovery, design, and development. This has resulted in a collection of loosely complimentary software to address different challenges in the field. These include examples such as Kadi4Mat, Galvanalyser, BEEP, PyBaMM, and the Battery Archive.

Kadi4Mat[83] is developed by the Karlsruhe Institute of Technology (KIT) to support the easy access, exchange, and interoperability of materials data. Kadi4Mat is a web-based application that combines the features of an electronic laboratory notebook (ELN) and data repository. The web-based node editor enables users to define simple workflows that can be executed locally. The infrastructure, shown in **Figure 3**, includes tools to upload, manage and exchange data, set flexible metadata schemes, and establish
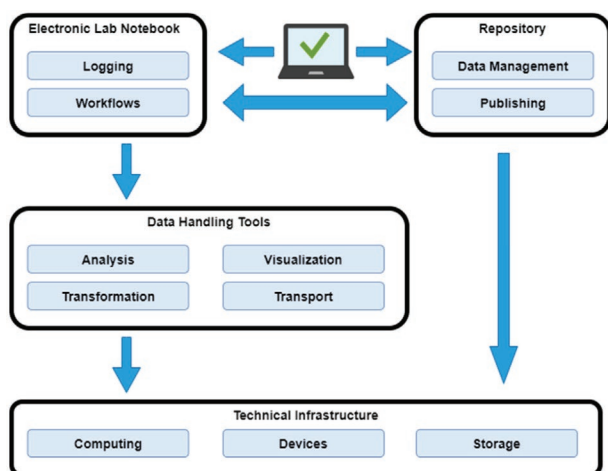
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Figure 3. Conceptual overview of the infrastructure of Kadi4Mat. The system is logically divided into the two components ELN and repository, which have access to various data handling tools and technical infrastructures. The two components can be used both graphically and programmatically via uniform interfaces.[86]

automated workflows. Although ostensibly geared toward the field of material science, the development of Kadi4Mat is supported by some of the leading German projects and clusters on battery research including FestBatt[84] and POLiS.[85] Kadi4Mat is open-source software, currently available for download and use in the community under Apache License 2.0.

Galvanalyser is a database solution for battery test data, which collects raw data from a variety of sources, parses it into a common format, and stores the data in a single PostgreSQL database.[87] Developed by researchers at Oxford University, Galvanalyser streamlines the process of gathering and querying data from different testing equipment. It supports access to the data through a web-based interface, which allows the user to search for datasets with certain properties and visualize them within the app. Open-source Python packages, like the battery evaluation and early prediction software package (BEEP)[88] and Python battery mathematical modelling (PyBaMM)[89] offer additional functionalities. BEEP is a framework for the management and processing of high-throughput battery cycling data, while PyBaMM is designed to allow for the simulation of cycling protocols *in silico*. While these packages offer solutions for developers interested in generating, managing, and modelling their own data, the Battery Archive[90] project run by the United States of America Department of Energy (DOE) compiles data and metadata from across many different studies to support model-based battery degradation predictions.

The digitalization of battery manufacturing benefits from the accelerating growth of battery manufacturing APIs. For example, the ERC-funded ARTISTIC project[91] develops a predictive computational platform of the impact of manufacturing parameters on the electrodes 3D texture and electrochemical performance. Such a platform encompasses physics-based and ML models describing each step of the manufacturing process (slurry, coating, drying, calendering, electrolyte filling, formation, electrochemical performance). The ARTISTIC project offers free online services to launch manufacturing simulations from an Internet browser.[92,93] Other example is the

DEFACTO project,[94] whose target is to create a basis for the digitalization of the battery manufacturing process, by developing multiphysics and multiscale modelling tools to improve the understanding of cell material behaviour and cell manufacturing process, and their impact on battery cell ageing. A further example of a commercial tool that stochastically generates electrode mesostructures is the software GeoDict.[95] A freeware alternative called INNOV is also available, which allows users to generate battery electrodes by controlling for example the shape of carbon-binder domain partially covering the surface of active material particles.[96–98]

2.2. Models

The second layer in the proposed DT structure presented in Figure 1 is related to models, which is defined as a representation of a system, through which relevant attributes are captured and is used to describe, understand, and predict the twin's operational states and behaviors. This paper differentiates between models describing machines and processes, following the criteria laid out in Ref. [58] *Machine models* are mostly focused on the representation of shop-floor elements (e.g., machines and equipment) through the modeling of mechanical, electrical, and hydraulic functions, while *process models* simulate the performance of an asset describing the creation and transformation of product characteristics. In any case, coupling of models across scales is required in the DT to analyze the interactions between machine processes and related machine tools, and later developed a virtual replica of the physical manufacturing chain. In this multi-level simulation, the different levels (battery cell, machine, and process chain) need to be addressed individually with a suitable modelling approach, based on physics-based mechanistic models and/or data-driven models where Machine Learning (ML) algorithms are implemented.

In general, the behavior and operation of each machine within the battery cell manufacturing process chain needs to be described by *machine models*. These models aim (1) to model machine operation over time according to the schedule provided by the process chain model; (2) to describe machine states of entire machines; (3) to provide demand profiles for energy carriers and resulting heat emissions, and finally (4) to model machine failure behavior.

When it comes to the *process models*, numerous factors during battery cell production influence the performance and quality of final cells; even product specifications of cells influence the operation of machines and process chains also affecting other production system element. Simulating these influences requires *process* models for describing the specifications and characteristics of processing units during production, as well as models for processes describing the creation and modification of product characteristics.

In the current LIB cell manufacturing processes, the electrode mesostructure (see **Figure 4**), defined as the way that the active material (AM), carbon additive and binder are distributed in the space and interfaces between them within an electrode, strongly controls the practical properties of the electrode and those of the cell, such as energy and power densities, lifetime and safety. Therefore, electrodes are the most complex
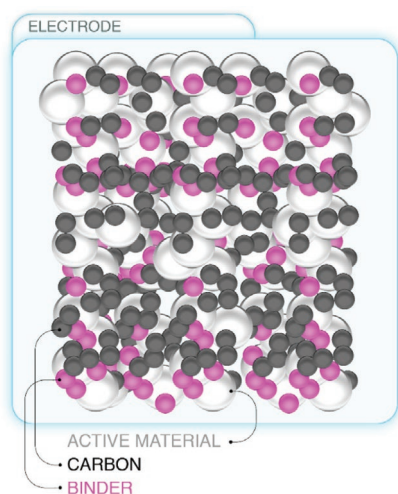
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Figure 4. Representation of the LIB electrode microstructure which is generally constituted of active material (AM), conductive additives (named "Carbon" in the figure) and binder.

components to manufacture in LIB cells and its fabrication process specially requires models capable of mimic the real manufacturing process to avoid the current time-consuming and costly trial-error approach.

Basically, three types of models have been developed and applied so far to predict electrode properties as function of a number of manufacturing parameters: stochastic models, physics-based models and data-driven models, i.e., ML models (see **Figure 5**). While the stochastic methods have been used from at least in the last 20 years in other electrochemical systems (e.g., solid oxide fuel cells),[99–101] application of physics-based and ML models to battery manufacturing is just emerging.[21,102,103] Because of their empirical character, stochastic models are the ones having the lowest computational cost, and the lowest prediction capability (since the electrode mesostructure generation forces the resulting mesostructure to match the experimental observables, such as the porosity). Physics-based models, depending on the number of spatial cartesian coordinates considered can have different computational cost and prediction capabilities: 3D models,[21] for example,

have the highest computational cost (usually several hours or days, depending on the hardware computational resources), and at the same time provide the highest prediction accuracies, while 2D, 1D and 0D models have lower computational cost, but also lower prediction capabilities. Finally, ML models usually need long times for their training from large data sets, although once they are properly trained, they can provide high accuracy predictions with ultralow computational cost (few seconds). Hereafter, the working principles of these three types of approaches and application examples in relation to battery manufacturing will be discussed.

2.2.1. Stochastic Models of Electrode Mesostructures Generation

When it comes to the study of LIB electrodes in three dimensions, the most intuitive approach to model their mesostructure is to assume particles as having polyhedral or spherical shape, and to artificially build an electrode by randomly (stochastically) packing them into a given volume, until reaching an experimental porosity or volume fraction (see **Figure 6**).[104–106] Usually, this process is repeated several times for different random seeds and the average mesostructure is retained.

A variation of this approach is the ballistic method, which has been proposed to be used for generating virtual electrodes and to estimate relevant structural and transport properties.[107] Overall, these approaches do not predict how the actual manufacturing parameters impact the electrode mesostructure, but they provide insights on how the mesostructure impact practical properties, such as the effective conductivities resulting from the particles percolation and the tortuosity factors. These effective outputs can be used as inputs of electrochemical models of LIB cells, such as the Newman's pseudo-2D approach.[108]

The stochastic approach finds also useful applications for all solid-state batteries.[109–112] Bielefeld et al.[113] studied the impact of carbon-free composite electrode formulation (active material/electrolyte ratio), porosity, particle size and electrode thickness on the formation of ionic and electronic percolation networks. Later, the same authors extended their work by incorporating binder in their analysis, studying the impact of binder content, active material particle size and porosity on the
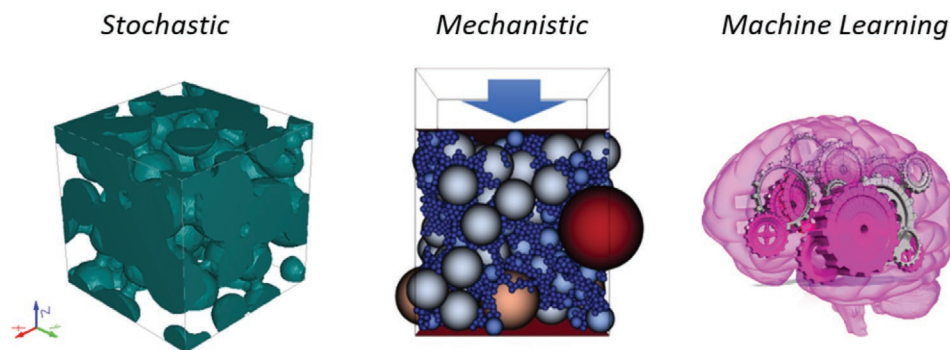

Figure 5. Different modeling approaches generate electrode mesostructures. Stochastic approach (left image) allows generation of electrode mesostructures by using as inputs experimental particle size distributions, formulation and porosity; mechanistic model, such as DEM (middle image), predicting electrode mesostructures as function of the manufacturing process parameters (e.g., formulation, drying temperature of the slurry, calendering pressure); ML approach (right image) for predicting the influence of manufacturing parameters on electrode mesostructure and performance properties.
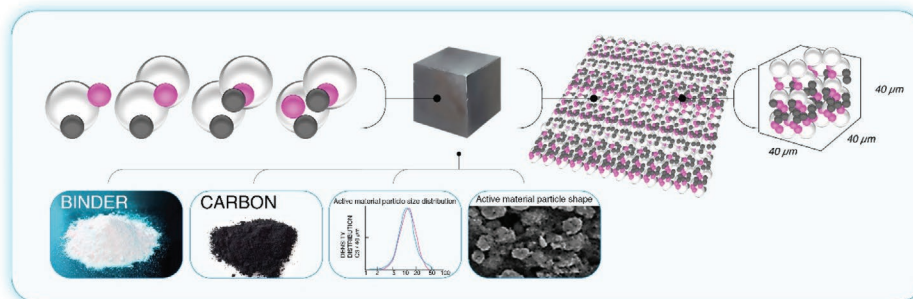
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Figure 6. Representation of the principles behind the stochastic generation of electrodes.

effective ionic conductivity and tortuosity.[114] They found that the binder, even if added in small amounts, negatively impacts the ion transport paths and the active surface area available for lithium insertion.

2.2.2. Physics-Based Models of the Manufacturing Process

In the first step of the electrode processing, an electrode slurry is obtained. Formed by a suspension of active material, carbon particles, binder and eventually dispersants in a solvent, with certain density, viscosity and stability that depend on the materials chemistry and the resulting complex interplays between van der Waals, Brownian and electrostatic forces, steric and hydrodynamic interactions.[21] Algebraic (or 0D) models for slurries have been proposed for estimating the viscosity of electrode slurries that incorporates colloidal forces such as van der Waals and polymeric steric repulsion forces.[115] Such kind of models can be very useful for fast understanding of the rheological properties of the slurries. Still, their empirical character does not allow creating truly 3D-resolved models accounting also for solvent evaporation, calendering and further manufacturing steps. Discrete particle approaches, such as atomistically-resolved approaches, could in theory provide this "understanding". However, in view of the wide diversity of sizes of materials involved in a slurry (~ μm for the active material, ~ tens of nm for the carbon additive, ~ few nm for a binder monomer) and consequently the millions of atoms involved, a fully atomistic-resolved approach simulating the interaction forces between them would have prohibitive computational cost and would be impractical for predicting slurry properties (e.g., rheology) in an appropriate way. Therefore, coarse-graining approaches, representing the particles suspensions and slurries through a collection of effective "beads" instead of atoms, have been used to investigate particle, polymer suspensions and slurries, in general.

Monte Carlo (MC) and kinetic Monte Carlo (kMC) methods can be used as that kind of coarse-graining approaches. MC methods were originally developed in the 1940s-1950s by Metropolis et al.[116,117] and since then they have become widely used for studying the statistical properties of discrete systems, allowing to close the gap between atomistic and continuum approaches. They are based on the extensive repetition of random executions to obtain results mimicking physical systems where the random character is inherent. Several MC

techniques have been developed, the most popular is the Metropolis algorithm consisting of performing random swaps from a given arrangement, e.g., spatial distribution of particles constituting a system, in order to search for the minimal energy configuration.[118–120] kMC methods are MC methods used to study the (temporal) evolution of systems.[121] While the primary outcome is the prediction of the time evolution, thermodynamic averages can also be obtained under equilibrium conditions. A kMC simulation relies on a set of discrete configurations and an a priori knowledge of a set of transition rate constants characterizing the transition events between these configurations. The states can be, for example, different arrangements of particles in a system and the events implemented as jumps of individual particles between positions. The events are assumed to obey "Poisson statistics", which is a statistical representation of random, uncoordinated rare-event (rate-limited) processes, also known as Markov processes. In this line, LiFePO$_4$-based electrode slurries and their drying have been simulated using an approach combining MC and kMC.[122,123] The approach optimizes the spatial arrangements of beads representing active material, carbon, binder, solvent, and pores (the latter in the case of solvent evaporation) based on energy calculations. It assumes a bi-dimensional system (in plane), that is, it does not describe the re-arrangement processes happening in the depth of the slurry upon solvent evaporation. Still, despite these geometrical approximations (e.g., active material particles represented like squares) the approach permits understand how solvent evaporation impact porosity evolution upon the slurry drying and allows studying the impact of mixing order on electrode mesostructure formation.

Brownian Dynamics (BD) method has been used to describe particles suspensions used for describing LIB electrode slurries, such as carbon additive, LMNO and silicon.[124–127] BD simulates the trajectory of interacting particles through empirically parameterized conservative forces, by solving a simplified version of the Langevin dynamics equation (usually used to describe Brownian motion), where no average acceleration takes place.[128] Publications reporting BD models to describe slurry particle suspensions have analyzed the effect of temperature, mass ratio between carbon and active materials on the resulting number of contacts between the conductive additive and the active material in the suspensions. However, these works have not addressed the presence of binder and do not account for very high solid-to-liquid ratios that one finds in actual slurries.

Originally developed in the context of complex chemical systems, like those found in biology (the original developers were awarded with the Nobel Prize of Chemistry in 2013),[129] coarse grained molecular dynamics (CGMD) constitutes another coarse-graining approach to simulate particle suspensions and slurries. CGMD is mesoscopic, i.e., it disregards all the degrees of freedom of smaller (atomistic/molecular) scales and "condensate" those degrees of freedom by some effective parameters. As for classical MD, CGMD models solve Newton equations then for beads or coarse-grained representations of smaller all-atom systems. The interaction forces (force fields) are determined by comparison between calculated and experimentally measured structural and thermodynamic or other macroscopic properties, and/or by using mathematical techniques to match the structural properties from CGMD simulations to those obtained from all-atom models. Measurements of properties, such as surface tension, wettability, and the zeta potential for the solid particles, as well as, the viscosity and the electric permittivity of slurry, may reveal also useful to support the force fields calibration work. Several coarse graining strategies exist to map the all-atom representation of the materials to the beads or coarse-grained representations, and to determine the force fields describing properly the physicochemical interactions between different compounds in suspensions.[130–135] In addition to this phenomenological approach, other well-stablished techniques, such as force matching,[136] iterative Boltzmann inversion,[137] and inverse MC[138] can be used to match the structural properties (Radial Distribution Functions) from CGMD simulations to those obtained from all-atom MD models. In the latter case, the reference all-atom MD simulations can be built with classical/semi-empirical force fields but, if needed, their refinement calculation by using ab initio methods in sufficiently small systems may be also considered. The adoption of ML algorithms to speed up the CGMD parameterization is also possible.[139] Because of a significantly reduced number of accounted degrees of freedom, CGMD can be used to perform simulations of much larger system sizes than what would be atomistically attainable. Still, due to the dependence on the detailed interactions between the materials, the CGMD method can capture the impact of the materials chemistries and initial volume or mass fractions on the resulting slurry mesostructure.

In the context of electrochemical energy conversion devices, CGMD has been first used to understand self-organization phenomena of polymer electrolyte fuel cell electrodes and proton conductive membranes.[140–143] Furthermore, CGMD was then applied to simulate NMC532-based slurries, as well as the subsequent electrode formation resulting from solvent evaporation, supported on a first tentative of experimental validation with one viscosity versus shear-rate curve.[144] Ngandjong et al. [145] extended this approach for NMC111, by predicting cathode mesostructures as a function of electrode formulation (weight percentage of active material and carbon-binder) and integrating the resulting electrode mesostructures in an electrochemical performance simulator coded in COMSOL Multiphysics, through a multiscale sequential-linking approach. In these CGMD models, slurries are represented as a mixture of spherical particles representing the active material and carbon-binder domain. The particles can overlap a given extent and are embedded in each volume with periodic boundary conditions. The models use interaction Lennard-Jones and Granular-Hertzian force-fields with empirical parameters. The resolution of the Newton equations allows converging to an equilibrium state representing the slurry, which can be characterized in terms of density and viscosity versus applied shear-rate, the latter using Non-Equilibrium MD simulations. In that sense, Lombardo et al.[146] reported a set of systematic computational methods to determine the parameters needed in the force fields to reproduce correctly experimental densities and viscosities, as function of the slurry formulation and solid-to-liquid ratio. Such methods include Particle Swarm Optimization (PSO), ML and a combination of both, which allows to accelerate tremendously (about 20 times) the time needed for the parameters' determination. In this approach, the effect of solvent evaporation has been modeled by shrinking the carbon-binder-domain (CBD) particles for a given extent in the slurries and solving again Newton equations to reach a new equilibrium state, corresponding to the dried electrode. As the slurry simulation starts from a random spatial distribution of particles, this implies a small uncertainty in the final spatial location of the particles in the predicted electrode mesostructures. In this context, Rucci et al.[147] have quantified such uncertainties propagation when the predicted mesostructures for different formulations are incorporated in a 3D-resolved electrochemical model. This work shows slight variations of calculated porosities for several CGMD runs for a same formulation and solid-to-liquid ratio, in good agreement with experiments repeated several times under the same conditions, while it induces significant variations in the predicted electrochemical performance upon galvanostatic discharge, also observed at the experimental level. Still, there is a good agreement in the trends and overall specific capacity values between simulated and experimental results.

The CGMD-predicted electrode mesostructures can be characterized by textural properties, such as porosity, pore size distribution, tortuosity factor, interfacial surface area of contact between AM and CBD, etc. Also, percolation theory and Fast Fourier Transform (FFT) methods[148] can be used for the determination of the effective conductivities of the calculated mesostructures. These quantifications can be used as further input to validate the CBD-shrinking drying approach and as input parameters of Newman-like electrochemical models. The predicted electrode mesostructures have been also incorporated in 4D- (three spatial dimensions + time) physics-based models resolving electrochemistry and transport processes in operating cells.[149,150]

Computational Fluid Dynamics (CFD) models have been proposed to simulate the drying process of the electrode coatings,[151] in particular to analyze potential binder migration upon solvent evaporation.[152,153] Such models assume 1D geometries and solve coupled heat and mass transfer equations. However, it is not unusual modeling reports with 0D representations, which can be used for process optimization in a faster way.[154] These models can provide useful and fast insights on the optimal drying conditions to avoid binder migration along the coating thickness. However, they cannot predict electrode mesostructures in 3D and/or heterogeneities in plane, like the discrete coarse-graining approaches described before, because of their 0D or 1D assumptions. Predicting those mesostructures

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in 3D is very important to understand heterogeneity and anisotropic electrode behavior in relation to performance limitation and ageing, for instance, and this having the same degree of interest than doing computer tomography of electrodes.[21]

Discrete Element Method (DEM) is a well-suited technique to address the particles rearrangement/deformations upon mechanical compression in granular materials.[155] DEM has already been used for the simulation of morphological changes of composite electrodes for solid oxide fuel cells[156] and, in combination with CFD, for the simulation of the flow of particles suspensions in semi-solid redox flow batteries.[157] In the recent years a number of DEM models have been proposed to simulate the calendering process of LIB electrodes. DEM explicitly accounts for the mechanical interactions between the individual particles and allows capturing particles deformation and cracking. This method allows simulating the interaction between discrete objects in contrast to the Finite Element Method (FEM), where the system is meshed and based on continuum mechanics. The DEM is much like MD: it solves Newton's equations for the trajectory of individual particles and/or aggregates from their mechanical properties and interaction mathematical laws accounting for stress-driven deformation. Mechanical stress testing can be performed for evaluating the level of accuracy of the model for predicting micro/mesostructural changes under mechanical stresses. The first DEM calendering model was proposed by Stershic et al.[158] for electrodes with spherical and ellipsoidal AM particles, starting from tomography images. Later, Sangrós-Giménez et al.[159–161] reported a series of DEM modeling studies to analyze the resulting particles assemblies as a function of the applied pressure and particles size distribution, in terms of active material particles percolation and associated properties of interest, such as the associated electronic conductivity, for the optimal battery cell operation. Such models have been considering explicitly only the spatial location of active material particles, and the CBD has been considered implicitly as affecting cohesive forces between active material particles. In addition, these models have been able to reproduce well experimental compaction curves, i.e., electrode porosity versus applied pressure. However, their implicit consideration of the CBD makes not possible the prediction of its spatial location, its spatial distribution affecting in a heterogeneous way the electrode operation.[146,162]. Recently, Ngandjong et al.[163] proposed the first electrode calendering DEM model able to account for the explicit location of both AM (NMC111) and CBD particles. Such model uses as an input an electrode mesostructure generated by the slurry and drying CGMD simulations described above, and a single set of force fields parameter values is found to fit simultaneously microindentation and compaction curves. The model can predict the spatial location of both AM and CBD, and the resulting mesostructures for different degree of compression are injected into a 4D-resolved performance simulator for predicting the influence of calendering on the lithiation upon galvanostatic discharge. Such chain of models (CGMD for the slurry and the drying simulation, followed by DEM for the calendering and the 4D-model for the electrochemical performance), constitutes the first workflow demonstrator of the LIB electrode manufacturing process based on physics-based models (**Figure 7**). Srivastava et al.[164] has also used DEM going directly from a random structure to an equilibrated one further pressed afterward to mimic the calendering. Despite this latter approach is not validated with experimental data, in particular regarding the impact of calendering pressure on the porosity, the authors were able to investigate the effect of CBD cohesion on the resulting electrode mesostructure, by analyzing a set of textural properties.

The electrolyte impregnation has been recently modeled using Lattice Boltzman Method (LBM), an approach which exists since more than 30 years in fields like fluid dynamics in porous media.[165] In LBM, a fluid is assumed to be composed of virtual particles moving and colliding with each other in a predefined lattice structure. Instead of treating these particles
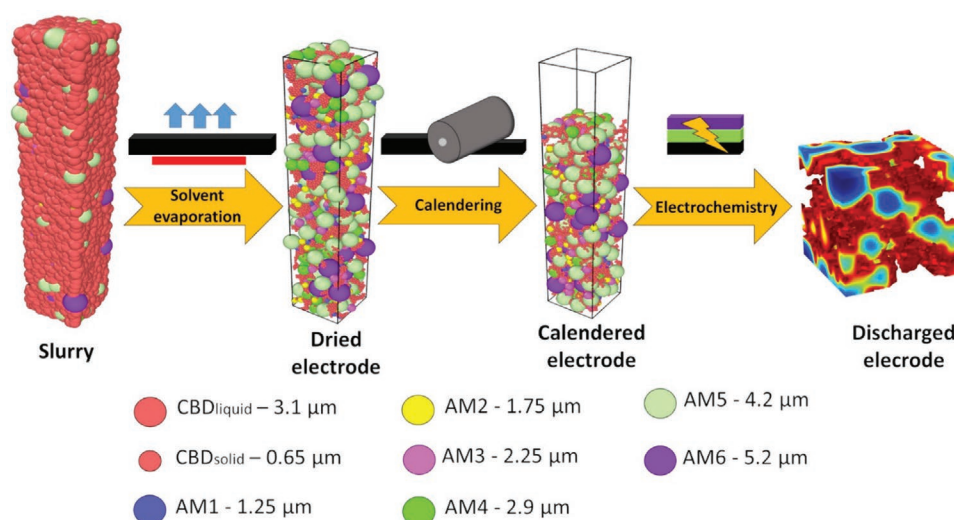

Figure 7. Workflow of LIB manufacturing, encompassing physical models for the slurry, drying, calendering and electrode electrochemical response. Different CBD and AM particle sizes considered are indicated. The discharged electrode image shows different lithiation states within the electrode. The fully lithiated state is shown colored in red, and the fully de-lithiated state is shown colored in blue. Reproduced with permission.[160] Copyright 2021, Elsevier.

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by their positions and velocities, the LB approach treats them by a distribution function with appropriate relation time collision operators, e.g., the Bhatnagar-Gross-Krook (BGK) model[166] and lattice schemes. This includes "bounce back" boundary conditions, capturing the interactions with the pores' walls, to enable the simulation of the electrolyte flow in the complex electrode mesostructures. Several experiments have been conducted to study the wettability by the electrolyte of LIB porous electrodes. For instance, Wu et al.[167] showed that the wetting, i.e., the spreading of electrolyte into the pores, is governed by the electrolyte viscosity and surface tension. Chu et al.[168] investigated the influence of compaction on the porosity and electrochemical performance of the positive electrode, which also suggested that the wettability has predominant effect at high C-rates. LBM has been used by Lee and Jeon[169] to simulate the electrolyte transport dynamics in electrode porous structures generated stochastically in 2D (**Figure 8**). The effect of the compression ratio of a porous electrode on wettability has then been explored with respect to variations of porosity and particle shape. Shodiev et al.[170] reported for the first time a 3D-resolved LBM model able to simulate electrolyte filling upon applied pressure of LIB porous electrodes obtained both from experiments (micro X-ray tomography) and computations (stochastic generation, simulation of the manufacturing process using CGMD and DEM). The model allows obtaining insights about the impact of the electrode mesostructure on the speed of electrolyte impregnation and wetting, highlighting the importance of porosity, pore size distribution and pores interconnectivity on the filling dynamics. Furthermore, the authors identify scenarios where volumes with trapped air (dead zones) appear and evaluate the impact of those on the electrochemical behavior of the electrodes.

2.2.3. Data-Driven Models of the Manufacturing Process

The DT of a manufacturing process aims to efficiently monitor and remotely manage the physical item, using data analytics and intelligence tools and technologies. It allows programming maintenance schedules, load balancing, and predicting failures and disruptions, in which the operational parameters of machine sensors or machine components must be rectified or adapted continuously in the operation stage of the manufacturing process. Additionally, using advanced ML algorithms and data analytics, the integration of the real-time streaming sensor data with other operational inputs to create an operational data-driven DT will be facilitated. This operational DT will provide a more holistic and dynamic virtual representation of the whole manufacturing system, end-to-end processes, and operations. Thus, these analytics are important to be combined with a DT to reduce system downtime, improve production efficiency, and perform predictive quality maintenance.

At the *machine level,* defect images can be identified using optical systems. In the production of goods, AI can be used to increase the performance of a production plant by means of collected production data or to find an optimal parameter configuration.[171,172] In this sense, a system that correlates the monitored process parameters with the quality characteristics, and independently learns to adjust the process variables to achieve the quality characteristics, is not yet known in battery cell production.[173] Thus, such system would offer great potential with respect to fast and flexible commissioning or retrofitting of production facilities.

Up to now, efforts to digitize production by means of algorithmic functions have often been implemented as isolated solutions in a plant and in a process state in production. When
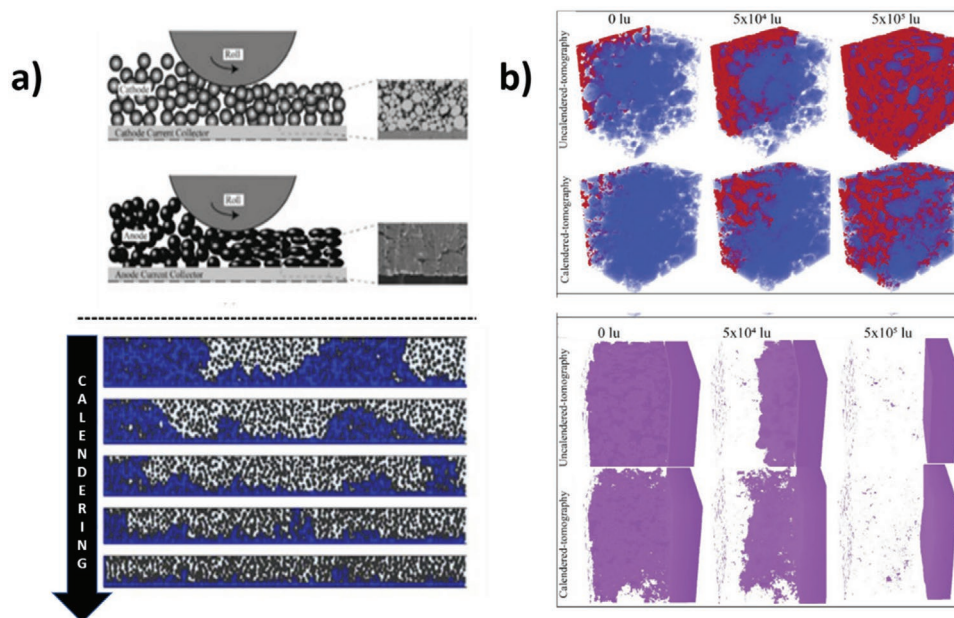

Figure 8. a) Top: Schematics of roll pressing process for positive (top) and negative electrodes (bottom); bottom: 2D-LBM calculated liquid electrolyte distribution in the cathode with different compression ratios. Reproduced with permission.[169] Copyright 2014, Elsevier. b) 3D-resolved LBM model of electrolyte infiltration on uncalendered and calendered electrode mesostructures arising from tomography; top: electrolyte (red) filling dynamics and bottom) air (purple) distribution dynamics. Reproduced with permission.[170] Copyright 2021, The Authors.

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the boundary conditions of the heterogeneous production landscape change, these functions usually must be adapted and trained again, with a great expense. In addition, productization for easy scaling has not been seen in the state of the art so far. Value creation through the use of ML algorithms is only possible when the latter can be applied cost effectively and reliably. This requires the provision of the necessary hardware and software IT infrastructure for the structured acquisition, and preparation of data for loading/learning and application, as well as for monitoring the required models at sufficient speed.

Defect detection in battery manufacturing is also key to ensure the required safety and lifetime properties of the battery. When manufacturing a LIB cell, an important step is the quality of the applied coating. Ideally, the coating is carefully grained and covers evenly and fully the substrate area. However, at this stage different defects may occur deviating from these ideal conditions. For example, when using the doctor blade equipment for achieving the coatings, a common fault is that it is clogged with agglomerates within the slurry mix. As a result, the applied coating may be not even and partially missing. At the usage stage, due to the defective electrodes the cells will suffer from severe degradation and even exothermic reactions can happen. To avoid these scenarios, optical methods can help in ensuring the quality of the electrodes. In addition, when developing research activities and novel slurry mixes are tested, electrodes can be poorly reproduced. In this other scenario, to provide a quality assurance of experimental slurry mixes, an optical inspection can be developed,[174] such as the one presented by Kapeller et al..[175] This inspection facilitates the quality assurance in the coating process of anode and cathode foils for battery cells. The developed system can acquire 2.5D images at speed of up to 500 mm/s with a lateral resolution of 50 µm/px. To achieve this, a tight coupling of transport movement, interleaved strobing of four-line lights, an image acquisition using an FPGA-based controller, and a photometric stereo surface reconstruction algorithm have been used and successfully developed.

Even though the defects may come in a specific step of the manufacturing process, the digitalization should be seen in the full process. In this regard, a recent publication[64] describes that through an analysis of the organizational structure, functional modules and information flow of a research pilot line, the requirements and modelling methods for an information model can be defined. This definition brings a division categorizing four functional modules, namely, production management, material management, equipment management and quality management. With similar approach, Thiede et al.[43,176,177] have reported several works on the use of ML at the LIB production process industrial scale. Overall, ML models were proposed to predict cell quality and performance as function of manufacturing machinery parameters and to assess energy efficiency involved the processing.

Focusing on the *process models*, still, the application of ML to battery manufacturing is emerging. Cunha et al.[178] reported for the first time ML models able to predict the loading and porosity of NMC111 electrodes as a function of manufacturing parameters. Such parameters include the slurry viscosity, solid-to-liquid ratio, and AM weight performance. The authors compared the prediction performance of three ML techniques,

namely, decision tree, support vector machine and deep neural network. The ML model based on support vector machine was able to predict classification multi-dimensional maps that can be visualized through intuitive slices in 2D. Such maps provide a useful guidance of which manufacturing parameters to adopt to prepare an electrode with low, medium or high loading or porosity. This facilitates the work of discovering interdependencies between parameters. The ML models were trained with only 80 experimental points of high quality, as each of them resulted from at least 3 experimental repetitions; prediction accuracy was above 80%. A similar approach, but this time using Gaussian process regression models, was reported later by Liu et al.[179] In that work the authors analyzed the effect of the AM content, solid-to-liquid ratio, viscosity and comma gap (i.e., the gap used during the coating process) on the electrode mass loading after the coating drying.

Primo et al.[180] recently reported an approach combining advanced statistics and unsupervised ML to unravel the correlation between parameters involved in the electrode calendering process and identify how their values impact electrode properties such as porosity, mechanical behavior, electronic conductivity, and capacity. Such parameters included applied pressure, roll temperature, and line speed, and the electrodes were NMC111-based. The authors found that that while porosity and the mechanical properties depend mainly on the applied pressure, the electrode's conductivity correlates mainly with the temperature.

Chen et al.[181] recently applied advanced statistics and ML models to optimize the manufacturing process of thin all solid-state battery electrolytes. ML models include unsupervised K-means clustering and supervised support vector machine. The combination of models allows predicting the impact of manufacturing conditions, such as the amount of solid electrolyte, liquid-to-solid ratio, and solvent composition, on the thin film electrolyte uniformity. The ML workflow shown in **Figure 9** is then used to design a suitable thin film electrolyte that has been tested in an all-solid-state-battery offering 100 cycles.

Encompassing high throughput experimentation, ML and physical modeling constitutes also an approach that has been proposed by Duquesnoy et al.[97] to develop digital twins of the electrode manufacturing process. The authors proposed an electrode stochastic generator able to predict how manufacturing parameters impact the electrode mesostructure in 3D. This is possible because the generator is informed by using both experimental and physics-based data (the latter arising from CGMD and DEM simulations as described above). Such generator can produce a massive number of electrode mesostructures that can be characterized in terms of textural and physical properties, like the surface area of contact between AM and pores, tortuosity of the porous media, conductivity, etc. This allows building a dataset of type "input = manufacturing parameters, outputs = electrode properties", which can be used for training ML models able to predict electrode properties from manufacturing parameters in the form of classifications or regressions. The authors demonstrated their concept for the electrode calendering step.

All in all, summary of the current modelling landscape has been added in **Table 1**. In addition, the main characteristics of each model are also introduced.
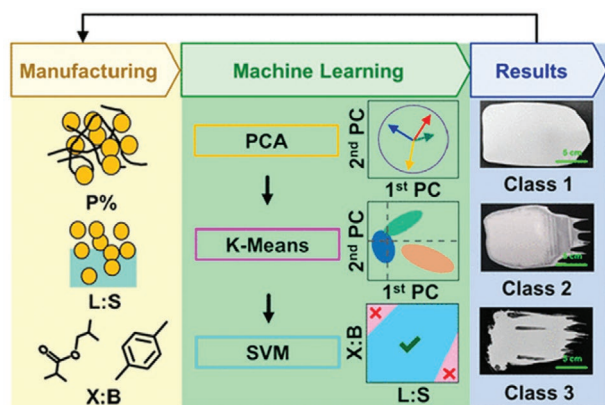
Figure 9. Application of ML to optimize the manufacturing of thin films for all solid-state battery electrolytes. Reproduced with permission.[181] Copyright 2021, American Chemical Society.

2.3. Standards Landscape for Smart Battery Manufacturing and Current Projects in Digitalization of the Battery Manufacturing Process

The third layer in Figure 1 is related to *Standards,* which can provide comprehensive self-assessment mechanisms to determine current digital twin readiness level and roadmap the steps that need to take to achieve a full digital twin approach.

In manufacturing industry, standards help establishing a solid foundation for a lifecycle spanning the development and manufacturing process. Here, in the framework of digital transformation and particularly in the digitalization of battery manufacturing process, standards are of prime importance. In this regard, numerous national, regional, and international standards development organizations (SDOs) are starting to focus explicitly on the needs for and impacts of the technologies fundamental to build a smart manufacturing, such as DT, Internet of Things (IoT), Cloud Computing, Big Data and analytics. In this category are international standards bodies, such as ISO,[182] IEC,[183] ASME,[184] ASTM[185] and IEEE SA[186] and national bodies including professional organizations, which define best practices. To the authors' knowledge, there is no

specific smart battery manufacturing standard available yet, and the standards developed so far are generic for any manufacturing industry. Taking this into account, this section provides a review of the existing standards, as well as the ones under development for digitalizing manufacturing industry in general.

Within ISO, the technical committee on automation systems and integration (TC184) has two subcommittees that are of particular interest in our landscape: SC4 and SC5. SC4 focuses on industrial data standards, where at the time this perspective is written 774 standards are already published and 37 of them are under development. Within this subcommittee, there is a specific Working Group (WG15)[187] that deals with the Digital manufacturing. Currently, they are working on the development of ISO 23 247[188] that provides an overview and general principles of creation of DTs of observable manufacturing elements including personnel, equipment, materials, processes, facilities, environment, products, and supporting documents.

Another aspect of smart manufacturing deals with the data science and analytical models to analyze real time production data from multiple sources, such as production machines, systems, and processes, and to accumulate this data into an automated manufacturing system.[189] To perform this vision of smart manufacturing, another requirement is to achieve interconnectivity across a diverse set of devices[52] and to acquire and integrate large amounts of data, which can be used to inform production decisions.[53] However, one of the main challenges in implementing this solution is establishing interoperability with each device. The technical committee ISO/TC 184/SC 5 has worked on defining 62 published standards and 4 under development.[190]. Particularly, within this subcommittee the standard ISO 15 746 is developed. This standard provides a framework and general functionality of a method for integration of advanced process control and optimization (APC-O) capabilities for manufacturing systems.

IEC, which historically has served the electronics industry, is also dealing with many standards in Information Technology (IT) for smart manufacturing systems, including sensor and device networks and user interfaces. IEC is working with ISO

Table 1. Summary of the current state of the art for models in the LIB manufacturing process.

Modeling approach	Predictability	Computational Cost (as for present computational technology)	Application examples (not exhaustive)
Empirical (0D)	Low (transferability to other materials and conditions)	Low	• Influence of formulation on slurry viscosity. • Influence of calendering parameters on electrode properties such as porosity.
Physics-based CFD (1D or 2D)	Intermediate	Intermediate	• Influence of drying rate on coating thickness.
Physics-based Discrete (3D)	High	High	• Influence of formulation and solid content on slurry rheology • Influence of drying rate and calendering conditions on electrode mesostructure in 3D. • Influence of electrolyte infiltration parameters on electrode wettability.
Physics-based Surrogate (3D)	High	High (for training)/Low (for prediction)	• Influence of electrolyte infiltration parameters on electrode wettability.
Machine Learning	High	High (for training)/Low (for prediction)	• Influence of manufacturing parameters on electrode textural properties and performance.

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under ISO/IEC JTC 1,[191] an international standardization committee in the field of Information Technology. In particular, the ISO/IEC JTC 1/SC 41 named "Internet of things and digital twin" is also working building the standards related to DTs. The activity of this committee related to DT has just started and the associated projects are at very initial stage of development. Other interesting standards subcommittees for manufacturing industry are ISO/IEC JTC 1/SC 42 Artificial Intelligence, ISO/IEC JTC 1/SC 7 Software and systems engineering—Business Process Management Initiative, ISO/IEC JTC 1/SC 27 Cybersecurity, ISO/IEC JTC 1/SC 32 Data Management and Interchange and ISO/IEC JTC 1/SC 38 Cloud Computing and Distributed Platforms.

Many ASTM International committees also support smart manufacturing technologies and applications. ASTM International staff and members from these committees are regularly working to break down silos through a high-caliber Smart Manufacturing Advisory Committee (SMAC[192]). Moreover, the SMAC is creating a more formalized structure of coordination and collaboration to share information and to identify new opportunities for new standards, programs and partnerships.

ASME has not any specific committee in the fields of smart manufacturing or DTs. Nevertheless, there are some subcommittees[193] that are approaching to this field, such as the subcommittee on Additive Manufacturing that develops standards to provide rules, guidance and examples of the design, manufacture, and quality assurance of additively manufactured part; and a subcommittee on Monitoring, Diagnostics and Prognostic for Manufacturing Operations, which develops standards and guidelines to advance the design and implementation of monitoring, diagnostic and prognostic capabilities, along with ways of verifying and validating their performance, enhancing adaptive maintenance and operational control strategies within manufacturing.

The *Institute of Electrical and Electronics Engineers Standards Association (IEEE SA)* has its own Association for Digital Transformation,[194] which is focused on such technologies as IoT, AI, Big Data, Virtual Reality (VR) /Augmented Reality (AR)/ Mixed Reality (MR)/ Extended Reality (XR) and DT. One of the most interesting projects is P2806 – System Architecture of Digital Representation for Physical Objects in Factory Environments[195] that defines standards for physical objects in a factory by defining its system architecture of digital representation. In addition, IEEE Computer Society Smart Manufacturing Standards Committee (IEEE C/SM SC)[196] is also working on the development of new standards for Smart Manufacturing (smart equipment, smart factory and smart services as an example). Established in September 2019, IEEE C/SM SC has the aim of supervising the development of IEEE Intelligent Manufacturing standards.

In **Table 2** we compile the current standard landscape in digitalizing any manufacturing chain that can be extrapolated to the particular case of battery manufacturing plants based on the previously described Asset Administration Shell (AAS) and the alignment between Standards and the Reference Architecture Model for Industry 4.0 (RAMI 4.0) Administration Shell concept. Table 2 is elaborated based on the information from,[194] where *Deutsches Institut für Normung* (DIN) along with other organizations, published the "Reference Architecture Model for Industry 4.0 (RAMI 4.0)" to align standards in the context of Industry 4.0, showing how standards are linked to certain submodels, e.g., identification, communication, or engineering[197] that might constitute the administration shells.

When it comes to the initiatives that works on promoting and accelerating the implementation of the Industry 4.0 approach in many fields, we have identified among others *German Platform Industrie 4.0*[199] which is shaping the digital transformation in manufacturing; *Alliance for Internet of Things Innovation (AIOTI)*[200] that was launched in 2015 by the European Commission to support the creation of an innovative and industry driven European IoT ecosystem; *Digital Twin Consortium (DG)*[201] that joints industry, government and academia to drive consistency in vocabulary, architecture, security and interoperability of digital twin technology; and finally Smart Manufacturing Platform[202] that supports collaborative activities integrating smart manufacturing applications. Another relevant initiative is the OntoCommons initiative[203] which is dedicated to the standardization of data documentation across all domains related to materials and manufacturing. OntoCommons takes a similar approach to the Industrial Ontology Foundry[204] (IOF) by first defining a top-level reference ontology, which acts as a source to grow industrial domain ontologies that use common terms and follow common principles. Battery domain ontologies BattINFO and BVCO, previously mentioned, are based on this initiative.

The digitalization of battery field is gradually following the same trend observed in many other sectors, where the growth of these kind of projects and efforts is increasing. At European level, besides the project ARTISTIC[91] funded by the European Research Council and the project DEFACTO[94] funded by the H2020 programme, both mentioned above, the project *eLAB: Big Data* in battery production by RWTH,[205] boosted by the Platform Industrie 4.0 initiative, aims at developing a procedure for plant linking and analysis of the cause-effect relationships. Various technologies will be integrated into the demonstration line for cell production in Aachen and a detailed approach will be developed together with the technology partners. Similarly, the project "DigiBattPro 4.0 – BW" – Digitized Battery Production 4.0[206] founded by Ministry of Economics, Labor and Tourism -Baden – Wuerttemberg aims at digitizing a battery cell production facility. Digitizing the entire process will make a significant contribution to improving and stabilizing the quality of lithium-ion battery cells. A particular focus of digitizing the battery cell production process is on developing a consistent traceability concept for tracking and assigning process parameters and product features.

European Li-Planet initiative[207] is another example in which the goal is to create a European innovation and production ecosystem by building a more competitive LIB cell manufacturing ecosystem. Also, the initiative aims to increase the production of LIB cells toward industrial scale, by bringing together the most relevant European Lithium battery cell pilot lines and the main stakeholders of the battery sector. The initiative includes also an Expert group aiming to define a roadmap toward battery manufacturing data standardization and digitalization.

Finally, BATTERY2030+ Initiative[208] suggested research actions to radically transform the way we discover, develop, and design ultra-high-performance, durable, safe, sustainable, and affordable batteries for use in real applications. Manufacturing

Table 2. Examples of norms and standards providing properties for sub-models of the Administration Shell[198].

Administration Shell	IEC TR 62 794 & IEC 62 832 Digital Factory
Identification	ISO 29 005 or URI Unique ID
Communication	IEC 61 754 Fieldbus Profiles Chapter 2 (Ethernet-real-time-enabled)
Engineering	IEC 61 360/ISO 13 584 Standard data element IEC 61 975 Data structures and elements ecl@ss Database with product classes
Configuration	IEC 61 804 EDDL IEC 62 453 FDT
Safety (SI L)	EN ISO 13 849 EN/IEC 61 508 Functional safety discrete EN/IEC 61 511 Functional safety process EN/IEC 62 061 Safety of machinery
Security (SL)	IEC 62 443 Network and system security
Lifecycle Status	IEC 62 890 Lifecycle
Energy Efficiency	ISO/IEC 20140–5
Condition Monitoring	VDMA 24 582 Condition Monitoring

of future battery technologies is addressed in this roadmap[209] from the perspective of Industry 4.0, where the power of modelling and of AI was proposed to deliver DTs both for innovative, breakthrough cell geometries, avoiding or substantially minimizing classical trial-and-error approaches, and for manufacturing methodologies.

2.3.1. Challenges and Opportunities

The process of digitalization is characterized by the transfer of analogue product features into digital values to enable an electronical and informational transfer, storage, and processing of the data. **Figure 10** shows a representation of the digital twin of the battery manufacturing plant that mimics the real manufacturing plant and is capable to make intelligent decisions over the plant. In the figure, the main three pillars of the DT can be identified: the real manufacturing plant (left side of the figure), the virtual replica (right side of the figure) and the connection of data and information (represented by lines) that ties the virtual replica and the real plant together. When operating, massive data may be extracted through the use of sensors from the physical assets, which can be transferred to the cloud for information systems to process. Then, big data analytics can support system management and optimization including supervision and control, having the means to interact with the physical asset through the actuators.

By a successful integration of digitalization approaches in an automated production line, the overall costs of the battery cell can be significantly reduced. Hereafter, we summarize the main challenges to be overcome to move toward digitalization of the LIB cell manufacturing plant.

Firstly, the use of *sensors and actuators* can increase the quality of the produced batteries, as well as the monitoring and control of the whole process. At this moment, their main purpose is mostly limited to basic safety functions, defect detection, automatic calibration of workpieces or simple measurement methods. However, as highlighted in the previous sections, the networking of intelligent sensors will enable enhanced functionality of existing production facilities. Sensors are one of the key concepts in the digital transformation phase, and precisely because of their importance and the limited implementation of these in battery manufacturing, it is necessary to further investigate and develop research activities in which the location, amount and purpose of the integrated sensors will be deeply studied. This research activities would bring not only novel sensors, but also novel machinery and effective adaptation of already in use machinery with the sensors to give manufacturers the opportunity to adopt agile methodologies, making real-time changes to processes that can increase battery cells performance.

The interaction between the physical components and the virtual data layer of a production system, by considering the corresponding technologies for *data acquisition, data storage*
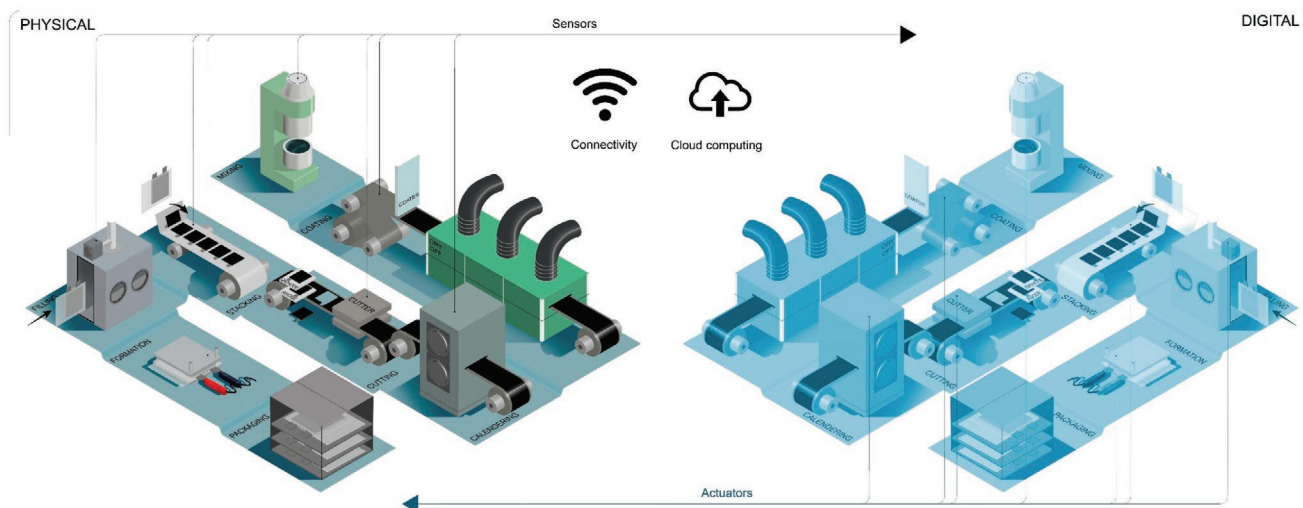

Figure 10. Digital twin of the LIB manufacturing plant (Wifi symbol: it represents the usage of wireless technology which encourage the communication. Cloud symbol: it represents the cloud computing technology).

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and data processing needs to be integrated in an efficient and sustainable manner. This full digital representation of the production system, including the sensors and actuators and the semi-finished products of the battery cell and of course the final product battery cell itself, will enable the prediction of the impact of changes in production on the structure of the battery components and consequently on the final cell performance.

Within the DT of a LIB manufacturing plant, the flow of data begins with the measurement of quantities via *sensors*. In the next step, data must be integrated into a common framework for data storage and processing to extract the necessary insight. This represents a challenge for a battery gigafactory, as the data generated is both voluminous and heterogeneous. A single gigafactory brings together many sub-processes and support laboratories, which may contain equipment from different manufacturers, each of them with their own software and file formats. There exists a need for tools to support the *interoperability of battery manufacturing data*. A similar challenge faces the *interoperability of models* used in the core simulator of the digital twins as they need to exchange and simulate models that were developed at different times, and in different modelling environments.

In addition, lessons learned from other industries, e.g., automotive and machining sectors, should be successfully implemented in the LIB cell manufacturing plants. In this way, *common languages,* interfaces, protocols, and usage of 5G or perspective 6G wireless technology is encouraged between different process steps or machines and material combination, pursuing a more efficient battery manufacturing process. Similarly, the use of standardized *communication protocols and sensors* will increase the generation and therefore the usage and management of data. In fact, the integration of these intelligent sensor systems will enable greater flexibility and higher reliability by combining available data sources with appropriate data analysis methods, such as ML and data mining. Accordingly, this continuous stream of data should be generated and managed from process parameters, information from peripheral devices and product characteristics, and later analysed using powerful algorithms and computing systems. The different steps of the manufacturing process need to be fully in line, assuring a proper integration between them and their communication.

Recently, substantial progress has been made optimizing the battery manufacturing process and the performance of battery cells separately. However, there is a relative death of work establishing the links between changes in measurable quantities in the manufacturing process with the performance of battery cells. In this sense, there is a need for *battery-specific APIs* that support decision making and operation control of battery manufacturing processes targeting desired performance of the cells. Identifying the links between battery manufacturing and cell performance is facilitated by taking a combined approach applying physics-based models with big data and semantic knowledge maps of two domains: manufacturing and electrochemistry.

As previously mentioned, *data interoperability* is another key aspect to reach the goal of the digitalization of the battery manufacturing process or developing a DT of a battery gigafactory. To do so, appropriate standards should be developed to address all the connectivity networks and APIs in a specific framework. The adoption of *ontologies* for both sharing data between computerized tools and establishing a standard vocabulary for efficient communication will be decisive in further development of ML models, in the digital transformation of LIBs manufacturing plants.

The battery manufacturing DT should enable more effective monitoring, optimization, and prediction of the physical counterpart. However, to develop a successful digital twin, deep understanding and planning of the production process and machines is crucial. The translation of key parameters into the full production system needs to be taken into consideration. Like this, a better and integrated predictive maintenance, fault, and error detection at both levels in the machinery, process and the product need to be developed. All this can be done through developing accurate, robust and efficient *physics-based and data-driven models*. One of the challenges associated to the physics-based models in general (and 3D-resolved models in particular), concerns to the reduction of computational costs. Depending on the size of the modelled system and the number of particles considered in techniques such as Coarse-Grained Molecular Dynamics (CGMD) and Discrete Element Method (DEM), computational cost can range from few hours to few days (also function of the type of hardware used for the calculations). One example of the reduction of the computational burden is presented by Lombardo et al.[146] where efficient algorithms were implemented to accelerate the parameters optimization of the electrode slurry models using CGMD. Another approach to build efficient models is to implement either Reduced Order Models (ROM) or surrogate models, which are used to establish predictive DTs that could be efficiently modeled based on embedded reduced order models or low-dimensional structures. An example of this approach is the recent work published by Shodiev et al.[210] on the use of a ML-surrogate model of electrolyte infiltration in 3D that takes few seconds instead of several days of computational cost by LBM, or even the work presented by Quartulli et al.[211] on the use of ensemble ML surrogate models for cell optimization purposes.

Another challenge is to develop more accurate and detailed models. Currently, discrete models such as CGMD and the most detailed DEM describe the LIB electrode materials as a collection of effective particles representing active material and carbon-binder domains (CBD). The latter consists in effective particles containing implicit representations of carbon additive particles and polymer. The remaining associated challenge is the explicit consideration of carbon additive and binder in these type of calculations without significantly increasing the computational cost. Such explicit consideration of the carbon additive and the polymeric binder as separate materials will permit a deeper analysis of their respective roles during the electrode operation.

On the other hand, the expected large deployment of ML models for battery manufacturing faces a new challenge associated with the availability of public databases. Such databases are needed for appropriate training and testing of such models. Academic initiatives, such as the ARTISTIC project,[91,92] is already making significant amount of battery manufacturing experimental and modeling data openly available and offer free online services for battery manufacturing simulations from an Internet browser. While this trend of giving open access to data

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helps in generating large volumes of data, and thus in building data-driven models, it is felt that it should be followed by the academia and industry as a whole in order to facilitate and accelerate the data-driven models implementation.

Another challenge constitutes the systematically reporting of quantified uncertainties and statistical errors in the experimental databases. This is important to develop ML models able to make predictions with high degree of confidence. Still, ML models will be as good as the quality of the data used to train them. An important challenge here is the setting of standards for battery manufacturing data reporting. In this regard, a recent text mining study by El-Bouysidy et al.[212] carried out on 13000 scientific articles on lithium ion and sodium ion batteries found that many articles do not report important manufactured electrode properties that are needed to reproduce reported experiments.

Computational workflows integrating at the same time physics-based and data-driven models to simulate the different battery manufacturing steps also constitute another challenge. Such approaches will encompass the advantages of physical (i.e., high fidelity models) and ML models (i.e., good prediction capability with low computational costs). Such computational workflows could have the advantage to allow the automatic definition of which kind of model to use depending on the problem of interest (type of material, manufacturing step, etc.).

Another remaining challenge is the incorporation of high-fidelity 3D-resolved physics-based models in system level modeling at the machinery level (including eventually robots); the integration of ML models not constituting a bottleneck by itself in view of their much less significant computational cost.

In any case, a clear definition of *interactions and information exchange between models* (process models and machine models), as well as the selection of suitable strategies for coupling and synchronization of the involved models result in new challenge, if we want to address the aim of the digital models as diagnostic tools, digitally highlighting circumstances that occur in the real manufacturing plant, and leveraged as a decision-making support tool.

AR and VR can be considered among the key technologies to create a detailed visualization of the assets.[213] In the battery field, VR and MR have been recently developed by Franco et al.[214] as powerful tools for teaching battery concepts and for analyzing results such as the 3D morphology of battery electrodes arising from tomography characterizations or physics-based simulations of their manufacturing process. VR offers fully immersive and interactive virtual environments powered with models of the physical world. The authors reported a series of VR serious games providing to the player the opportunity to interact with materials, electrodes, and batteries during their operation. Such serious games incorporate physical models describing the operation principles and allow to ease performing modeling computations (such as the evaluation of an electrode geometrical tortuosity) because such computations are performed just by playing. The authors shown that their VR and MR serious games and tools allow to significantly ease the understanding of the complex battery concepts and operating principles, and significantly raises the engagement and motivation of students.[91,215] Such VR tools, but also Augmented Reality (AR) superposing digital information in real

environments, have definitely a strong potential to facilitate the training of operators working in battery production lines. Furthermore, the integration of physics-based and ML models in these tools can ease the use of computational models in battery R&D and the control of the manufacturing machines, concepts being developed in the ARTISTIC project.[91,210,216]

Standards for smart battery manufacturing are another important aspect, which are seen of capital importance to reach a complete digitalization of the battery manufacturing process. Although, there is a growing awareness of the need for standards to power industry 4.0, this presents an opportunity to the case of the smart battery manufacturing in order to better share existing best practice, and avenues for influence, in a more readily accessible way. In addition, certain standards have been developed to support the general interoperability of data and models within a digital twin framework, including the asset administration shell (AAS) and functional mock-up interface (FMI). However, more work is needed to adapt these approaches to the specific needs of the battery manufacturing industry. Another important goal to keep in mind is the international harmonization of Standards. A degree of global agreement around core standards is needed to create greater business certainty, facilitate trade, and support global innovation.

Finally, it is worthy to highlight the importance of a circular economy with respect to recycling and the steps of reuse and remanufacturing. Manufacturing and recycling steps are closely related. Accordingly, the digitalization and enhancement of the production processes may clarify and give key insights on how to develop concepts for a reuse of certain battery cells or a remanufacturing, for example, of battery modules and finally a safe and sustainable recycling process. Recent proposals call for the establishment of a Battery Identity Global Passport (BIGP) to support battery recycling. The BIGP is envisioned as a digital asset that accompanies the battery over its lifetime, from manufacturing to recycling, and should provide to recyclers the necessary information about the materials that are included in the cell, so that it can be processed in a tailored recycling process. In this scenario, battery manufacturers will likely be asked to mint the BIGP for their cells, which again underscores the need for common data structures to support interoperability, not only internally within a gigafactory, but across the entire battery value chain.

All in all, the next big leap in smart battery manufacturing requires cooperation and compromise among scientists and manufacturers. The biggest roadblock to proper Industry 4.0 implementation is the ability for machines and equipment to work together and share data. This can be avoided through standardization of machine-to-machine communication, IIoT communication and considering software database and communication protocols for MPR, ERP, MES, etc. Once this is achieved, then battery manufacturing will turn into a fully modular and interchangeable set of software and hardware.

Overcoming all these challenges will bring about truly connected battery manufacturing plant, where the DT will be capable of reproducing a physical asset or process accurately in the digital world and will enable more effective monitoring, optimization, and prediction of the physical counterpart, throughout its lifecycle, making what once cost billions to establish, now become the current trend.

3. Future Trend: Toward Chemistry Neutral Battery Manufacturing Digital Twins

Regarding smart battery manufacturing, a new paradigm anticipated in the BATTERY 2030+ roadmap[209] relates to the generalized use of physics-based and data-driven modelling tools to assist in the design, development and validation of any innovative battery cell and manufacturing process. In this regard, battery community has already started developing efficient and robust models able to simulate the battery cell design and the main and more critical manufacturing steps. This is being already covered for the optimization of LIB cell designs, but is limited to conventional LIB cell manufacturing processes.

In view of the expected rapid emergence of new battery technologies, such as all-solid-state batteries, lithium-sulfur batteries, and metal-air batteries, among others, and the poorly understood physics of their manufacturing process and scalability, it is necessary to take a step forward versus existing and short-term incoming manufacturing modeling solutions. Therefore, it is needed to develop an integrative modeling approach able to simulate and optimize fabrication processes of this new generation of battery technologies and their manufacturing processes. All in all, in order to meet the above targets, we envision that the academia should be emphasizing on the following aspects:

- Development of an integrative software solution able to interface individual building simulation blocks pertaining to battery manufacturing processes in a wide diversity of fields beyond batteries themselves (e.g., additive manufacturing, chemical vapor deposition, extrusion, spark plasma sintering and dry process). Such approach should also be able to integrate the optimization of the cell design features in connection to the "virtually" adopted manufacturing processes.
- In addition, the developed tool should couple both physics-based and data-driven models of the cell design and manufacturing process in favor of developing modular modeling of manufacturing processes. This would allow predicting the impact of the unusual combination of disparate process techniques (chosen from virtual libraries built from different technical fields) on the resulting electrode texture and associated electrochemical performance.
- And, last but not least, such modeling tools will have to be developed in strong synergy with the remaining disciplines such as the data acquisition sensorization, interoperability, communication and ontology.

More information on future trends about chemistry neutral battery manufacturing DT will be available in the corresponding review paper[217] belonging to the dedicated special issue to BATTERY 2030+ in this journal.

4. Conclusions

With the current trend of digitalization and demand for customized, high-quality batteries in highly variable batches, with short delivery times, the battery industry is forced to adapt its production and manufacturing style toward the Industry 4.0 approach. Going digital will provide an invaluable set of tools in the fight to improve battery quality and reduce the production costs, as the DTs have the potential to predict failures before they affect or damage the products, to enable manufacturers with instant troubleshooting by adjusting the parameters along the production line in the twin, and they also allow the engineers to commission and diagnose the batteries in real-time. Additionally, the models behind the DT will provide mechanistic insight into the full manufacturing process, for each of the individual steps, as well as the interdependencies in the context where the battery cell manufacturing process is highly complex.

Based on our technology watch, we can conclude our analysis emphasizing there is still plenty of room to reach the level acquired in some other industrial sectors, and we also provide certain recommendations for reaching the goal of having fully connected battery manufacturing facilities, including the concepts of considering chemistry neutral approaches:

- Coupling of the multiscale models: building machine models interconnected to the process models, with the aim to depict the machining process as realistically as possible and to display the relevant process characteristics in local resolution, to describe the physical and technological phenomena over the whole process.
- Combining complementary strengths in physics-based and data-driven modeling approaches, the hybrid analysis and modeling framework will become particularly appealing for developing robust DT platforms and will enable battery researchers and manufacturers to make more informed decisions into the battery manufacturing chain, mitigating the challenges relevant to physical assets.
- Building flexible digital twin capable to be adapted to new and disruptive manufacturing and advanced chemistries.
- A reliable working of any DT will require data arising from different components, such as sensors and models; therefore, advanced communication technologies for keeping the data always synchronized will be required to make sure the two twins remain synchronized, data remains protected and secured.
- Additionally, we would like to highlight the importance of standardization. In a fully connected and interactive battery manufacturing plant, different physical assets will be interacting with each other, and the corresponding digital twins will also have to interact with the physical assets. To facilitate these interconnections, there will be a need for standards cutting across different domain areas. Even interoperability aspects are of paramount importance in the Industry 4.0 framework.
- Moreover, the digitalization procedure should move toward the inclusion of the human factor while digitalizing manufacturing processes.

To conclude, it is undeniable that DTs are an emerging trend in many sectors and, although their technology is still at its infancy, further research efforts toward testing and implementation of DTs will facilitate the digital transformation of the battery manufacturing plants, with the aim to achieve the required targets in saving expenses and ensuring sustainability.

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Conflict of Interest

The authors declare no conflict of interest.

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