Journal of Power Sources 631 (2025) 236158

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Integration of lithium-ion battery recycling into manufacturing through digitalization: A perspective

Imelda Cardenas-Sierra [a,b,1], Utkarsh Vijay [a,b,e,1], Frederic Aguesse [c], Néstor Antuñano [d], Elixabete Ayerbe [c,e], Lukas Gold [f], Aleksandra Naumann [g,h], Laida Otaegui [d], Nadir Recham [a,b], Simon Stier [f], Sandro Süß [g,h], Lalitha Subramanian [i], Nicolas Vallin [j], Gabriela Ventura Silva [g,h], Nicolas Von Drachenfels [g,k], Dennis Weitze [a,b], Alejandro A. Franco [a,b,e,l,*]

[a] *Laboratoire de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne, 80039, Amiens Cedex, France*
[b] *Réseau sur le Stockage Electrochimique de l'Energie (RS2E), Fédération de Recherche CNRS 3459, Hub de l'Energie, 15 rue Baudelocque, 80039, Amiens, Cedex, France*
[c] *CIDETEC, Basque Research and Technology Alliance (BRTA), Paseo Miramón 196, Donostia/San Sebastián, 20014, Gipuzcoa, Spain*
[d] *Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Alava Technology Park, Albert Einstein 48, 01510, Vitoria-Gasteiz, Spain*
[e] *ALISTORE-European Research Institute, Fédération de Recherche CNRS 3104, Hub de l'Energie, 15 rue Baudelocque, 80039, Amiens Cedex, France*
[f] *Fraunhofer Institute for Silicate Research ISC, Neunerplatz 2, Würzburg, 97082, Germany*
[g] *Battery LabFactory Braunschweig (BLB), Technische Universität Braunschweig, Langer Kamp 19, 38106, Braunschweig, Germany*
[h] *Institute of Machine Tools and Production Technology (IWF), Technische Universität Braunschweig, Langer Kamp 19b, 38106, Braunschweig, Germany*
[i] *Dassault Systèmes America, 175 Wyman Street, Waltham, MA, 02451, USA*
[j] *Dassault Systèmes SE, 10 Rue Marcel Dassault, 78140, Vélizy–Villacoublay, France*
[k] *LiPLANET e.V., Volkmaroder Str. 5, 38104, Braunschweig, Germany*
[l] *Institut Universitaire de France, 103 Boulevard Saint Michel, 75005, Paris, France*

HIGHLIGHTS

- Lithium-ion batteries require lifecycle management due to their extensive use.
- Battery recycling reduces waste and recovers valuable materials.
- Digitalization can transform recycling processes by increasing their efficiency.
- Digitalization helps integrating recyclability into the manufacturing processes.

ARTICLE INFO

Keywords:
Lithium-ion cells
Battery
Recycling
Digitalization
Circular economy

ABSTRACT

The lithium-ion batteries (LIBs) industry has expanded quickly despite technological constraints. Additionally, raw materials supply, end-of-life (EoL) management, and the creation of LIB manufacturing policies are receiving attention. All these concerns could be addressed simultaneously by integrating recycling of EoL cells from the early stages of the LIB manufacturing. This article presents perspectives on how to achieve this holistic integration through the means of digitalization. Various challenges of LIB recycling, and different digitalization tools are discussed, shedding light on the latter's potential applications and outcomes. Through the use of the discussed tools to create advanced Digital Twins, it would be possible to screen different recycling processing conditions and materials to achieve higher efficiency, increased safety, at a lower cost. In this regard digitalization of the recycling process for LIB cells, emerges as the key for achieving a collaborative, sustainable, and efficient battery value chain in the European Union. Lastly, in the view of the growing LIB market, this article is thought to be of interest for recycling stakeholders as they move towards a more circular economy model.

* Corresponding author. Laboratoire de Réactivité et Chimie des Solides (LRCS), CNRS UMR 7314, Université de Picardie Jules Verne, 80039, Amiens, France.
E-mail address: alejandro.franco@u-picardie.fr (A.A. Franco).

[1] These authors contributed equally to this work.

https://doi.org/10.1016/j.jpowsour.2024.236158
Received 23 October 2024; Received in revised form 14 December 2024; Accepted 30 December 2024
Available online 25 January 2025

1. Introduction

1.1. Context

To comply with the sustainability goals of reducing carbon emissions, the European Union has proposed the "Fit for 55" proposal, which acts as one of the factors that is steering the automotive industry towards electrification. This proposal establishes that by 2035, all cars and vans registered in Europe will be mandated to be zero-emission [1]. As a reaction of this proposal, a competitive race has started to create the batteries that will power the engines of the next generation of electric vehicles (EVs). The players of this race range from emerging battery manufacturers, well-established vehicle manufacturers, as well as partnerships between both of them.

Within this context of increased demand for lithium-ion batteries (LIBs), we find the birth of the gigafactory, a term used to describe a factory that focuses on the massive production of rechargeable batteries. It gets its characteristic name from the multiple lines required for cell assembly and finishing that are coupled together to produce an annual output of several GWh of battery cell capacity [2].

The increase in the market's demand for batteries will naturally result in an increased number of gigafactories, and with this augmentation, the consideration of a proper waste management system arises. Given that these factories produce their goods out of expensive and critical raw materials, both end-of-life (EoL) cells, as well as production scrap need to be considered.

A solution to this escalating waste problem is to conceive the totality of a battery's life-cycle from its product design, putting particular emphasis on integrating recyclability into the development chain. In this specific context, we highlight the use of digitalization as a tool to ease the integration of recyclability aspects into the manufacturing process of LIB cells.

1.2. How to navigate this article

The goal of this article is to offer perspectives on how the LIB recycling process can be eased by repurposing state-of-the-art battery digitalization tools, currently applied to different steps in the battery manufacturing chain. Since large scale recycling processes are still being developed and scaled up, and computational modeling of these processes is basically on its infancy, this article offers perspectives for redirecting the computational modeling efforts towards the creation of an autonomous, smart and circular battery value chain. In order to do so, the article is divided into different subsections covering the spectrum of topics presented in Fig. 1.

After a brief introduction to the problem at hand, tackled in this Section 1, the state-of-the-art on recycling techniques, the challenges that this sector faces for its scalability and automation, are discussed in Section 2, in addition to the ways in which digitalization of the recycling process can help to complement circular economy goals.

In Section 3, current optimization approaches at different stages of the LIB cell production are presented by describing the computational modeling efforts and techniques. In this same section, some perspectives on how these techniques could be reoriented as tools for the digitalization of the LIB cell recycling process are also discussed.

Finally, Section 4 outlines the current status of LIB recycling in the European Union by making a critical analysis of the current standardization initiatives and reviewing some of the current public funded projects adjacent to the topic of LIB cell recycling.

2. Battery recycling

2.1. Circular economy approach for battery cell recycling

Recycling battery cells is a topic that has gained popularity in the past decade, given that the notion of sustainability was introduced to energy storage devices, with a specific focus on LIBs in the 2010s by Larcher & Tarascon [3]. This visionary review suggested greener battery chemistries as well as insisted on the need for novel recycling methods.

In recent times, sustainability efforts have been developed outside of academia and have been one of the main driving forces behind governmental actions for developing the European Battery Industry. One example is the "Strategic Action Plan on Batteries", an effort by the European Commission for ensuring a sustainable and competitive battery value chain. In the report for this action plan, the circular economy approach for the value chain is highlighted and deemed achievable by fostering the re-use and recycling of cells [4].

Embracing a circular approach by targeting the utilization of EoL batteries is expected to contribute to a reduced strategic dependency on primary raw materials and resources that, with very few exceptions, come from geographic regions outside Europe. This dependence of Europe on raw material reserves outside its geographical boundary often leads to conflicts with European goals in protecting basic human rights, environmental protection and other ethical dilemmas [5]. Moreover, with some of those materials coming from politically unstable regions, the ingredients for fabricating the current and future batteries (generations 4 and 5), have highly fluctuating prices.

Alongside this, one of the EU's directive proposals will require to recover 95 % of cobalt, copper, and nickel, and 70 % of lithium from spent LIBs (for traction applications) by the year 2030 [6]. In this way, the Circular Economy, as well as the Life Cycle Assessment (LCA) concepts have gained more and more prominence in the context of LIBs value chain [7,8] to support efficient utilization starting from cradle to grave.

In the past, LCA has been considered as a tool to analyze the supply chain, forecast environmental impacts, and support sustainability decisions, however, Cilleruelo Palomero et al. [7] have highlighted the importance of considering circularity calculations alongside LCA, for having a complete perspective of supply chains.

Applying this concept to the battery industry, what is currently needed by manufacturers, is a way to actively incorporate the concept of recycling from the early stages of conceiving the scale-up from pilot line to large-scale production.

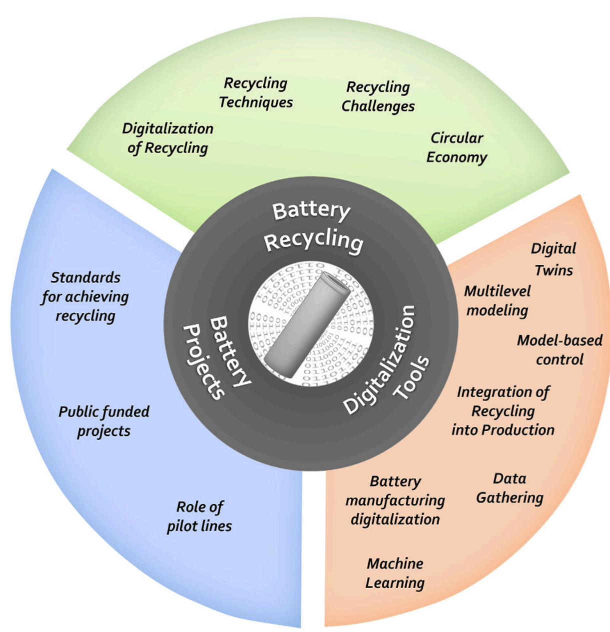

Fig. 1. Visual summary of the main topics discussed in this article.

2.2. Battery recycling techniques

From a Circular Economy perspective, recycling aims to obtain materials suitable for the manufacturing of a new battery cell from a spent one, bringing economic, environmental, health and humanitarian benefits to the battery business through the use of recycling techniques.

EoL batteries represent a corrosive, explosive and overall hazardous waste according to the U.S. legislation, as they contain toxic chemicals and a remaining electric charge, which remains as one of the cornerstones for battery recycling companies [9]. Aside safety issues, there is a problem concerning the existence of many different form factors, and a wide variety of chemistries, common ones for electrodes including Nickel-Manganese-Cobalt (NMC), Lithium Iron Phosphate (LFP), Nickel-Cobalt-Aluminium (NCA). Having said this, the composition of the EoL battery cells is one of the most important factors to consider, given its influence on the technical, economic, and environmental feasibility of the different recycling processes.

Currently, battery recycling focuses on the recovery of the most valuable metals such as nickel, cobalt, copper and manganese, making NMC electrodes attractive for recycling. Nevertheless, this approach is slowly changing, depending on the targeted electrode composition to be recycled. A fully circular business model, in addition to recovering active materials, should also address the treatment and recovery of the less valuable components of spent batteries (such as binders, conductive additives, electrolyte salts and solvents, separators) [10]. Moreover, several EVs manufacturers have announced their plans for the use of LFP electrodes in their future batteries; thus, strategies for the recycling of LFP (which are currently not economically as attractive as NMC) will be needed [11].

To achieve high recovery yields of all the components of a battery cell, and fully embrace the zero-waste concept, it is essential to integrate novel recycling steps that consider the non-active materials, in addition to ensuring a proper liberation of the enclosed active materials [12]. The development of disruptive pretreatments and recycling processes will help to provide a significant increase in the number of elements that can effectively be recovered from EoL batteries (see Table 1) without affecting the recovery yields of the active materials.

Table 1
Some of the current materials used in commercial LIB cells.

Battery Component	Battery Element	Material used
Positive Electrode	Current collector	Aluminum foil
	Binder	Polyvinylidene fluoride (PVDF)
	Additives	Conductive carbon/s
	Active Material	LCO ($LiCoO_2$)
		NMC ($LiNi_xMn_yCo_{1\text{-}x\text{-}y}O_2$)
		NCA ($LiNi_{0,8}Co_{0,15}Al_{0,05}O_2$)
		LMO ($LiMn_2O_4$)
		LFP ($LiFePO_4$)
Negative Electrode	Current collector	Copper foil
	Binder	Styrene-Butadiene Rubber (SBR) + Carboxymethyl cellulose (CMC)
	Additives	Conductive carbon/s
	Active Material	Graphite
		Graphite/Si
		Graphite/SiO_2
		LTO ($Li_4Ti_5O_{12}$)
Electrolyte	Solvent	Mixture of cyclic and linear carbonates
	Salts	Lithium hexafluorophosphate ($LiPF_6$)
		Lithium Bis(trifluoromethanesulfonyl) imide (LiTFSI) and its derivatives
Separator	Membrane	Polyolefin-based (PO) polymers
	Coated membrane	PO + PVDF
		PO + Ceramic
Casing (depending on the format and geometry)	Pouch	Aluminium + Polymers
	Cylindrical/ Prismatic	Steel

As for the battery cell recycling processes applied directly to the active materials, several technologies (Fig. 2) have been developed to tackle the different challenges in recycling:

(i) Pyrometallurgical method:

Pyrometallurgy is a combination of different processes and technologies for metals recovery through the use of high temperature chemical reactions (calcining, roasting, smelting and refining). After dismantling EoL battery packs, the recovered cells and/or modules are heat treated, which avoid the need of sorting or other pre-treatments. In this way, the batteries are rapidly thermally deactivated, the organic compounds (*e.g.* plastics, solvents, graphite or binders) are removed, and the most valuable metals (cobalt, nickel, manganese and copper) are recovered in the form of alloys by a process of reductive smelting. One of the major drawbacks of this route relies in the difficulty to recover Li from the slag at a viable cost together with high energy consumption and expensive gas treatments to avoid toxic emissions [13]. In some cases, this technique is used for the obtention of black mass product, obtained at lower working temperatures (400–800 °C). Depending on the temperature, the final powder product may consist of a mixture of the active materials, conductive carbons, metal impurities coming from the current collector materials, and even binder and some electrolyte components [14].

(ii) Hydrometallurgical method:

Hydrometallurgical processes are focused on dissolving valuable metals in order to separate, purify and finally obtain precursors of new active materials. The active materials are concentrated in the form of black mass through discharging, crushing and fractionatiing spent batteries, followed by lixiviation (mainly inorganic or organic acids) and purification steps (selective precipitation ion-exchange and/or solvent extraction, etc.), which enables high purity of the products. However, this approach requires sorting and mechanical pre-treatments which can be dangerous. In general, this route is more complex than pyrometallurgical one and overall costs are higher [15].

(iii) Direct recycling method:

Direct recycling includes novel methodologies developed to recover, regenerate, and reuse the active materials of the electrodes while keeping their chemical structure intact. After processing, these recovered and regenerated materials are intended to be returned to the battery supply chain without additional, or in some cases, limited processing [16]. The high cost-effectiveness and low environmental impact of this disruptive recycling route are evident, but these benefits are currently outweighed by the challenges of solving the technical difficulties and large-scale implementation.

The current status of industrial and research process for recycling EoL batteries can be mainly classified in two process routes: a combination of pyrometallurgy and hydrometallurgy, or a mechanical treatment followed by hydrometallurgical process [17]. Both recycling alternatives have been developed with the aim of increasing the recovery yield of the most valuable metals, leaving aside the treatment and valorization of low-density plastics, metal scraps, graphite, electrolytes (salts and organic solvents), binders and separators, among others. In this way, the recycling rate of the batteries is really low with a huge reduction in circularity and sustainability because complex materials, including halogenic and organic compounds, as well as some strategic battery materials are lost.

2.3. Challenges in recycling

In addition to the recycling procedure itself, certain recycling routes call for careful sorting preprocessessing like sorting and pretreatments,

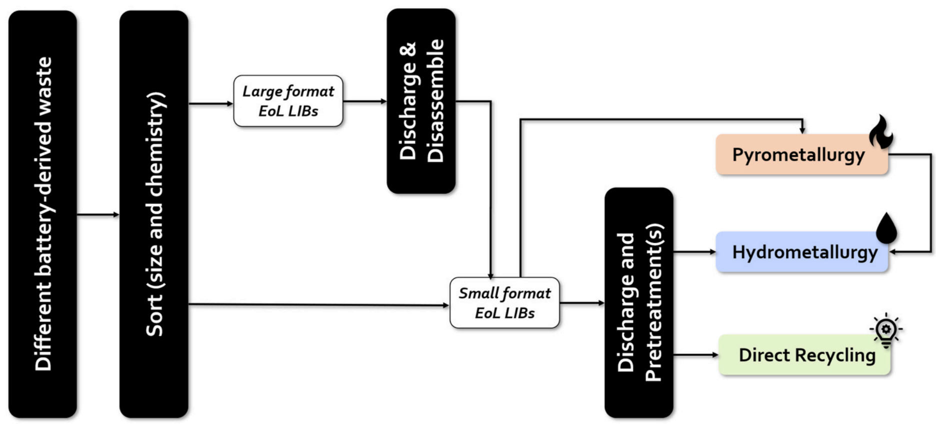

Fig. 2. The different recycling routes for battery-derived waste.

which are difficult to fully automatize due to the different commercially available cell/pack designs available, as well as a lack of information supplied by the battery manufacturers. Insights have been provided on the type of data to which recyclers and second life experts would like to have access to perform their activities [18]. Battery chemistry, disassembly options and instructions as well as product design information is some of the desired information by recyclers. On the other hand, the reasons for battery manufacturers not disclosing this information are mainly competitive concerns, confidentiality contracts, and legal pressure. In this regard, a holistic approach has been proposed by Kintscher et al. [19] for an information exchange architecture among the different relevant partners which play a role in the supply chain of EV batteries. An information marketplace in which information or datasets relevant for the recycling process can be sold or bought is developed.

All in all, the technical, economic and environmental feasibility of battery recycling processes need to ensure the treatment of EoL batteries of different chemical compositions, geometries and designs, efficiently recovering as many elements as are contained into the cell in order to reintroduce them into a new one. Herein, it is considered that an effective integration of digitalization of recycling processes emerges as a key factor for achieving this, in addition to building a collaborative, sustainable, efficient and complete battery value chain in the European Union.

Nonetheless, each of the recycling methods mentioned above has its own limitations, and the ever-growing demand of batteries will only intensify these limitations, making them more pronounced in relation to the available information. This information includes origin of the cell, aging condition, nature and composition of anode and cathode electrode materials as well as the state of the cell at the EoL [20]. Additionally, the segregation or sorting process is a key challenge. The main obstacle at hand is to facilitate the correct implementation of the recycling process. However, providing key cell information (such as the cathode chemistry and its residual capacity at EoL) can lead to a more efficient and tailored recycling route based on the available data.

Similarly, different batteries involve different material compositions, that require the extraction of specific elements. These factors lead to difficulties in recycling and require a number of experimental steps to get the right composition [21]. The most discussed example is the recycling of black mass, which is a mixture of the active material powders of both electrodes, which is very complicated to either separate or regenerate directly. This challenge is intensified in the case where the transition metals are sensitive to reduction by carbon if a heating stage is required [22].

Other of the areas of the process that affects the recyclers in a significant way is the safety, often combined with proper handling and disposal of the EoL battery cells. As the disposed battery cells may still contain stored energy and lead to accidents if improperly handled.

In a nutshell, it can be said that prior and proper information on all the areas mentioned above, may help recyclers in designing better experiments, reduce accidents, and recycle more efficiently. In this context, integrating a digital pipeline into the recycling sector can help industry partners to combine both empirical and digital tools to move towards the Green Chemistry context in the field of battery recycling [21,23].

2.4. How digitalization of recycling can complement circular economy goals

When we consider the battery value chain from the extraction of raw materials to the final disposal of EoL batteries, managing its complexity would need an integrated and interdisciplinary approach [24]. Integration of digitalization technologies in the domain of recycling is thus envisioned to enhance processes efficiency, battery product quality, and sustainability. Such an approach will need to encompass automation through the use of sensors, analytics, and data-driven tools to optimize steps like waste sorting, material recovery, and resource utilization. Although conventional approaches are always an option, digitalizing analytics of different areas in the value chain would complement the recycling process and accelerate development.

For example, combining Machine Learning (ML) algorithms with the LCA analysis of a LIB cell's life-cycle, will be useful for data-driven decision-making in the choice of cell designs. By assessing environmental impact especially, one can optimize the material choice, energy consumption, and emissions. LCA insights and eco-design digital tools can help manufacturers with information to create more sustainable battery cells, thus utilizing efficient resources and minimizing waste [24,25].

A second example of how leveraging the digital approach, using data-driven decision-making tools might transform the optimization, is to use a twin of the manufacturing process to give insights into each step of it. In this context, these twins are being used in battery cell manufacturing for minimizing defects and scrap rates [26]. For instance, studying and improving the most crucial steps of manufacturing through computational simulations, would aim to increase efficiency and minimize waste. Additionally, in the era of Artificial Intelligence (AI), it is envisioned that an intelligent quality check during manufacturing is exported to the recycling process and ensure minimum waste and improved material recovery process.

Similarly, digitalizing the process and its corresponding data specifications can help manufacturers and recyclers to benefit from transparency, ensuring a proper recycling and recovery during the battery cell's lifecycle. Supported by incentives, digital campaigns to educate product users about LIB cell recycling, can also help manufacturers for an eased collection through urban mining, recovering the most valuable materials. To achieve this, accurate information regarding the specific impact of battery materials or processing, can assist in developing regulations and standardizations.

Furthermore, data from digital tools could help to make well-informed decisions on environmental effect mitigation by considering the technical, economic, and design perspectives across the battery cell value chain. Additionally, digitalization can offer a holistic ecosystem for sustainable repurposing, reusing, and recycling of battery cells. As an example, a centralized information database which includes incentivization mechanisms for collection of both data and battery products (Fig. 3), can facilitate stakeholder collaboration and overall help the transition of the battery chain from linear to circular.

All the points previously mentioned get their importance when we consider that observations indicate that from EV scrap, LIBs alone could contribute to a total annual waste generation of 4 million tons by the year 2040 [27,28]. Most importantly, with ongoing research for new energy storage technologies including next generation LIBs, all solid-state batteries (ASSBs) and post LIBs, challenges related to raw material depletion, high scrap rates, and associated environmental impacts will escalate. Therefore, it will remain important to leverage both the advancement and advantages of digitalization in this field.

In conclusion for this section, along with improvements in recycling methods and technologies, the need for sustainable practices through collaboration is greater than ever in the current world. As we move closer to the principles of Circular Economy, digitalizing battery recycling process and associated data might impact the ways in which the LIB industry develops, in order to promote a more sustainable use of our resources while still providing an effective technology [27,29].

3. Digitalization techniques: from cell production to recycling

Simulation techniques along the battery value chain have found their use in many applications; from simulating the dynamics of active material particles upon slurry drying at the lowest of levels, to analyzing the thermal behavior of a battery pack, at one of the highest levels (Fig. 4). However, despite the apparent diversity, all these modeling efforts find their commonality by aiming in the same direction: reducing iterative experiments, saving both time and resources, and finally, accelerating the development, design and optimization of the battery cells as products.

In the fast-evolving field of batteries, it is not rare for the techniques applied in one specific use case to find new relevance in another one. In this context, the following Section discusses how modeling techniques applied to battery design, research, and optimization can be repurposed to shed light on the LIB recycling process and its digitalization.

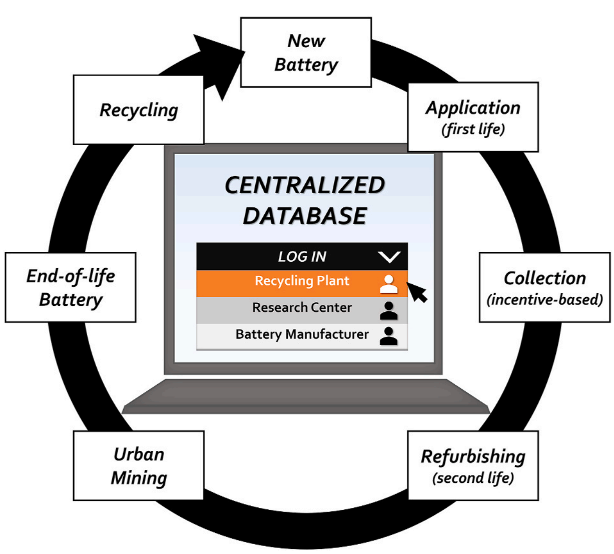

Fig. 3. A proposed user acceptance model, based on a centralized database and incentives.

For a comprehensive analysis, we discuss the modeling techniques spanning from the process level all the way down to the physicochemical level. Following a brief overview of these techniques current employment in the battery manufacturing field, each technique's transferability for application in recycling is discussed.

3.1. Digital twins and virtual twin experiences for efficient recycling

In an era where the productive processes are starting to switch to methodologies like Smart Manufacturing, Digital Twins (DTs) are a concept that has gained popularity in the recent years [30]. This growing interest is understandable, as it is a technology that aims to connect modeling technologies (in a virtual space) to products/processes located in the physical space [31].

DTs have been previously described as a digital representation of a real-world entity or system, in the form of a software object or a model that mirrors a physical object, process or organization. Going deeper on this idea, Virtual Twins (VT) have surged as something further from a mathematical representation of an object or a system. VTs consider an entire system of systems, including the environment in which the physical object exists. This VT technology makes it possible to visualize, model, and simulate virtual worlds, along with the consequences that each modification of an individual component has within the entire model.

These twins have been proposed as a key tool to plan, construct and operate gigafactories [32]. Recently, several reports in the press have stated that battery manufacturers are starting to partner with companies that offer modeling and simulation solutions to create digital twins for their processes [33–38]. Currently, the terminology is evolving fast, and we have taken several steps forward from DTs to virtual twin experiences (VTEs). These technologies have been previously targeted towards the cell design, optimization and manufacturing process. However, it is intended to extend these concepts to the recycling process to allow an integrated end-to-end digitalization from battery cell design and production to second life, end of life, and finally recycling.

Taking the example of battery makers, they can start to use VT technology to design their batteries in a system of systems, with VTs representing the chemistry level of the cell, to the 3D engineering level of the cell, pack, module, and device. Once each of those VTs are done, they can be subjected to simulation protocols to check, for example, how resistant the design is to external elements. VTs will respond to the virtual testing and reveal how the battery cell or pack would perform under cold weather conditions as an example. This will enable engineers to determine if they need to change the chemical formulation within the cell or the padding used around the cell, etc. Once the design is ready to move into the manufacturing process, they can use a VT to investigate how to improve the gigafactory layout to mitigate scrap and lower energy consumption; or how different suppliers impact the overall carbon emissions levels of the end product and how the supply chain will be impacted by their choices.

Another major differentiator of a VT is that it establishes a continuous feedback loop, with data coming in from the product or process in its real-world usage. Teams can analyze this data, run additional tests and make changes to create constant improvement, always aiming to prevent unexpected downtime.

In summary, a DT can be understood as an image of the working process. However, a VT ties together all aspects of the system, the processes, and the responses and is made available in a single platform. Instead of just a digital representation, it is possible to track and respond to all of the requirements in one space. Thus, VTs, subjected to virtual testing, allow a complete and powerful VT experience. This convergence of the virtual and real worlds and the continuous cycle of information between the two creates a closed-loop capability that enables optimization of products and processes through these VTEs.

However, creating these technological breakthroughs is only part of the entire solution, as there are plenty of areas of opportunity in

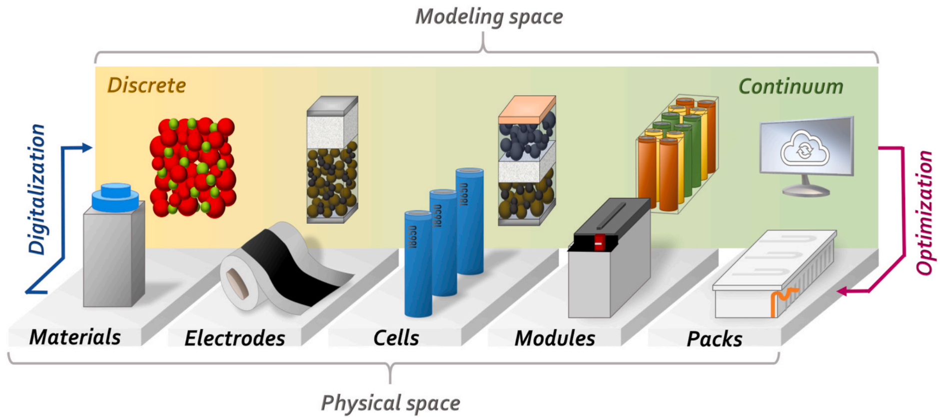

Fig. 4. Modeling techniques for battery manufacturing optimization span multiple scales, reflecting the different scales of battery components in the physical world. These techniques range from discrete to continuum in the corresponding virtual models.

different industry sectors to integrate them [30]. As a way of forecasting the trends, this paper aims to present perspectives that hopefully give some ideas on how to apply the approach of VTEs to one of the crucial steps of the battery life-cycle, recycling. This approach is believed to accelerate the process of closing the loop to foster a circular battery economy.

More than 40 million electric cars are expected to be sold in 2030 by the largest automakers [39]. With this growing demand along with shortage of virgin cell materials, battery manufacturers must consider recycling and recovering chemicals to build batteries. This requires safe and efficient processes, starting from the battery disassembly, or the collection of scrap materials during cell production, to the extraction of the materials. A "model-first" approach through VTEs helps industry to achieve the crucial step of proactive "design-for-circularity" batteries for cost-effective and efficient disassembly and collection processes for recycling and recovery.

During cell production, the amount of scrap materials generated can be significant. VT experiences can help mitigate the amount of scrap materials, as well as to control and optimize production. Digital continuity between cell design and manufacturing process engineering will bring visibility on the performance of the manufacturing process. Virtual models of each step of the manufacturing process can provide insights on the efficiency of each step [26]. This allows virtually designing and virtually testing improvements for each step towards an optimized solution that will potentially reduce the amount of scrap materials. VTEs can also be applied at the line level, with solutions like factory flow simulations, to optimize the flow of materials across all the process steps. Such solution helps not only to identify production bottlenecks but also define mitigation paths for scrap materials, using methods like direct recycling, or optimizing the route for scrap material flows. Manufacturing Operations Management systems can execute such plans for materials traceability, quality controls or warehouse management. The integration of such a comprehensive tool chain is possible, bringing digital continuity from product and process engineering to manufacturing operations, so cell makers can improve material reuse and recyclability.

Using modeling and simulations as well as generative AI and ML techniques for materials design and process optimization, informed decisions can be made on the second life performance of the recycled chemicals. VTEs for the choice of the mechanical and chemical technologies for recycling, converting precious metals in the battery to high-purity raw materials, enabling the production of new batteries from recycled materials, and ensuring that the second life battery performs as good as the batteries made from virgin materials are all necessary for successful circularity. By performing "what/if" virtual experiments, several scenarios can be virtually investigated prior to deploying them in the physical lab.

By designing specific VTEs, battery circularity can be planned, optimized and automated before batteries reach the end of its first life. Fig. 5 represents the digital thread connecting materials resilience, materials traceability and second life eligibility. By simulating supply chain fluctuations, price hikes as well as market demands, raw material resilience can be built. With VTEs covering battery materials chemistry, formulation and design, the most appropriate raw materials and process can be chosen, which are cost efficient while maximizing performance and lowering environmental footprint. VTEs where modeling and simulations are combined with generative AI and ML allow to screen the phase space of second life materials and predict cell performance allowing to assess the potential battery health, safety and lifetime.

The VTEs allow to visualize, model, and simulate the entire environment of a sophisticated experience, facilitating sustainable business innovation across a full product's life-cycle. VTs cover a range of length scales, starting from cell chemistry at the nanometer scale to the micrometer scale, and cell and pack engineering covers millimeter to meter scales. To cite some examples, a few recent publications that used different software like BIOVIA Materials Studio [40] at the cell chemistry scale, are highlighted [41–43].

Fig. 5. Virtual Twin Experiences loop for recycling and recovery.

3.2. Multilevel modeling

Battery cell production consists of heterogeneous processes coupled by converging and diverging material flows, resulting in the propagation of cause-effect relationships along the process chain and affecting product, process, and production performances. Consequently, alterations in one process located at the beginning of production may lead to changes along the chain [26,44,45].

This applies similarly to battery cell recycling. The majority of LIB battery recycling processes are characterized by a combination of different disassembly processes, followed by mechanical, thermal, and hydrometallurgical processes. The resulting material flows within the process chain are complex, particularly as varying cell chemistries are fed into the process chain, leading to volatile process outputs in terms of quality and achieved material fractions. In order to make techno-economic decisions in this context, it is necessary to employ digitalization-empowered methods and tools that take the complexity of the material flows into consideration. The handling of this complexity necessitates a high degree of transparency of the process chain and data infrastructure for the seamless integration of data from various stages of the recycling process in order to create a comprehensive overview that supports informed decision-making.

Modeling approaches can enable the reproduction of complex cause-effect relationships in the chain as well as the investigation and quantification, for example, of the interconnections between manufacturing process parameters (*e.g.*, temperature and speed) and structural parameters (*e.g.*, mass loading and porosity) at a process level.

Independent process models can be coupled to investigate the process-structure relationships along the process chain. A further coupling of these models with electrochemical or production models enable the investigation of interdependencies on the battery cell properties [26,46,47,84] or production performance (*e.g.*, machine utilization, energy and material consumption) [48]. With that, cause-effect relationships on a product, process, and production levels are quantified by coupling at a multilevel approach. For the specific problem at hand, we propose a framework like the one shown in Fig. 6.

Since physics-based (*i.e.*, mechanistic) modeling provides the reproduction of known phenomena, existing and validated models may be extrapolated to other scenarios, such as new chemistries or process configurations. In addition, this approach allows the consideration of interdependencies in planning activities, which in turn facilitates the selection of better parameters, the improvement of battery cell quality, and the avoidance of material and energy losses associated with the production of battery cells of poor quality.

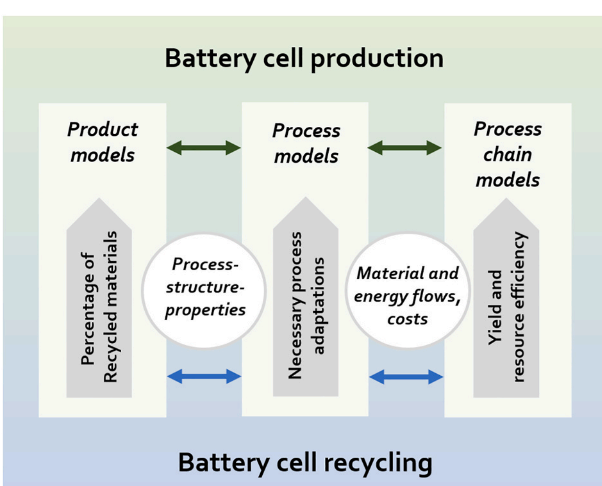

Fig. 6. Proposed coupling of different models involved during production and recycling of LIB cells, considering product, process and process chain models.

Over the past years, the investigation of battery cell recycling has become increasingly important as a response to the growing efforts to increase circularity and comply with the new regulations. Battery cells can be recycled in different routes, with varying yields and resulting quality. Understanding the process-structure relationships in recycling is mandatory for improving the efficiency of recycling processes and increasing the quality of recycled materials. The majority of current investigations regarding the recycling process are focused on experimental work [49–51]. Other studies investigate the effect of process configurations and yield by modeling the material flow with published data [52] or the effects of recycled materials in battery cell production with economic and environmental focus [53–55]. Work based on experimental data is currently limited by low recycling rates of batteries after the use phase and low maturity level of recycling technologies. The multilevel physics-based modeling approach, developed for battery cell production, could be extended to recycling processes to support the investigation and comparison of different recycling routes in the yield and quality material. As there is currently limited experimental data on recycling processes, especially in larger scales, the advantages of mechanistic modeling could be transferred to recycling and thus used to consider new scenarios for which there is still a lack of information. Moreover, the linking of process chain models for battery cell recycling and production in a circular approach could support the investigation of usage of recycled material. This investigation has so far only been carried out as part of work focusing on the circular economy [56] and there is a lack of further analysis on the exact impact of recyclates on battery cell quality and process configurations. With this, the percentage of used recycled materials could be determined considering their quality and impact on the final battery cell properties and resource consumption.

3.3. Model-based control

The utilization of both descriptive and predictive data-based approaches is key to understand interrelations within the process chains and controlling them effectively supporting ecological and economical goals. Descriptive methods enable a cross-process understanding to evaluate the most important factors within the process chain. These parameters can then be used as levers for the prediction of the final quality parameters of the cell. An application example is the early declaration of scrap based on the product feature prediction and general process knowledge gained through descriptive methods [57][81]. It can prevent the addition of further material onto an intermediate product that is not going to be able to provide a functioning product.

In general, the determination of more parameters for error prevention along the process chain is associated with higher costs. A compromise must therefore be found between the costs of prevention and the costs of errors that actually occur. Quality gates are a concept that sets inspection and decision points along the process chain to evaluate the quality of an (intermediate) product [58]. Quality itself can be defined as a "… degree to which a set of inherent characteristics or features of an object fulfills requirements" [59]. This set of characteristics can *e.g.* relate to a process or an (intermediate) product. A distinction must therefore be made between those two. It is however important to acknowledge the influence of the process parameters on the product features which is why both the process and product quality need to be considered. Especially for large-scale production inline inspections with automated evaluation are most suitable for potential decision making with regard to the control of downstream processes [58]. The right determination of the most important parameters and features however can be based on experience and historical data using feature selection methods like recursive feature elimination [60].

The interrelations found by *e.g.* data mining of the historical data at the quality gates can be utilized on different levels of control. On the one hand, single processes can be enhanced, on the other hand, these interrelations enable cross-process control that utilizes the knowledge regarding the process chain to control the downstream processes based on the intermediate product features and process parameters. Currently, these approaches are mainly found in production but not recycling. The main focus is often the relationship between process parameters and intermediate product features as well as the prediction of features [57, 60–62]. This is the main basis for the mentioned quality gates building a foundation for decision support within the production. In contrast to production, recycling processes follow more variable routes since different chemical and physical techniques of material extraction are usually necessary [63]. The current focus is still on understanding the individual processes.

Model-based control systems considering both battery cell production and recycling as consequence of production are currently scarcely addressed in research. Making the link from recycling back to production can provide helpful insight of the interrelations between both process chains adding more complexity to the overall system but also including decisions that have to be made in when passing material between the process chains [64]. An example would be exclusion of highly contaminated material that cannot be handled by an in-house recycling route. Scenarios like these can be very facility-dependent and individual but are necessary to be considered long-term due to the growing importance of a high secondary materials share driven by demand and politics. Additionally, the concept of circulation factories combines both process chains under one roof offering the advantage of independence from recyclers, while also providing rejected parts of known chemistry for recycling. The extension of control systems to include recycling is therefore favorable since the material passed on between the process chains highly influences the product quality, especially considering the imperfect or unknown process quality of the recycling processes. Enhancing transparency with data-based approaches therefore benefits the factory overall.

3.4. Integration of recycling into the production at the system level

Besides the aforementioned connection of process chains on a control level, circulation factories connect all flows of production and recycling including information, material, energy and personnel. All of them can benefit from working within a common factory under the right circumstances while also reducing the travel distance.

The complexity of the most useful in-house recycling line is determined by various factors like the individual company prerequisites and the scope they want to act in. On the one hand, company prerequisites include, for example, the scrap rate, return options for own or known batteries, existing relationships with recyclers and political conditions such as subsidies or recycling quotas in the respective country. On the other hand, the motivation to operate a recycling line in the first place or even take on a more advanced recycling line is determined by factors such as establishment and preservation of intellectual property within the company or ecological goals. It is also unknown which requirements companies will face in the future. To have working structures established at an earlier stage might save time and could be a competitive advantage.

Linking production and recycling through information flows within a circulation factory supports the aforementioned data-based methods helping to identify the most important influences on the process chains as well as the recycling effort. This supports not only the operation of the plant but also planning processes of the plant or the product design.

3.5. Data gathering and storage as basis for data-based and physics-based modeling

It is important to ensure that managing the data across intricate manufacturing steps presents significant challenges, chiefly in maintaining the data consistency and connectivity. A promising solution lies in creating a semantic layer over the whole manufacturing infrastructure. This concept has been explored in research projects such as KIproBatt [65], ViPro [66], and DataBatt [67], guiding the path towards comprehensive machine-readable process data.

The cornerstone of these initiatives should be a process-centric data model, as suggested previously by the General Process Ontology (GPO) [68]. Complementing this is the peripheral, an inventory description that includes machine and material metadata using Battery Interface Ontology (BattINFO) [69] and various data sources and digital assets. This strategic approach can significantly impact integration time, AI application, and closed-loop process/value chain optimization, including recycling. Furthermore, it offers interoperable data for other domains, particularly sustainability research.

3.6. Overview of current digitalization of battery manufacturing

The state-of-the-art of modeling techniques applied to battery manufacturing mainly rely on the use of physics-based models (PBMs) and AI/ML. These models allow researchers to study complex phenomena occurring on a wide array of scales [70,71]. However, for the purpose at hand, this subsection will focus on the simulation of recycling at the micro- and macroscopic scales and will shed light on how computational tools can be used to optimize our ability to both efficiently and sustainably recycle battery materials.

As an example of the current battery manufacturing modeling approaches, Fig. 7 shows an illustration of a simplified and experimentally validated PBM used for an electrode manufacturing pipeline. This model has been developed in the context of the ARTISTIC Digitalization Initiative, initially supported by a European Research Council project [72]. The steps within this modeling framework involve the simulation of the electrode slurry followed by a drying and consequent calendering process at different compression degrees. Each step of this simulation pipeline is carefully parametrized for different slurry and electrode properties (like density, porosity, and thickness). The final output are 3D-resolved electrode microstructures which are also characterized for textural properties like tortuosity factor [73–75].

Depending on the desired electrode material and experimental data, different types of active material particles can be considered inside the simulations (e.g. NMC [73], Graphite [76]) and the framework has been extended for the electrode manufacturing simulations of other battery technologies such as ASSBs [77,78]). The additional electrochemically inactive materials such as the conductive additives and the binder can also be considered explicitly in this modeling framework, through an entity named as Carbon Binder Domain (CBD) [79]. The data generated at each step of the ARTISTIC pipeline are further utilized for manufacturing process optimization (inverse design) via the use of various AI tools [26,80–85]. In a nutshell, by leveraging pilot line experimental data, physics-based simulations at the mesoscale and AI/ML, this combined approach demonstrates a powerful tool for manufacturing optimization with the goal of reducing scrap rates at source [26]. It is important to underline that, because of its mesoscopic character, the ARTISTIC approach bridges the gap between the materials and the cell device scales.

In terms of leveraging this type of methodology for the development of battery cell recycling through digitalization, an idea that comes to mind is to get inspiration from this framework and thus create a connected modeling pipeline that mirrors the sequential steps of the recycling pipeline of interest. However, depending on the type of the recycling approach and number of steps utilized, there could be a variety of ways of translating this approach to the recycling value chain. For this reason, in the following Sections we discuss the perspectives of particular modeling tools and our envisioned use of these techniques in the recycling landscape.

3.7. Discrete simulations for recycling digitalization

Since the recycling of the electronic or ionic conductors forming electrochemical cells has been the focus of recycling efforts, use cases of discrete modeling methodologies applied for electrodes and electrolytes

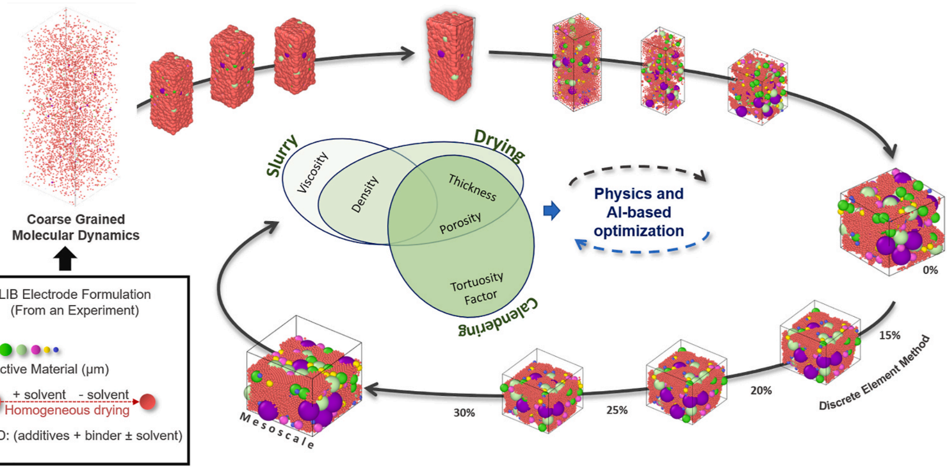

Fig. 7. One of the physics-based manufacturing simulation frameworks for LIBs developed in the ARTISTIC project. Based on the experimental formulation specifications (e.g. material and composition), Coarse-Grained Molecular Dynamics (CGMD) is applied to simulate the electrode slurry and its drying, and Discrete Element Method (DEM) is used to simulate calendering at different compression degrees, all in a sequence. The physics-based data are further utilized for manufacturing optimization using AI tools (inverse design).

are herein presented. After this brief description, a perspective on how these modeling methods could be adapted to describe the recycling approaches is discussed.

Within battery cell recycling, a deep understanding of the micro- and macroscopic phenomena occurring at each step of the process is essential to identify the parameters with the highest impact, and thus, optimize the efficiency and sustainability of the process line. This subsection will focus on the simulation of recycling from micro-up to macroscopic scales and will shed light on how computational tools can be used to optimize our ability to recycle the materials inside the cells.

To narrow down on the possible perspectives inside the wide topic of LIBs recycling, for discrete simulations, the light is shed to apply the techniques onto the recycling of electrode scraps after undergoing coating (as they are envisioned as the scrap with highest rejection rates). Hydrometallurgical recycling and direct recycling processes are proposed for potential application in this area [86]. On the next subsections, perspectives for both recycling methodologies will be discussed.

3.7.1. Perspectives of discrete methods for the simulation of direct recycling methods

Scrap recycling is often performed by using high temperatures, but even then, binder dissolution remains a problem, as it is a process that can take anywhere between minutes and hours [87–89]. To scale up this type of recycling methodology, and achieve industry relevance, it is important to focus on methods that will target reduced time and energy requirements.

Computational approaches represent a cost-effective method to study this target requirements and the efficiency of different recycling methods. As an example, molecular dynamics simulations of polymer dissolution have been already reported [90,91] and can be used to simulate structure-property relationships of bulk systems of polymers in a solvent [92,93]. Promising work has already been done on the computational screening of solvents and temperatures as well as their effect on polymer dissolution [94,95].

Such approaches typically consist of generating a polymeric structure with steric interaction and assessing the trajectory of the polymer with respect to the solvent quality. Based on the sampled trajectories conforming to the simulated ensemble, structural properties can be extracted from the resulting topology and conclusions about the dissolution behavior of a polymer in such a solvent can be reached.

Molecular dynamics simulations can thus be performed to screen different binders, relevant to battery production, based on their solubility. Based on this, researchers can garner knowledge on material behavior, thus allowing them to use their knowledge to minimize energy and time requirements to recycle scrap electrode material. In addition, free energy calculations can also be promising to simulate the dissolution of the same binders by their use with Monte Carlo simulations to determine optimal structure-property relations. In this way, green and non-toxic solvents can be computationally screened for their viability.

Zooming out of the molecular approaches, at the mesoscopic and macroscopic scales, the usage of hydrodynamic interactions can be envisioned to calculate further properties. Coupling of computational fluid dynamics (CFD) and DEM appear to be good choices for studying certain interactions between materials and target environments or experimental conditions. This will allow the improvement of property intuition for scientists and engineers and a more targeted approach for reducing energy and time requirements for the separation of materials.

3.7.2. Perspective of discrete methods for the simulation of hydrometallurgical recycling

The hydrometallurgy approach is used in LIB recycling for recovering metals waste materials using aqueous solvents. It consists of a leaching, solution concentration and purification, and a step responsible for the recovery of metal salts. During leaching, acids or bases are used at low temperatures to oxidize or reduce and dissolve the metals. During the purification step, the desired metal is separated from impurities. Physics-based simulations can be used to computationally model each step and to establish optimal properties for hydrometallurgical recycling and thereby maximize the rate of metal extraction and even the safety of researchers and engineers.

Firstly, the use of molecular dynamics simulations finds its importance in studying metal-ion solvation and complexation processes to elucidate how metallic ions interact with aqueous solvent molecules and reveal their adsorption to metal surfaces. By performing these simulations, one might gain further insight into the surface coverage and aggregation of the metal and thus allow for a targeted prediction of the separation process. Such simulations have already been performed to study gold recovery [96], and are an important element when it comes to developing efficient hydrometallurgical extraction processes. By further studying thermodynamic quantities and reaction-diffusion processes, it is possible to analyze the time evolution of the system under study and identify reaction pathways [97]. This ultimately allows for a better understanding of all the processes involved. ML tools may also be a useful addition to learning reaction rates from molecular dynamics simulations and ultimately allow for faster solvent screening, thus allowing researchers to quickly find suitable solvents for leaching processes [98].

3.8. Hybrid methods

CFD may also be considered as a useful tool to study hydrometallurgical processes on a macroscopic level and can be particularly useful in helping engineers and scientists to optimize performance and scale of these processes to industrially relevant sizes, always targeting more efficient and safe processes.

In specific, the use of simulations for stirred tank reactors might help to optimize reactor design and thereby to optimize miscibility efficiency. Thereby, scientists and engineers can be guided by numerical models to develop optimal leaching vessels for better miscibility. Work on such optimization processes already exists [99] and has the potential to guide researchers in the future.

Furthermore, multiphase fluid models have been used to simulate the effects of solid particles present in the aqueous solution on its effect on gas-liquid flow as well as heat transfer within the reactor vessel [100, 101]. It could be fruitful to perform parameter studies for materials used in hydrometallurgical recycling of batteries to optimize cell recycling. Using a fluid dynamics simulation or a coupled CFD and DEM simulation, one may simulate the flow of the leaching solution through the recycled metal, thereby predicting the concentration of the metals within the solvent. To enhance safety of hydrometallurgical recycling, CFD simulations may also be performed to understand acid and dust pollution occurring during the recycling process and to design emission control systems.

Ultimately, it is a worthwhile endeavor to combine both experimental and simulated datasets of the structural effects of solvents on polymers to create a database of dissolution properties for recycling, like the one developed recently by Zhou et al. [95]. On the one hand, this will allow scientists to develop an intuition on which solvents can best be used to dissolve a given binder. On the other hand, ML approaches can then be employed to connect structure-property relations to the feasibility of recycling of products and thereby reduce time and energy requirements for maximal throughput.

3.9. Continuum methods

Expanding on other modeling tools beyond discrete methods, we can find the use of techniques to model the phenomena happening at the continuum space. In this regard, we highlight the use of electrochemical PBMs, as mathematical representations of the inner workings of a battery cells that consider both physical and chemical phenomena. The first works of PBMs applied for battery materials dates back to 1962, when the current distribution in porous electrodes was studied by Newman and Tobias [102], later referred to also as "Doyle-Fuller-Newman" (DFN) models, making reference to the authors [103].

The basis of these models consists of setting up a set of partial differential equations (PDEs) based on given physics laws, with the purpose of predicting the internal behavior of a cell under different conditions [104]. A well posed and well-parametrized model can allow to study the evolution in time of the internal variables in a way that is not possible with current in-operando experimental techniques applied to batteries [105]. For example, some internal variables that are possible to track areconcentration of the lithium ion in the electrolyte and of its metallic counterpart in the active material. Additionally, the potential and current distributions in both the electrolyte and electrodes can also be monitored.

Nowadays, these models are so advanced as they are being used in an array of applications ranging from understanding and improving electrochemical performance of electrodes, to the design optimization of full cells and battery packs. We can highlight the use of these models for relating electrochemical performance with manufacturing process parameters of electrodes as shown recently [106].

Going further, PBMs have evolved to account for additional physics in addition to tracking the evolution of internal electrical potentials and concentrations. As an example, we highlight reviews of collection of models that focus on mechano-chemical degradation [107], thermal degradation [108], and even real-time state of charge (SoC) and state of health (SoH) monitoring for batteries [109].

In the scope of this article, we picture the utilization of PBMs as a cost-effective and straightforward method for conducting quality control of the electrochemical properties of electrodes produced from recycled materials. Quality control is particularly important in this landscape, given that soon, battery manufacturers will be required to comply with mandatory minimum levels of recycled metallic elements in their products, as stipulated by the European Union [110]. To foster a circular and sustainable battery value chain, the inclusion of waste from battery manufacturing processes into the production of new batteries will also be considered as part of the recycled content. In the ideal case, newly manufactured batteries would be made in their entirety from recycled batteries, or battery scrap materials. Still, given the state-of-the-art, it would be easier to comply with the regulation by combining both recycled and pristine electrode materials into a single hybrid electrode formulation.

For achieving this idealistic goal of creating electrodes with both pristine and recycled active materials could pose two main challenges. First one, that the performance of the recycled material can be unsuitable to meet customer demands (in terms of energy or power). The second one, lays in finding the optimal proportion of pristine and recycled material, since this procedure could be time consuming and may require iterative experimentation.

Electrochemical models could serve as an effective tool to first evaluate the performance of recycled products vs. pristine ones, and second, select their correct integration into hybrid electrodes. To overcome the first challenge, a model can help to decouple the intricate link between the chosen recycling process, the obtained physical and chemical properties, and electrochemical performance.

Depending on the goals, degree of accuracy and available computational resources, different model types can be chosen. As an example, manufacturers could choose to work with low dimensional models like the Single Particle Model (SPM) or Pseudo 2-Dimensional (P2D) model, due to their advantage of offering fast, reliable, and computationally inexpensive results [105]. However, if structural features and inhomogeneities in electrodes are relevant to the electrochemical performance, the use of fully resolved 3D models (with defined geometry, like shown in Fig. 8), would be preferred, even if they are usually more computationally expensive.

Regarding the second challenge for creating hybrid recycled electrodes, PBMs could be used as a probe tool to study the electrochemical performance of the recycled material alongside the pristine one. A crucial role of these models will be to elucidate the electrochemical fingerprint of these new hybrid electrodes, since describing each active material by a set of coupled equations can allow to decouple the contribution of each component to the total measured voltage, following the approach of blend electrodes [111–113].

Having discussed these two challenges and how models could help introducing digitalization into the recycling process, it is proposed that a combined experimental and modeling approach will appear at several gigafactories, since companies are realizing that performing full experimental studies for a single product are costly, involves complex procedures, and are typically realized in large quantities. Due to the need for modeling batteries in an easier and ready-made way, different software companies have come up with modules, packs or libraries that can help to develop different types of electrochemical models [114–116].

3.10. Machine learning methods

ML has emerged as a valuable tool for addressing numerous challenges along the entire battery value chain, albeit with a primary emphasis on battery design, manufacturing, and utilization.

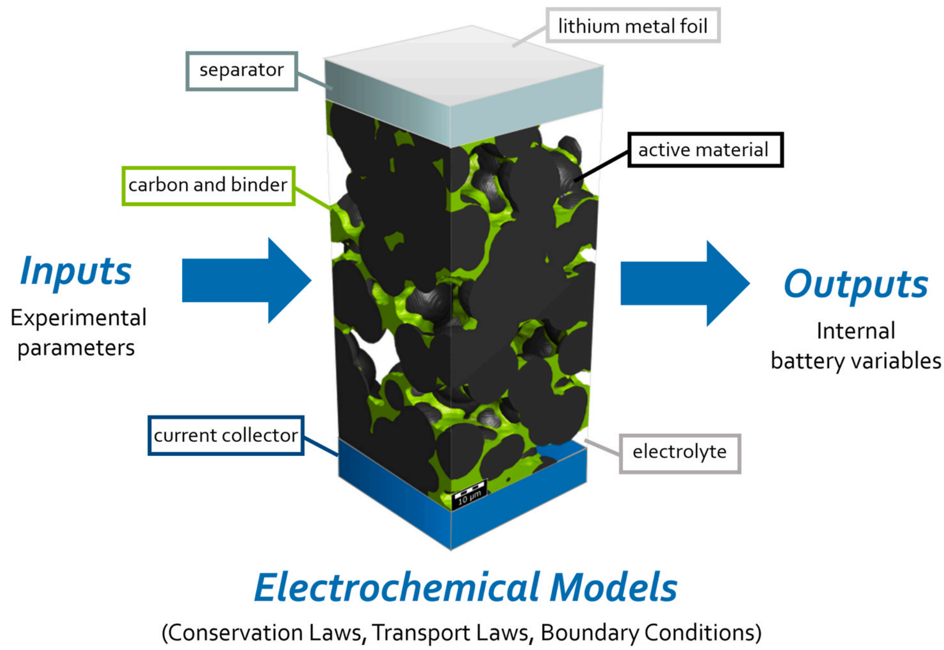

Fig. 8. Illustrative image of the appplication of an electrochemical model to an electrode microstructure.

Numerous works have been undertaken to tackle each stage of battery development: from the automatic discovery of complex battery mechanisms [117–120], prediction of the rest of useful life (RUL) [121–123], evaluation of SoH [124,125], providing insights into battery production processes and their interdependencies [81–84,126], guiding battery design [127,128], optimizing cycling profiles [129,130], early prediction of the battery cell lifetime [131], approximating failure distributions [132] or prediction of lifelong performance immediately after cell manufacturing [133].

However, in the context of battery cell recycling, the utilization of ML has remained relatively constrained. Only a small number of studies have delved into ML techniques specifically targeting various stages of the recycling process. This scarcity is often attributed to the inadequate availability of comprehensive battery data, especially for batteries that have undergone cycles until the EoL stage.

The following sections contain various examples and advantages of ML in the field of battery manufacturing followed by some use cases and perspectives of ML for its integration in the battery recycling process.

3.10.1. Machine learning and physics-based continuum models

It has been previously highlighted that in regards to LIBs used for EVs, there is a clear opportunity for recovering the materials inside these batteries by the use of automated processes and intelligent characterizations [134]. As we approach this new era of digitalization, our battery modeling tools continue to improve, and the combination of several computational tools is expected to maximize the most out of the available experimental data. In here, we identify the combination of continuum PBMs alongside ML methods as one of the most promising combinations.

Two different use cases for this particular combination are identified. The first case is to use data driven methods like ML in order to exploit the results obtained from performing physics-based simulations, while the second case relies on the implementation of physics equations into the ML architectures to create what is known as "physics-informed" ML models.

(i) Machine learning for exploiting data arising from physics-based simulations

Data driven techniques are increasing in popularity due to their ability to arrive to accurate and reliable interpolation results. However, these types of techniques require big and reliable datasets to do so. In addition, obtaining these extensive datasets experimentally, is not a trivial task. As an alternative, utilizing datasets coming from validated and robust PBMs, would enable the use of ML algorithms.

In the particular LIB context, it is of interest to integrate the results of electrochemical modeling results into ML architectures, in order to accelerate result acquisition capabilities of the models. This idea has been previously explored for PBMs with different levels of complexity. For example, a combination of these techniques was implemented by Dawson-Elli et al. [135], where researchers studied the use of data coming from a P2D PBM to train different ML algorithms like decision trees (DTs), random forests (RFs), and gradient boosted machines (GBMs). This research highlights the use of these models for time critical applications, since introducing ML can increase execution times while keeping a high accuracy for predicting discharge profiles.

Another relevant example was presented by Li et al., where a combination of techniques was done by training recurrent neural networks (RNN) by using a synthetic dataset coming from a P2D model, in order to predict SoC, and estimate the internal battery variables at different spatial locations [136]. This was achieved by training on a large dataset coming from an electrochemical-thermal model. The goal of tracking internal concentrations and potentials of both electrodes based only on inputs of current, voltage and temperature was achieved, demonstrating the ease of use of these types of models for the final user.

A more sophisticated approach was studied by combining a 3D physics-based modeling dataset with ML through the use of convolutional neural networks (CNNs) by Marcato et al. [137]. In this work, a proof of concept of a time dependent discharge simulation of a 3D resolved lithium ion battery electrode microstructure was presented. This model was key to show that these ML surrogate models are not only capable of predicting battery metrics like voltage or current, but also are capable of unveiling the dynamics of the battery electrodes by showing the evolution of the lithiation on a three-dimensional microstructure.

More recently, another study focused on tracking the SoH of batteries under fast cycling conditions was published by Weddle et al. [138]. In this work, a synthetic dataset coming from P2D PBMs was used to create full cycling profiles. The profiles were posteriorly used to train a deep learning algorithm to identify the aging modes. Herein, a CNN was used to identify the features of the cycling as to map the aging modes. At the end, this methodology allowed to build a robust and reliable model to enable a rapid, and continuous aging assessment under different charging conditions.

All these studies represent an important background on how accurate, and fast surrogate models can be built from training ML architectures using PBMs datasets as inputs. However, the choice of algorithm and the fidelity of the training data will affect the interpolation capabilities of the surrogate model, and it is important to mention that all of the previously mentioned works have different tradeoffs between accuracy, training times and prediction abilities.

For the perspective of exporting this approach into the digitalization of the recycling process, it is expected that this hybrid methodology proves useful as well. PBMs are expected to be a key component to create large datasets and thus accelerate the quality control workflows by coupling them with data driven techniques. It is envisioned that to accelerate development, a modeling workflow could consist of first, performing enough experimental characterizations to parametrize and validate a PBM. After that, the obtained data would be fed into a ML capable of extracting meaningful results for different conditions and use cases. Going further, this coupled approach could also be implemented in conjunction with powerful cloud computing power and Internet of Things technologies (IoT) with the purpose of creating a sophisticated VT experience of the recycling process line.

Expanding on this, the ideal integration of IoT into the recycling pipeline would be to equip all machinery with state-of-the-art sensors (prioritizing advanced robotics), and the use of in-operando characterization techniques [134]. In this way, each sequential task of the recycling line would be carefully monitored. Advanced cloud computing power would give the power to take the real-time inputs measured by the sensors and incorporate them into a model that is able to compute the predicted performance based on the received inputs.

A ML model acting as a surrogate model of the PBM, will basically calculate results based on synthetic data or hybrid datasets (involving experimental and synthetic data),[26], and if parametrized correctly, it would be able to help the process engineers to make decisions on whether to change a step of the process or leave it unchanged according to the predicted results. To go even further in the automation dream, another model could be coupled to the fully automated line, in order to be smart enough to tweak the machine specifications if it detects at some point that the measured parameters has a negative correlation to the battery performance. In this way, we could have a truly holistic DT that can be controlled to get the targeted performance.

(ii) Physics-informed machine learning

Apart from profiting on ML to accelerate the interpolation predictions of PBMs, there exists another way to integrate physics equations into data driven techniques. Physics-informed Machine Learning (PIML) is a modeling methodology which combines both PBMs and ML algorithms, to improve generalization and extrapolation capabilities, even when data is limited [139]. These type of hybrid models are built by providing the data driven algorithms with different types of biases during the learning process in order to identify solutions that are physically consistent [140].

For the particular case of adapting the highly non-linear physics of electrochemical models into a complex data driven architecture, in the specific case of working with neural networks, is to inform the loss functions with the residual of the physical equations. This particular approach has been previously discussed in a study of adapting deep learning functionalities to solve problems involving PDEs [141].

In the case of LIB cell simulations, the goal is to enable highly accurate voltage/capacity predictions while preserving the low computational complexity. If we compare this approach to other models used to simulate the voltage profiles of a battery cell, the target performance would be achieved by combining the high physics fidelity and low volume of needed data that PBMs offer, with the low computational cost of the trained ML models to get the best tradeoff between the techniques (Fig. 9).

Some examples of this methodology have already been applied to batteries, and focus particularly in the domain of estimating the SoH, aging, and the RUL of LIBs. Nascimiento et al. demonstrated a hybrid modeling tool created by directly implementing physics of discharge (Nernst and Butler Volmer equations) into a deep learning approach [142]. This hybrid model used deep neural networks (DNNs) along with a reduced order PBM to predict the discharge curves, as well as end-of-discharge of batteries under different loading conditions. In particular, we highlight the high-flexibility of the ML component to correct for some of the missing physics and account for uncertainty in some model parameters.

Other approaches for introducing physics into an AI architecture were shown by Xu et al. [143]. In this research paper, a PIML prognostic model was created and coined with the "PIDDA" name. The main advantages when comparing this model —which can forecast the secondary variables of discharge, capacity, and SoH throughout the battery's life— to traditional ML methods, was an improvement in the prediction accuracy, and the decrease of necessary input data.

Other examples of PIML models include the use of alternative data inputs. In this case, Kohtz et al. showed that a partial charging segment under constant current (corresponding to less than 300 s of data) was able to be taken as input for a multi-fidelity battery model with SoH prognostic capabilities [144]. In this work, it was demonstrated that it was possible to estimate the SoH in just minutes by using this hybrid approach.

A more recent study, focused on exploring online estimation of degradation modes in addition to battery capacity [145]. Thelen et al. made this possible by considering differential capacity curves (associated with different degradation modes), as well as inputs of early-life experimental and simulated data. The results suggested that this approach may enable quick, accurate, and automated online degradation diagnostics of LIBs, for its possible implementation on new generation battery management systems with online estimation capabilities.

The hybrid PIML methodology was used by Shi et al. to model the degradation trend and posteriorly obtaining a RUL prediction for LIBs [146]. This was achieved by combining a physics-based calendar and cycle aging (CCA) model with a long short-term memory (LSTM) layer. The main advantage of using the PIML approach in this case, was the accurate prediction of the capacity fade by learning the effect of the

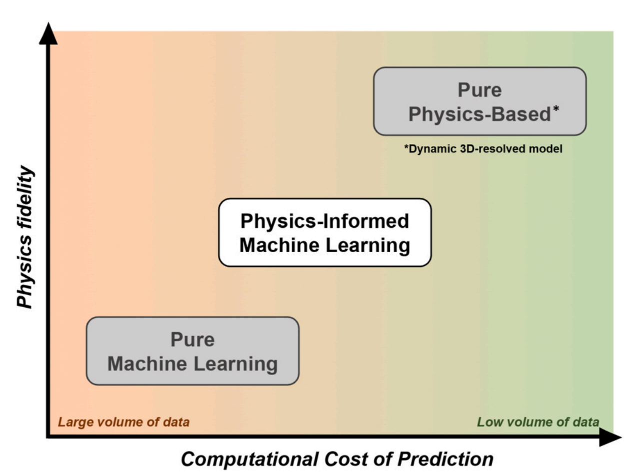

Fig. 9. Comparison of the ML, physics-based, and physics-informed ML approaches for modeling LIB cells. This schematic illustrates the general relative physics fidelity and computational cost of prediction for these approaches. A dynamic 3D-resolved model is used as an example of high-fidelity physics-based approach.

different operation stress factors on the battery's health condition and degradation.

Posteriorly, Tu et al. demonstrated the use of different hybrid feed-forward neural networks (FNNs) [147]. Two different types of hybrid models were studied, and shown to have as high voltage prediction accuracy throughout the LIB cycle at different C-rates. It was found possible to combine these models along with bulk thermal models to predict the electrochemical and thermal behaviors simultaneously. After that, an extra awareness of the aging condition was also embedded on top, by making the ML informed of the battery's SoH. The proposed frameworks on this work while combining several different models, is able to generalize and predict precisely even beyond training datasets. The rationale behind this work was to make the neural network informed of the battery's internal state in order to have results that are physically sound.

Another work by Ma et al. [148], focused on predicting the rest of useful life by the input of a single charging curve. In this study, a DNN was informed with the input of a PBM which predicted voltage vs capacity. This PBM was in charge of characterizing the ageing behavior of the curves, subsequently, this information was encoded into the program via the use of a particular parameter set. The main advantages of this model were found to be the transferability to various operating conditions (C-rates, temperature, active material and even partial charging data).

A physics-informed neural network (PINN) was also studied based on its capacity to treat both physical information as well as synthetic data on the ML performance and the SoH estimation abilities, by Hofmann et al. [149]. In this paper, they concluded that a combined dataset was the best for the PINN training, since the inclusion of internal states in the simulation dataset increases the performance.

Moreover, Wang et al. incorporated a hybrid approach of battery PBMs with a LSTM-based network to create a temperature prediction model for studying cells throughout their useable life [150]. Parameters of the electrical, heat, and thermal models were automatically learnt during the training stage. They concluded that temperature prediction could be done at different operating conditions and that one of the advantages of the hybridization was the transferability and generalization of the model, due to the deeply embedded physics.

Given said that, exploring the use of the PIML approach for the digitalization of recycling techniques is expected to aid in the creation of relevant recycling models that incorporate the key aspects of PIML into traditional data driven tools. This is anticipated to result in models that are, relatively, computationally inexpensive and highly accurate, even if they are trained with smaller datasets than the ones used for traditional ML.

As an example, for modeling hydrometallurgy approaches and screening solvents, incorporating physics laws related to solvent dissolution into a data driven approach could accelerate the acquisition of the key parameters to optimize the recycling process. In addition, if we consider the scope of direct recycling methodologies, it could be possible to come up with different suggestions to apply a hybrid methodology like PIML, therefore, it is up to researchers to identify the key challenges of each process step, and select the most appropriate modeling technique that can help achieving this goal.

3.10.2. Machine learning for battery sorting

Battery sorting, a process that screens, selects, and regroups batteries based on key sorting indices such as capacity and internal resistance, proves to be an effective method in reducing inconsistencies among batteries and thereby enhancing overall battery performance. Typically, battery sorting and regrouping involves two stages. In the first stage, sorting indices like capacity and internal resistance are acquired from historical or testing data. Subsequently, in the second stage, batteries are chosen and regrouped according to specific sorting and regrouping criteria and the obtained indices [151].

Establishing an efficient collection system for EoL batteries is a fundamental component of a successful recycling strategy [152]. On one hand, the disassembly and recovery potential of batteries depend on various parameters, including their EoL health state, typically indicated by metrics like SoH, SoC, and RUL. Incorrect estimation of these parameters can result in disassembly failures and diminish sustainable benefits [153]. On the other hand, the initial phase of the battery recycling process, which involves collection and sorting, presents a significant challenge due to the substantial variation in the chemistries and states of batteries, influenced by their wide application and usage scenarios [154]. Therefore, accurately identifying and classifying batteries based on their chemistry and state becomes a pivotal step before the recycling process can commence.

Sorting methods tailored for rechargeable batteries intended for second-life applications have been developed in recent years. For example, Schneider et al. introduced a visual inspection method complemented by DC electrical measurements to discern batteries suitable for reuse across various applications [155]. Additionally, alternative non-destructive testing methods have been proposed. Xiong et al. discussed three commonly used methods for aging diagnosis: disassembly-based post-mortem analysis, curve-based analysis, and model-based analysis [156]. Typically, post-mortem analysis serves for cross-validation, while curve-based and model-based analyses offer quantitative insights. Pastor-Fernandez et al. explored prevalent non-invasive diagnosis techniques such as pseudo Open Circuit Voltage, Incremental Capacity - Differential Voltage (IC-DV), Electrochemical Impedance Spectroscopy (EIS), and Differential Thermal Voltammetry to quantify degradation modes [157]. EIS, ultrasonic testing [158], and X-ray computed tomography [159] have also been extensively employed for the same purpose. Nevertheless, there are still gaps in achieving intelligent testing and sorting for high-throughput processes.

Among the existing methods for battery sorting, ML methods stand out with superior merits, which avoid conspiring the complex internal electrochemical reactions inside batteries thus establishing the relationship between features and battery capacity directly. In addition, ML could achieve fast and reliable sorting on the basis of fast testing data or historical data. At present, the application of ML methods in battery sorting has made significant strides, gradually surpassing classical sorting methods reliant on experimentation. In such approaches, voltage curves serve as the primary source of input features [160,161], with LIBs being the most commonly studied technology. Moreover, neural networks emerge as the dominant method [161], varying from simple three-layer models (most prevalent) to sophisticated deep learning architectures.

One of the most recent examples is the work by Tao et al. [162], who embarked on a cathode material sorting initiative for retired batteries. They leveraged existing battery data from various collaborators, including battery manufacturers, practical application operators, academic research institutions, and third-party platforms. Employing a collaborative and privacy-preserving ML approach, they developed a federated ML model. This model was trained using only one cycle of field-testing data from a unique dataset comprising 130 LIBs spanning 5 cathode materials and 7 manufacturers. This was accomplished through a standardized feature extraction process, without prior knowledge of historical operational conditions. The study compared the predictive power of their federated ML model with independently learned local models, under both homogeneous and heterogeneous battery recycling circumstances. To address the heterogeneity issue, the authors proposed a Wasserstein-distance voting strategy, which effectively mitigated cathode sorting errors to 1 % and 3 %. Additionally, an economic evaluation of retired battery recycling was conducted using the proposed federated ML framework, highlighting the importance of accurate sorting in the recycling process. Finally, the study delved into model interpretability, battery recycling implications, and the broader prospects of integrating federated ML into future recycling practices.

Xia et al. proposed a novel Lithium Metal Battery (LMB) sorting method leveraging two-dimensional sequential features and deep learning [151]. This method comprises a hybrid LSTM-CONV1D model (combining long short-term memory unit and one-dimensional convolutional layer) to estimate the sorting index capacity, alongside a cycle-based inference method employing a voting ensemble approach. Initially, segments of discharging curves during battery activation are generated as training and validation samples. Subsequently, the model undergoes training on a segment-based training set and optimization on a validation set, facilitated by a greedy strategy. Finally, the model and the cycle-based inference method are validated across battery cycles in the training, validation, and test sets.

3.10.3. Machine learning for battery disassembly

During the initial phase of disassembly, when the vehicle case is removed, the battery packs present varying shapes due to the diverse range of EV models available in the market. Furthermore, these battery packs comprise complex battery management systems, cooling systems, and insulation packages, with the arrangement of these components differing among various manufacturers. Additionally, modules and cells within the battery pack are arranged and interconnected in specific configurations to achieve the desired voltage and capacity, with series and parallel connections being commonly utilized, albeit with potential variations between EV models and manufacturers [163]. Moreover, manual disassembly of EoL LIBs is impractical due to the potential exposure of workers to toxic substances such as cobalt, lithium, or organic electrolyte, as well as the risk of battery explosion. Such exposure can result in significant negative health effects on workers. Moreover, manual disassembly is both costly and time-consuming, and it is susceptible to noise sensitivity.

As a preferable alternative, automatic disassembly without human intervention is advocated for the pre-processing of EoL batteries for the subsequent recycling process.

Following automatic disassembly, Lu et al. [164] demonstrated a cyber-enabled and ML-enhanced battery disassembly system. The system utilized computer vision to classify different types of batteries based on their brands and sizes. Real-time temperature data captured from a thermal camera was then combined with a data-driven prediction model to forecast cutting temperature patterns. Subsequently, a closed-loop control mechanism was implemented to prevent temperature spikes by timely adjustments to cutting variables. Moreover, quality control was ensured through the use of a computer vision model to detect and mitigate cutting defects.

The value of AI in the disassembly steps has been also thoroughly assessed and confirmed through a systematic review conducted by Meng et al. [165]. The review demonstrates that AI holds significant potential to enhance the entire EV-LIB disassembly process, contributing to the establishment of a sustainable circular economy within the EV-LIB industry. AI's primary appeal lies in its capacity to address safety concerns, accommodate diverse battery types, and navigate uncertainties inherent in the disassembly process. By leveraging AI, disassembly efficiency and adaptability can be improved, while pollution and hazards can be minimized, ultimately leading to enhanced profitability. The review identifies and discusses both the opportunities and challenges associated with intelligent EV-LIB disassembly. It highlights areas such as EV-LIB state prognostics, disassembly planning and decision-making, and target detection as particularly promising for future research and development towards an intelligent era. However, challenges persist in achieving extensive autonomy in EV-LIB disassembly due to inherent limitations in AI, as well as the mechanical and chemical complexities of EV-LIBs, and concerns surrounding sustainable benefits. Practical insights and forward-looking perspectives are provided to advance intelligent EV-LIB disassembly, including the analysis and comparison of primary intelligent methods in the field. The review emphasizes the importance of carefully selecting and applying intelligent methodologies and techniques in EV-LIB disassembly, proposing a comprehensive framework to guide this process. Moreover, the review suggests remote human-robot collaboration with learning capabilities as a pragmatic approach to address safety and uncertainty concerns. In summary, Meng et al.'s systematic review underscores the transformative potential of AI in EV-LIB disassembly, while also highlighting the need for thoughtful consideration of challenges and practical implementation strategies to realize its full benefits.

3.10.4. Machine learning and knowledge graphs

To enhance several aspects of ML, Knowledge Graphs (KGs) can serve as a tool to directly impact data preprocessing in scenarios requiring the exploit of diverse, dynamic, and large-scale data collection [166]. They do so by automatically constructing data pipelines based on the semantic descriptions of data sources and sinks.

When it comes to parameter selection, KGs can automate the optimization process of iterative parameter selection by utilizing machine-readable process specifications —which typically include parameters and expert knowledge annotations— related to correlations. This leads to more accurate and efficient selection of these parameters.

In terms of model or method selection, KGs can pick suitable AI/ML models based on machine-readable information on data (either small-data or big-data) and the availability of models (like physical equation/simulation). This ensures the most effective model is chosen for a given dataset.

Furthermore, KGs can improve validation and quality by combining expert knowledge with statistical approaches. This not only accelerates the usage of AI but also enhances the quality and explainability of the models, making them more reliable and understandable.

The use of this tool is expected to play a key role in automation of recycling pipelines, since they could help reduce the time and effort required in manual data handling. In the recycling field, they have been studied for robotic disassembly of EoL batteries of EVs [167], but could also prove useful for classification purposes, since a multitude of influx battery-derived waste needs to be properly classified into different categories due to composition, SoH, RUL, or other parameters.

3.10.5. Machine learning applied to hydrometallurgical recycling

The hydrometallurgical recycling of LIBs involves the dissolution of metallic components, primarily sourced from the active material (a mixture of cathodes and anodes). This dissolution is typically carried out using mineral acids, followed by metal separation techniques such as solvent extraction, ion exchange, and precipitation [152]. Additionally, a thermal pre-treatment, involving pyrolysis or calcination, can be applied as well [168]. Leaching serves as the initial step in the hydrometallurgy process, following mechanical or thermal pre-treatment. In this regard, only a few examples are found in the literature where ML techniques are applied to enhance the leaching process itself. Niu et al. proposal is one of these approaches [169]. They utilized ML techniques to streamline the efficient leaching of metals from spent LIBs. They comprehensively analyzed all operational factors, including 20 input features related to the leaching process, encompassing both raw material properties and technological parameters. These factors were used to predict the output variables, namely the leaching efficiency of lithium, cobalt, manganese, and nickel. To gather data for ML analysis, the authors meticulously reviewed published references spanning from 2005 to 2022, accumulating a total of 17,588 data points related to the hydrometallurgy recycling of spent LIBs. To enhance prediction accuracy, they employed four ML algorithms: XGBoost (XGB), Random Forest (RF), Support Vector Machine (SVM), and AdaBoost. Subsequently, they developed and compared 16 models based on these algorithms. Building on the optimal models, the researchers designed a user-friendly graphical user interface (GUI) to aid researchers in swiftly obtaining metal leaching parameters from spent LIBs. This GUI only requires experimental measurements of particle size (screening) and waste feed composition, eliminating the need for extensive leaching experiments. Finally, the reliability of the GUI was verified through a series of experiments.

3.10.6. Machine learning perspectives for recycling digitalization

While ML is currently being studied for the hydrometallurgical recycling route, there is still an opportunity to address the preprocessing parts of the LIB recycling process, like the mechanical separation, or even other recycling processes and techniques such as the pyrometallurgical and direct recycling one have yet to be implemented.

(i) Machine learning applied to mechanical process

Since mechanical processing and other pretreatments are indispensable prerequisites preceding the hydrometallurgical treatment of batteries, we highlight it as a key research topic to focus for the next coming years.

This process involves the separation of metals such as iron, cobalt, copper, aluminum, lithium, and nickel (referred in conjunction as black matter). The objective of this step is to increase the surface area by crushing the components, thereby enhancing the efficiency of metal dissolution during posterior acid leaching [170].

Equipment such as rotary shears and hammer mills are employed to pulverize battery components. Subsequently, various separation techniques are utilized to segregate the metal shreds. These typical steps include an initial magnetic separation to remove the steel casing. Subsequently, density separation, froth flotation, sieving, and vibrating drum screens are additional methods thay may be utilized for metal component separation.

However, it's important to mention that prior to subjecting batteries to crushing and other mechanical processes, they must first be deactivated and discharged, as performed in the disassembly and pyrometallurgical phases. Incorrect execution of this step poses a risk of battery explosions or fires. Should the thermal deactivation phase be omitted, pulverization can be conducted under cryogenic conditions or in an inert atmosphere to prevent metal oxidation and combustion. However, this method is considerably costlier [163].

It is envisioned for ML techniques to be applied at a multitude of the different steps of the recycling pipeline, however certain proposed ideas include the utilization of modeling techniques for improving separation of spent battery components of varying chemistries and/or size requirements. A recent example of modeling applied to this part of the process was shown by Punt et al. [171]: in this reference, the authors investigated models for a cutting mill and zig-zag-sifter in conjunction with dynamic flow sheet simulations. We foresee that in the future, these types of modeling approaches will be complemented by ML techniques to further optimize these models, and thus, the overall recycling process.

(ii) Machine learning applied to pyrometallurgical recycling

In the pyrometallurgy route, the main objectives of this step are to deactivate batteries and improve worker safety [13]. This process involves a high-temperature furnace, initially emptied and then filled with pure nitrogen gas, within this furnace, metals and oxides in the battery are melted and converted into a copper, cobalt, iron, and nickel alloy, through the use of redox reactions occurring at temperatures of approximately 500–600 °C.

Subsequent separation processes are needed after the pyrometallurgical treatment, with hydrometallurgical processes being preferred to recover these metals. Aluminum and lithium oxides typically become part of the slag and are not recovered. If aluminum is to be retrieved in its pure metallic form, the process must be conducted under vacuum conditions. Consequently, the output of this process comprises materials in the form of alloys, gases, and slag [170,172].

The way computational tools could improve the process of the pyrometallurgical route is to test different process conditions occurring at different temperatures, different atmospheres and quantities. Computational thermochemistry approaches like the one studied recently for other fields involving metallurgical processes [173] could be applied for LIB recycling in conjunction to ML tools in order to further optimize the recycling process design while also reducing the energy consumption.

(iii) Machine learning applied to direct recycling

Direct recycling, based on chemical relithiation methods, presents a promising approach to address compositional and structural defects in degraded cathodes without sacrificing the embedded energy in the materials. This method enables the production of cathodes that are directly useable in the assembly of new battery cells, eliminating the need to resynthesize cathodes from their precursors. Compared to pyro- and hydro-recycling routes, direct recycling offers significant advantages in terms of energy consumption, safety, cost, flexibility, and economic returns, attracting considerable attention from academia and industry.

Recently, some researchers reviewed the state-of-the-art direct recycling technologies of spent LIBs, placing significant emphasis on various relithiation routes and the importance of sustainable recycling compared to conventional metallurgical methods. However, critical obstacles hindering the practical implementation of direct recycling have been overlooked [163].

In this regard, ML can propose a streamlined optimization of the challenges that keep direct recycling from being scaled up. Collecting data of experiments dealing with direct recycling methodologies and using ML for identifying the most relevant parameters for a recycling potential prediction remains as an area of opportunity in this sector.

Ultimately, it is important to highlight that AI, specifically ML methods, represent important tools for screening the most ideal conditions for a specific step during the recycling process. However, the capacity of ML to identify potential synergies between different steps of the pipeline should not be overlooked.

4. Lithium-ion battery cell recycling digitalization via funded initiatives

In the pursuit of achieving a fully functional, sustainable and interconnected manufacturing-recycling LIB value chain, the efforts for standardization, sustainability aspects and different funded initiatives have been put into place to drive innovation. In this section, we aim to describe the sustainability and standardization aspects that are a cornerstone for the design of the present recycling processes and highlights the key public research initiatives that are shaping the future of the processes that will established in the following years.

The European Commission champions projects that align to the sustainable development goals, and the main aim here is to establish safe, and economically sustainable battery cell recycling supply chains. In terms of improving the way in which our current LIB affects the ecosystem, we find different topics of interest that involve the participation of people from different fields.

Out of the most important areas that are currently being targeted we find the initiative of developing a robust, flexible, and sustainable direct recycling processes for various waste streams, since direct methods aim to recover the materials directly from electrodes of battery cells without shredding components, enhancing overall resource efficiency.

Moreover, projects on the development of an all-encompassing process, capable of treating all types of batteries are positively valued. This comprehensive ensures flexibility in managing diverse battery cell chemistries and states, contributing to a more efficient and inclusive recycling ecosystem.

Additionally, other efforts are focused on optimizing the collection and reversed logistics to enable efficient diagnostics. This is targeted due to the potential that streamlining these processes has on the identification and handling of batteries, facilitating their recycling and reducing environmental impact. This topic also involves the general population, since the education of citizens is necessary for their participation in collection programs.

Furthermore, the projects prioritize decreasing the carbon footprint of innovative battery systems. By implementing sustainable practices throughout the battery life-cycle, environmental impact is minimized, supporting a transition to cleaner energy solutions.

Lastly, projects promoting the development of novel biotechnological processes for producing various bio-ionic liquids and optimizing their extraction methods are currently ongoing. These innovations offer sustainable alternatives for battery cell production, contributing to a greener and more circular economy.

4.1. Standards for achieving recycling

In order to achieve a holistic incorporation of battery cell recycling into the LIB value chain, effectively implementing standardization measures is key to ensure the selection of the right recycling techniques, and most of all, drive innovation in the automatization sector. This in turn, will also help to overcome the main concerns of scalability and safety of the recycling processes.

From this point of view, the development of a digital product passport that helps to effectively label and identify a product of the battery industry by means of automation is a key focus of European projects like CIRPASS and DigiPass [174,175]. These initiatives aim to streamline and digitize product information, enhancing data transparency, traceability and interoperability.

Battery-specific implementations are being explored in the BatteryPass [176] and BASE projects, which are working towards creating a property list and architecture draft. A categorized list of the properties that are taken into consideration within BatteryPass, is visualized in Fig. 10. As an example, we highlight that this initiative aims to make available the data that the material composition and manufacturer in addition to more detailed information like the performance and durability of the product, it's carbon footprint, the circularity and resource efficiency of the product, etc.

Looking forward, the plan is to define a common language for all by annotating ontology terms to the different product properties, such as the BattINFO and BVCO initiatives [177] were set to do inside the BIG-MAP project. This will expand the scope beyond final product data and offer also a zoomed-out value chain perspective.

As evidenced by the Catena-X prototype implementation, the execution of these battery standardization projects should also take into account the Gaia-X and International Data Spaces reference architectures and make use of uniform linked data schemas [178]. Following this approach will ensure a comprehensive and integrated digital solution for creating useful product passports, that can help to achieve a truly automated, safe and efficient pipeline through automation.

4.2. A bird's eye overview of public funded projects in the EU

The European Commission and public bodies across EU countries are significantly investing in projects related to battery cell recycling. This focus aligns with the EU's broader goals of promoting sustainability, reducing environmental impact, and advancing the circular economy. Since 2019, 145 projects have been recounted both at EU and national levels [179]. Several funding mechanisms are available. For example, at EU level, Horizon Europe, H2020, and the European Innovation Council are the main funding mechanisms. At the national level, each country has their own funding bodies. One can mention the "Agence National de Recherche in France" (ANR) in France [180], the "Bundesministerium für Bildung und Forschung" (BMBF) in Germany [181], the "Centro para el Desarrollo Tecnológico y la Innovación" (CDTI) in Spain [182], or "UK Research and Innovation" (UKRI) in the United Kingdom [183]. The contribution of each country to different types of LIB recycling projects is visually shown in a pie chart Fig. 11.

The granted projects cover the points established in the next sections.

4.2.1. Battery repurposing and second life applications

Around recycling and circular economy, one alternative initiative focuses on the development of second-life batteries. The EoL of an EV battery is considered when less than 20 % of its initial capacity is lost [184]. For this reason, the reuse of these batteries in stationary energy storage applications is one of the alternatives studied to improve the lifetime and total cost of EVs batteries. Different testing and verification methods have been developed to determine the potential reuse of these batteries.

By refurbishing and repurposing these batteries, valuable resources are conserved, and environmental impact minimized. As an example, repurposing batteries from EVs into other sources enables their use in smaller-scale transportation solutions, bolstering urban mobility sustainability. It also supports battery reuse in medical devices, recognizing

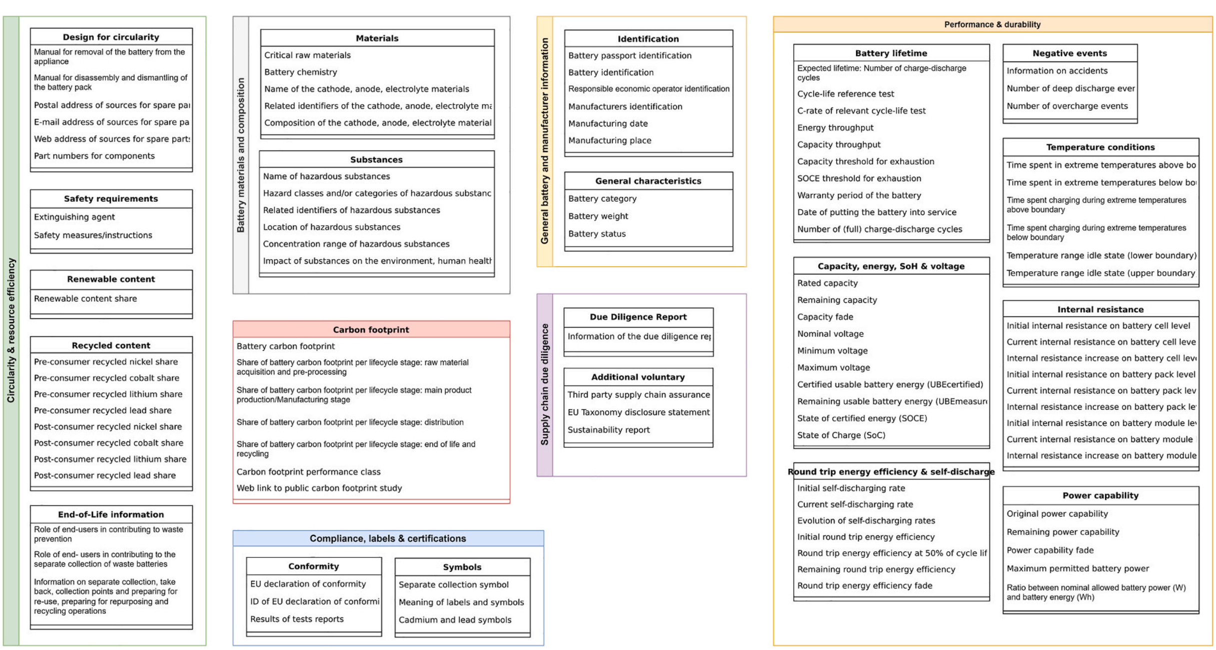

Fig. 10. Visualization of the attributes listed and categorized by BatteryPass. Created from BatteryPass "Data Attribute Longlist", available online under CC BY-NC 4.0 license [176].

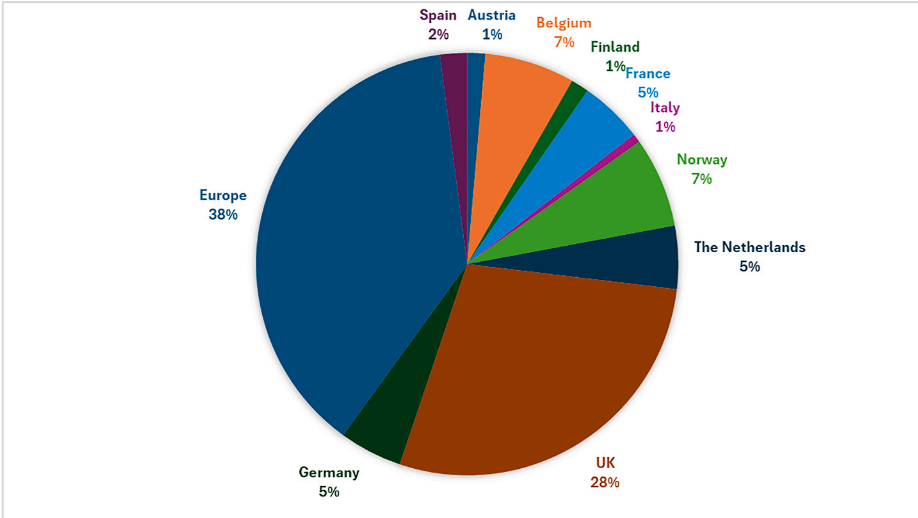

Fig. 11. Distribution per country of projects on battery recycling topics funded by the European Commission or other public funding bodies among 145 projects.

the potential to extend their lifespan and reduce waste in healthcare.

Furthermore, several projects emphasize smart sorting and dismantling systems for LIBs. These systems automate classification and disassembly, identifying and separating functional battery modules for reassembly into new batteries for second life applications. It is necessary to design a methodology for the rapid identification of EoL batteries as a useful tool for collection, handling and pre-processing infrastructures. The value of the active material content, recyclability and remanufacturing costs for a second use determine the best management option for EoL batteries (second life or recycling).

Additionally, project calls are focused on advancing streamlined collection and reversed logistics for automatic dismantling of EVs and stationary batteries. Optimizing collection and logistics processes aims to facilitate efficient dismantling and repurposing, promoting circular economy principles in the battery industry. Through these initiatives, the European Commission and other national public funding bodies drive innovation in battery reuse and repurposing, contributing to resource conservation, waste reduction, and the transition towards a more sustainable and circular economy.

4.2.2. Recovery and reuse of battery materials

Innovative projects to enhance the sustainability and efficiency of battery cell recycling and reuse have been funded. These initiatives focus on key areas to improve the life-cycle management of batteries. The concepts of safe and reliable remanufacturing-reuse-recycle platforms are largely adopted in projects, facilitating systematic and secure battery handling throughout their life-cycle. The reuse and recycling of EoL batteries is another critical focus. Advanced techniques to refurbish and repurpose batteries aim to extend their lifespan and reduce waste. Specifically, the recovery of lithium as battery-grade lithium hydroxide monohydrate is promoted to ensure high-purity lithium can be reused in new batteries, maintaining the supply chain and reducing reliance on raw materials.

The recovery and reuse of graphite electrodes are also prioritized, enabling reintegration into new battery cell production. Public funding bodies advocate for green, low-cost, and low environmental impact recycling methods for various battery cell chemistries, including NMC, LFP, and sodium-ion batteries (SIBs). These methods aim to minimize environmental impact and reduce costs while efficiently recovering valuable materials.

Finally, the recovery of solvent and electrolyte from EoL batteries is encouraged to enhance the overall efficiency and sustainability of the recycling process. Through these efforts, the European Commission is fostering a robust and sustainable battery recycling ecosystem, addressing environmental concerns and resource security for the future.

4.2.3. Innovative recycling processes and technologies

Public funding of European countries and the European Commission are promoting groundbreaking initiatives to revolutionize battery recycling, promoting sustainability and efficiency in waste management. Central to these efforts is the development of new recycling processes designed to enhance resource recovery and minimize waste. Amongst the granted projects, one significant focus is on hydrometallurgical methods to process black mass, which allow for the efficient extraction of critical metals like lithium, cobalt, and nickel from EoL batteries. Cleaner alternatives offer higher recovery rates and reduce environmental impact. Additionally, microwave-assisted treatment of battery waste is being promoted to improve material recovery efficiency and reduce energy consumption. Projects aim for replacing pyrometallurgical recycling with water-based processes to eliminate undesired side products, making recycling safer and more environmentally friendly. The use of molten salts as solvents in dissolving battery cathodes is another innovative approach proposed, enabling selective recovery of metals and enhancing purity and yield. Efforts to promote low-cost and green recycling processes are aimed at recovering materials from various battery types, reducing the carbon footprint, and improving economic sustainability. Advanced pre-treatment techniques like electrohydraulic fragmentation and ultrasonication are also riding high in Europe, which ensure high material purity and efficiency. Furthermore, several public funded projects support the development of disruptive biotechnological processes for bioleaching and metal recovery from batteries. Utilizing microorganisms, these methods provide a sustainable and environmentally friendly alternative to traditional extraction techniques.

4.2.4. Development of circular economy solutions

National funding entities and the European Commission on top are driving forward initiatives aimed at revolutionizing the battery industry towards circular economy principles. One significant focus is on developing and demonstrating new circular economy solutions tailored specifically for the European battery value chain. These solutions seek to establish closed-loop systems that minimize waste and maximize resource efficiency throughout the life-cycle of batteries. In addition, funded projects support the development of innovative processes for waste remanufacturing, leveraging techniques such as hydrothermal and microwave treatments. These processes aim to extract valuable materials from waste streams, promoting sustainability and reducing reliance on raw materials. Moreover, the Commission emphasizes design considerations for EoL batteries such as the design-for-recycling concept, ensuring that batteries are designed with recyclability and sustainability. By incorporating EoL considerations into battery design, the Commission aims to facilitate easier and more efficient recycling processes. Projects are also addressing the development of advanced methods and algorithms to optimize the recovery of mixed waste streams of batteries. These methods enable more precise sorting and processing of battery components, increasing resource recovery and minimizing waste. Furthermore, projects aim at establishing a safe, economically sustainable battery cell recycling supply chain. This includes initiatives to improve collection and reverse logistics processes, ensuring efficient diagnostics and transportation of batteries for recycling. Finally, projects are committed to decreasing the carbon footprint of innovative battery systems. By promoting the adoption of environmentally friendly practices and technologies, a major outcome would be to minimize the environmental impact of battery cell production and recycling processes.

4.2.5. Automation and robotics in recycling

Europe is spearheading initiatives aimed at optimizing the reverse logistics of batteries and revolutionizing the dismantling and sorting processes for EoL batteries. One key focus area is the development of more efficient and universal methods for battery discharge and initial diagnosis during reverse logistics (from end-users back to the manufacturer). By streamlining these processes, projects aim to improve the efficiency of battery cell recycling and minimize delays in the transportation and handling of EoL batteries. The transportation of these batteries is especially important, since in literature, even if the cost estimates vary widely, analysis of different studies has identified an average 41 % of the total recycling cost being associated to transportation [185].

Moreover, public funding bodies are investing in the deployment of robotic systems designed for flexible product manipulation, dismantling, and sorting. These advanced robotic systems enable precise and efficient disassembly of battery packs, maximizing resource recovery and minimizing manual labor. Such development goes in line with the implementation of smart sorting and dismantling systems capable of automated classification and dismantling of LIBs. These systems leverage cutting-edge technologies to identify and separate battery components, optimizing the recycling process. Furthermore, there is a strong need to establish pilot lines equipped with robotized and automated disassembly of battery packs. These pilot lines serve as testbeds for innovative dismantling technologies, paving the way for scalable and efficient battery cell recycling operations. In this view the integration of AI into automated dismantling processes, can enable more accurate sorting and classification of battery components. AI-driven dismantling systems enhance the precision and efficiency of battery recycling, improving resource recovery rates. Adaptable and safe dismantling and sorting of EoL batteries and components using robotics, ML, and other Industry 4.0 technologies are of paramount importance. These advanced systems ensure the safe handling and processing of batteries, mitigating risks associated with manual dismantling and sorting processes.

4.3. Perspective on the role of pilot lines in production and recycling digitalization

Driven by the upcoming EU regulations, sustainability imperatives, and resource security concerns, there is a growing recognition among many players in the battery ecosystem of the necessity to investigate both battery production and recycling processes. Such investigations are inherently risky and costly when conducted directly on production systems. To address these challenges, two key strategies are essential. First is the focus on digital tools and methods to accompany investigations, as outlined in this paper. Second is the use of R&D pilot lines to develop, employ, and test innovations, underscoring the critical role of pilot lines in this context. For this reason, this paper considers that investing in pilot lines as well as in funded projects and standardization initiatives, is essential.

Pilot lines are indispensable within this ecosystem, providing a versatile platform for the development, validation, and optimization of the innovative methods and tools discussed herein. They serve as a testbed for the methods outlined in this paper, offering the necessary data to implement tools like model-based control strategies and ML-driven techniques.

Within this role, the scope of research topics covered by pilot lines continues to expand, necessitating more interdisciplinary research and development efforts. To maximize their effectiveness, pilot lines must integrate expertise from digitalization specialists, facilitating the development and calibration of models with different degree of complexity.

Effective knowledge and data exchange are paramount, requiring organized platforms for collaboration. This can be achieved through joint projects or networks of pilot lines, such as the LiPLANET network [186], which has brought together the experts contributing to this paper.

In summary, pilot lines play an essential role in:

(i) Generating the necessary data for the development of digitalization tools for production and recycling;
(ii) Acting as a testbed for the technological advancements from the digitalization domain;
(iii) Establishing platforms for knowledge exchange by connecting expert's production, recycling and digitalization R&D;
(iv) Fostering interdisciplinary collaborations and transdisciplinary R&D.

5. Conclusions

The purpose of this article has been to guide both research and industry towards more sustainable battery development by emphasizing the key role of digitalization to achieve a fully circular battery economy. We envision that the inclusion of recycling from the initial stages of the electrode and cell production by the use of state-of-the-art modeling techniques, represents a promising topic inside the vast LIB field.

When it comes to processing EoL and waste LIB cells, three main recycling approaches have been found useful. Currently, the state-of-the-art techniques concern hydrometallurgy, pyrometallurgy or direct methods. However, the choice of the technique will be mainly decided on the cost-effectiveness which is in turn based on the targeted electrode chemistry, the number of steps in the process, energy expenditures, and desired final product.

Even if these techniques are quickly evolving, we consider that there are still many opportunities for improvement in the recycling process for all aforementioned techniques, specifically in the areas of safety and handling, as EoL batteries are regarded as hazardous, explosive, and corrosive waste. By introducing the use of advanced robotics empowered with AI, and sensors to automate the recycling process in a smart fashion, a part of the risk might be reduced, and its development accelerated.

To achieve the complex goal of seamlessly integrating recycling into the already complex batterymanufacturing process, it is necessary to take advantage of current technology and look forward to the evolution of the industrial processes. In the past decade, advances in manufacturing processes and the introduction of concepts such as Smart Manufacturing and DTs have highlighted the possibility of real-time process control through the implementation of an intricate network of sensing and monitoring devices.

In here, we propose that focusing on recycling methods should be among the next priorities of digitalization efforts, due to its pivotal role for achieving a circular battery economy. A digital transformation is crucial, and by steering research on this topic, we can anticipate the needs of the future market.

The consideration of design, manufacturing and recycling in a holistic fashion offers an opportunity to push the boundaries of research and innovation. By replicating environments, processes, and phenomena in virtual settings, scientists and engineers can simulate complex scenarios with precision and efficiency. This opens new avenues for experimentation, discovery, and problem-solving. As technology continues to advance, digitalization approaches are well poised to revolutionize how we invent sustainable products and optimize processes, thus promising exciting prospects for future scientific endeavors. The creation of these digital recycling ecosystems will require the integration of different modeling tools (applied at different scales). Overall the digitalization efforts will require an interdisciplinary participation from specialists in several scientific domains.

Given that the cell recycling models and cell performance models involve the same materials, in this article we suggest that this digital transformation can be carried out by evaluating the recyclability of battery cells by using the modeling toolkits we currently have for the simulation of battery cell manufacturing and performance.

We also provide an analysis of these modeling techniques starting from the highest level (process scale) up to the smallest one (material level), carefully discussing each modeling approach and then its envisioned integration for its application in recycling of LIBs.

In the field of process engineering we identify that in order to integrate recycling alongside the state-of-the-art battery manufacturing process, multilevel modeling and control-based modeling will be key players to enable an early detection of scrap and thus enhance resource efficiency. Furthermore, the consideration of recycling under inside a single facility, or at least inside the same company, will lead to more effective recycling, since battery chemistry of own scrap and/or EoL batteries is understood, and resources can be shared between the different steps and machinery.

We also find that recycling digitalization could find its inspiration from state-of-the-art battery cell manufacturing process model pipelines, either by including recycling materials with different parameters into this already existing framework, or create a parallel type of framework but for the different steps of battery cell recycling processes.

The utilization of more specific modeling techniques was discussed by starting with the use of discrete modeling techniques, which find their usefulness to model interactions from the micro up to the macroscale, *e.g.* CGMD, and even coupling it with other methods like DEM or CFD, to get insights at the mesoscopic and macroscopic scales. An example of this combination of techniques is discussed for achieving a targeted approach at optimizing separation methods for LIB recycling. In addition, these simulation techniques could also be used to screen different types of green and non-toxic solvents while optimizing for lower energy and time requirements.

On a different note, continuum PBMs are also discussed, since they provide a window into the internal battery states, which allows for the optimization of cycling conditions and electrode design. The study of battery performance in connection to manufacturing parameters is one of the main focus of the current research. As of right now, a number of researchers have shown that modeling pipelines that use of data generated by physics-based simulations to train AI surrogate models. However, integrating physics-based simulations and AI to create novel physics-informed ML approaches, can also be a valuable strategy to optimize training data requirements, as we can lower the amount of data bias and increase accuracy by using physics equations as biases. As a perspective, the utilization of the discussed approaches as a way to perform quality control for recycled electrode materials or hybrid electrodes containing both pristine active materials and recycled ones is proposed as an interesting topic of research.

In addition to the aforementioned modeling methods, another important tool for achieving recycling digitalization, relies on harnessing the power of data driven approaches, in particular those based on AI. These techniques, find their predictive power due to the high volume of data used to train the models. If applied correctly, these models could find their usefulness in multiple different steps of battery recycling. However, we emphasize their ability to be used to train robotics to perform the most dangerous processes that can expose workers to the highest amount of risk, being sorting and disassembly and mechanical processing, some of them.

In addition to reducing workplace hazards, ML algorithms are envisioned to be used for predicting the outputs of different recycling methods, optimize the process, increase yield, in the cases where enough data is readily available.

At the end, thanks to the anticipation of a large volume of both EVs and consumer products powered by batteries, key players in academia, industry and government, have identified the potential of LIB recycling. However, the interest on this topic is not only driven by the possible economic gains of recycling, but also by the recent introduction of strict sustainability policies. A clear example are the directives and regulations targeted to batteries in the EU, emphasizing the mandatory use of recycled elements like lithium in newly manufactured batteries.

For managing to achieve the complex goal of having a circular battery economy, different funded initiatives have been started. First, project initiatives aim to create digital product passports in order to streamline the standardization and labeling of different battery products. These projects are heavily linked with the definition of a battery ontology to define common terms as the goal.

As for the publicly funded projects in the EU, adjacent to battery cell recycling, the topics deal with the repurposing and second life applications, and also the recovery and reuse of materials used for battery manufacturing. For the projects directly targeting recycling, the focus is on studying innovative processes, developing circular economy solutions, improving automation and robotics. Lastly, we end by highlighting the importance of pilot plants as mediums for testing, developing, validating and optimizing different recycling techniques, generating useful data for digitalization efforts, and fostering interdisciplinary collaboration.

Finally, it is important to note that while this article focused on discussing perspectives for LIBs recycling digitalization, this approach is chemistry agnostic and is also encouraged to ease of recyclability of other battery chemistries, *e.g.* sodium ion batteries, or even to other battery technologies like ASSBs.

CRediT authorship contribution statement

Imelda Cardenas-Sierra: Writing – review & editing, Writing – original draft, Conceptualization. **Utkarsh Vijay:** Writing – review & editing, Writing – original draft, Conceptualization. **Frederic Aguesse:** Writing – review & editing, Writing – original draft. **Néstor Antuñano:** Writing – review & editing, Writing – original draft. **Elixabete Ayerbe:** Writing – review & editing, Writing – original draft. **Lukas Gold:** Writing – review & editing, Writing – original draft. **Aleksandra Naumann:** Writing – review & editing, Writing – original draft. **Laida Otaegui:** Writing – review & editing, Writing – original draft. **Nadir Recham:** Writing – review & editing, Writing – original draft. **Simon Stier:** Writing – review & editing, Writing – original draft. **Sandro Süß:** Writing – review & editing, Writing – original draft. **Lalitha Subramanian:** Writing – review & editing, Writing – original draft. **Nicolas Vallin:** Writing – review & editing, Writing – original draft. **Gabriela Ventura Silva:** Writing – review & editing, Writing – original draft. **Nicolas Von Drachenfels:** Writing – review & editing, Writing – original draft. **Dennis Weitze:** Writing – original draft. **Alejandro A. Franco:** Writing – review & editing, Writing – original draft, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

A.A.F and I.C.S acknowledge funding from the French National Research Agency (ANR) on the context of the “France 2030 program” and the Priority Research Programs and Equipment (PEPR) “Batteries” (Grant ANR-22-PEBA-0002, Project BATMAN).

U.V. and A.A.F., as a part of the DESTINY Ph.D. program, acknowledge funding from the European Union’s Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Actions COFUND – Grant Agreement No: 945357.

S.Sü. acknowledges the German Ministry of Education and Research (BMBF) for funding the project DiRectION (03XP0358A).

S.St. and L.G. and A.A.F. acknowledge the European Union for funding the project Battery 2030+ CSA under grant number 101104022 in the Horizon Europe research and innovation program.

A.A.F and D.W. acknowledge the European Union’s Horizon Europe Research and Innovation program under project PULSELiON (Grant Agreement no. 101069686).

A.A.F. acknowledges Institut Universitaire de France for the support.

The authors acknowledge the LiPLANET network and its coordinator, Prof. Arno Kwade, for providing a forum for discussion on topics related to battery pilot lines. This paper originated from the work of the Expert Group on Digitalization, Measurement Methods, and Quality, coordinated by Prof. Alejandro A. Franco, within the LiPLANET network.

Data availability

No data was used for the research described in the article.

References

[1] Directorate-General for Climate Action, Fit for 55: EU Reaches New Milestone to Make All New Cars and Vans Zero-Emission from 2035, European Commission News Article, 2023. https://climate.ec.europa.eu/news-your-voice/news/fit-55-eu-reaches-new-milestone-make-all-new-cars-and-vans-zero-emission-2035-2023-03-28_en.

[2] F. Degen, M. Schütte, Life cycle assessment of the energy consumption and GHG emissions of state-of-the-art automotive battery cell production, J. Clean. Prod. 330 (2022) 129798, https://doi.org/10.1016/j.jclepro.2021.129798.

[3] D. Larcher, J.M. Tarascon, Towards greener and more sustainable batteries for electrical energy storage, Nat. Chem. 7 (2015) 19–29, https://doi.org/10.1038/nchem.2085.

[4] European Commission, Implementation of the strategic action plan on batteries. Building a Strategic Battery Value Chain in Europe, 2019. Brussels, https://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:52019DC0176&from=ES.

[5] S. Helen Davies, P. Christense, T. Holberg, J. Avelar, O. Heidrich, in: S. Passerini, L. Barelli, M. Baumann, J. Peters, M. Weil (Eds.), Emerging Battery Technologies to Boost the Clean Energy Transition, Springer International Publishing, Cham, 2024, https://doi.org/10.1007/978-3-031-48359-2.

[6] S. Doose, J.K. Mayer, P. Michalowski, A. Kwade, Challenges in ecofriendly battery recycling and closed material cycles: a perspective on future lithium battery generations, Metals 11 (2021) 291, https://doi.org/10.3390/met11020291, 2021, Vol. 11, Page 291.

[7] J. Cilleruelo Palomero, L. Freboeuf, A. Ciroth, G. Sonnemann, Integrating circularity into life cycle assessment: circularity with a life cycle perspective, Clean. Environ. Syst. 12 (2024) 100175, https://doi.org/10.1016/J.CESYS.2024.100175.

[8] P. Strothman, G. Sonnemann, Circular economy, resource efficiency, life cycle innovation: same objectives, same impacts? Int. J. Life Cycle Assess. 22 (2017) 1327–1328, https://doi.org/10.1007/S11367-017-1344-5/METRICS.

[9] ERG Inc. and JSE Associates, EPA “summary report” lithium-ion battery disposal and recycling stakeholder workshop. https://www.epa.gov/system/files/documents/2022-03/final_lithium-ion-battery-workshop-public-report_508web.pdf, 2021.

[10] M.-M. Titirici, P. Johansson, M.C. Ribadeneyra, H. Au, A. Innocenti, S. Passerini, E. Petavratzi, P. Lusty, A.A. Tidblad, A.J. Naylor, R. Younesi, Y.A. Chart, J. Aspinall, M. Pasta, J. Orive, L.M. Babual, M. Reynaud, K.G. Latham, T. Hosaka, S. Komaba, J. Bitenc, A. Ponrouch, H. Zhang, M. Armand, R. Kerr, P.C. Howlett, M. Forsyth, J. Brown, A. Grimaud, M. Vilkman, K.B. Dermenci, S. Mousavihashemi, M. Berecibar, J.E. Marshall, C.R. McElroy, E. Kendrick, T. Safdar, C. Huang, F.M. Zanotto, J.F. Troncoso, D.Z. Dominguez, M. Alabdali, U. Vijay, A.A. Franco, S. Pazhaniswamy, P.S. Grant, S.L. Guzman, M. Fehse, M. G. Mestres, N. Antuñano, Roadmap for sustainable batteries, J. Phys.: Energy (2024), https://doi.org/10.1088/2515-7655/AD6BC0, 2024.

[11] T. Zhao, W. Li, M. Traversy, Y. Choi, A. Ghahreman, Z. Zhao, C. Zhang, W. Zhao, Y. Song, A review on the recycling of spent lithium iron phosphate batteries, J. Environ. Manag. 351 (2024) 119670, https://doi.org/10.1016/J.JENVMAN.2023.119670.

[12] D. Amalia, P. Singh, W. Zhang, A.N. Nikoloski, Liberation of valuable materials from spent cylindrical lithium-ion batteries via semi-autogenous attrition, Miner. Process. Extr. Metall. Rev. (2023), https://doi.org/10.1080/08827508.2023.2259576.

[13] A. Holzer, S. Windisch-Kern, C. Ponak, H. Raupenstrauch, A novel pyrometallurgical recycling process for lithium-ion batteries and its application to the recycling of LCO and LFP, Metals 11 (2021) 149, https://doi.org/10.3390/MET11010149, 2021, Vol. 11, Page 149.

[14] C. Hanisch, T. Loellhoeffel, J. Diekmann, K.J. Markley, W. Haselrieder, A. Kwade, Recycling of lithium-ion batteries: a novel method to separate coating and foil of electrodes, J. Clean. Prod. 108 (2015) 301–311, https://doi.org/10.1016/J.JCLEPRO.2015.08.026.

[15] D. Latini, M. Vaccari, M. Lagnoni, M. Orefice, F. Mathieux, J. Huisman, L. Tognotti, A. Bertei, A comprehensive review and classification of unit operations with assessment of outputs quality in lithium-ion battery recycling, J. Power Sources 546 (2022) 231979, https://doi.org/10.1016/J.JPOWSOUR.2022.231979.

[16] S. Sloop, L. Crandon, M. Allen, K. Koetje, L. Reed, L. Gaines, W. Sirisaksoontorn, M. Lerner, A direct recycling case study from a lithium-ion battery recall, Sustain. Mater. Technol. 25 (2020) e00152, https://doi.org/10.1016/J.SUSMAT.2020.E00152.

[17] M. Kaya, State-of-the-art lithium-ion battery recycling technologies, Circular Econ. 1 (2022) 100015, https://doi.org/10.1016/J.CEC.2022.100015.

[18] K. Berger, J.P. Schöggl, R.J. Baumgartner, Digital battery passports to enable circular and sustainable value chains: conceptualization and use cases, J. Clean. Prod. 353 (2022) 131492, https://doi.org/10.1016/J.JCLEPRO.2022.131492.

[19] L. Kintscher, S. Lawrenz, H. Poschmann, P. Sharma, Recycling 4.0-digitalization as a key for the advanced circular economy, J. Commun. 15 (2020) 652–660, https://doi.org/10.12720/jcm.15.9.652-660.

[20] N. Hayagan, I. Gaalich, P. Loubet, L. Croguennec, C. Aymonier, G. Philippot, J. Olchowka, Challenges and perspectives for direct recycling of electrode scraps and end-of-life lithium-ion batteries, Batter Supercaps 7 (2024) e202400120, https://doi.org/10.1002/BATT.202400120.

[21] T. Ouaneche, L. Stievano, L. Monconduit, C. Guéry, M.T. Sougrati, N. Recham, The art of Lithiation Revisited: solvent-free room temperature reaction, Energy Storage Mater. 70 (2024) 103507, https://doi.org/10.1016/J.ENSM.2024.103507.

[22] G. Hong, H. Park, A. Gomez-Flores, H. Kim, J. Mi Lee, J. Lee, Direct flotation separation of active materials from the black mass of lithium nickel cobalt manganese oxides-type spent lithium-ion batteries, Sep. Purif. Technol. 336 (2024) 126327, https://doi.org/10.1016/J.SEPPUR.2024.126327.

[23] T. Ouaneche, M. Courty, L. Stievano, L. Monconduit, C. Guéry, M.T. Sougrati, N. Recham, Room temperature efficient regeneration of spent LiFePO4 by direct chemical lithiation, J. Power Sources 579 (2023) 233248, https://doi.org/10.1016/J.JPOWSOUR.2023.233248.

[24] N.B. Manjong, V. Bach, L. Usai, S. Marinova, O.S. Burheim, M. Finkbeiner, A. H. Strømman, A Comparative Assessment of Value Chain Criticality of Lithium-Ion Battery Cells, vol. 36, 2023, https://doi.org/10.1016/J.SUSMAT.2023.E00614, 36.

[25] N. von Drachenfels, J. Husmann, U. Khalid, F. Cerdas, C. Herrmann, Life cycle assessment of the battery cell production: using a modular material and energy flow model to assess product and process innovations, Energy Technol. 11 (2023) 2200673, https://doi.org/10.1002/ENTE.202200673.

[26] J.F. Troncoso, F.M. Zanotto, D.E. Galvez-Aranda, D.Z. Dominguez, L. Denisart, A. A. Franco, The ARTISTIC battery manufacturing digitalization initiative: from fundamental research to industrialization, Batter Supercaps (2024) e202400385, https://doi.org/10.1002/BATT.202400385.

[27] M. Goyal, K. Singh, N. Bhatnagar, Circular economy conceptualization for lithium-ion batteries- material procurement and disposal process, Chem. Eng. Sci. 281 (2023) 119080, https://doi.org/10.1016/J.CES.2023.119080.

[28] J. Baars, T. Domenech, R. Bleischwitz, H.E. Melin, O. Heidrich, Circular economy strategies for electric vehicle batteries reduce reliance on raw materials, Nat. Sustain. 4 (1 4) (2020) 71–79, https://doi.org/10.1038/s41893-020-00607-0, 2020.

[29] K.S. Ng, A. Yang, N. Yakovleva, Sustainable waste management through synergistic utilisation of commercial and domestic organic waste for efficient resource recovery and valorisation in the UK, J. Clean. Prod. 227 (2019) 248–262, https://doi.org/10.1016/J.JCLEPRO.2019.04.136.

[30] L. Duan, L. Da Xu, Data analytics in industry 4.0: a survey, Inf. Syst. Front (2021) 1–17, https://doi.org/10.1007/S10796-021-10190-0.

[31] Q. Qi, F. Tao, Digital twin and big data towards smart manufacturing and industry 4.0: 360 degree comparison, IEEE Access 6 (2018) 3585–3593, https://doi.org/10.1109/ACCESS.2018.2793265.

[32] M. Bakker, E. Horetsky, D. Luchtenberg, Batteries included: building and operating sustainable gigafactories, McKinsey&Company, 2022. https://www.mckinsey.com/capabilities/operations/our-insights/batteries-included-building-and-operating-sustainable-gigafactories. (Accessed 30 April 2024).

[33] N. Flaherty, Siemens, LG Team on Digital Twin of Battery Factories, EeNews Europe, 2021. https://www.eenewseurope.com/en/siemens-lg-team-on-digital-twin-of-battery-factories/. (Accessed 30 April 2024).

[34] N. Flaherty, Siemens Digital Twins for ACC Battery Gigafactories, EeNews Europe, 2022. https://www.eenewseurope.com/en/siemens-digital-twins-for-acc-battery-gigafactories/. (Accessed 30 April 2024).
[35] N. Flaherty, Verkor Signs Dassault for Digital Twin of Battery Gigafactory, EeNews Europe, 2022. https://www.eenewseurope.com/en/verkor-signs-dassault-for-digital-twin-of-battery-gigafactory/. (Accessed 30 April 2024).
[36] N. Flaherty, Morrow, Gamma Team on Battery Digital Twin Tech, EeNews Europe, 2023. https://www.eenewseurope.com/en/morrow-gamma-team-on-battery-digital-twin-tech/. (Accessed 30 April 2024).
[37] N. Flaherty, €680m Battery Test Plant with Digital Twin for Germany, 2024. https://www.eenewseurope.com/en/e680m-battery-test-plant-with-digital-twin-for-germany/. (Accessed 30 April 2024).
[38] Dassault Systèmes, The 3DEXPERIENCE Platform, 2024, p. 2024. https://www.3ds.com/3dexperience (accessed May 31, 2024).
[39] IEA, Global EV outlook 2021 Paris, 2021. https://www.iea.org/reports/global-ev-outlook-2021 (accessed May 31, 2024).
[40] Dassault Systèmes, BIOVIA materials Studio, 3DEXPERIENCE, 2024. https://www.3ds.com/products/biovia/materials-studio (accessed May 31, 2024).
[41] S.T. Dix, J.S. Lowe, M.R. Avei, T.R. Garrick, Leveraging molecular dynamics to improve porous electrode theory modeling predictions of lithium-ion battery cells, J. Electrochem. Soc. 170 (2023) 083503, https://doi.org/10.1149/1945-7111/ACECA8.
[42] Y. Mabrouk, N. Safaei, F. Hanke, J.M. Carlsson, D. Diddens, A. Heuer, Reactive molecular dynamics simulations of lithium-ion battery electrolyte degradation, Sci. Rep. 14 (2024) 1–12, https://doi.org/10.1038/s41598-024-60063-0, 2024 14:1.
[43] A. Usman, G. Murtaza, A. Ayyaz, M. Shafiq, M.I. Piracha, H.S. Arif, M. Zulfiqar, Investigation of zinc and chromium substitution nickel-rich LiNi1−x−yZnyCrxO2 cathode materials to improve the redox reaction of lithium-ion battery: a first-principles study, J. Electrochem. Soc. 171 (2024) 030504, https://doi.org/10.1149/1945-7111/ad2d19.
[44] M. Thomitzek, O. Schmidt, F. Röder, U. Krewer, C. Herrmann, S. Thiede, Simulating process-product interdependencies in battery production systems, Procedia CIRP 72 (2018) 346–351, https://doi.org/10.1016/J.PROCIR.2018.03.056.
[45] G. Ventura Silva, M. Thomitzek, M. Lippke, T. Heckmann, H. Karaki, C. Lischka, F. Möhlen, D. Mayer, J. Hagemeister, R. Daub, J. Fleischer, H. Nirschl, D. Schröder, P. Scharfer, W. Schabel, A. Kwade, C. Herrmann, Digitalization platform for sustainable battery cell production: coupling of process, production, and product models, Energy Technol. 11 (2023) 2200801, https://doi.org/10.1002/ENTE.202200801.
[46] A.C. Ngandjong, T. Lombardo, E.N. Primo, M. Chouchane, A. Shodiev, O. Arcelus, A.A. Franco, Investigating electrode calendering and its impact on electrochemical performance by means of a new discrete element method model: towards a digital twin of Li-Ion battery manufacturing, J. Power Sources 485 (2021) 229320, https://doi.org/10.1016/J.JPOWSOUR.2020.229320.
[47] H. Karaki, M. Thomitzek, T. Obermann, C. Herrmann, D. Schröder, Optimizing the microstructure and processing parameters for lithium-ion battery cathodes: a use case scenario with a digital manufacturing platform, Energy Technol. 11 (2023) 2201032, https://doi.org/10.1002/ENTE.202201032.
[48] G.V. Silva, T. Heckmann, T. Abraham, P. Scharfer, W. Schabel, C. Herrmann, Model-based process design under consideration of production performance for battery cell production: a coating and drying study, Procedia CIRP 120 (2023) 780–785, https://doi.org/10.1016/J.PROCIR.2023.09.075.
[49] C. Hanisch, J.-H. Schünemann, J. Diekmann, B. Westphal, T. Loellhoeffel, P. F. Prziwara, W. Haselrieder, A. Kwade, In-production recycling of active materials from lithium-ion battery scraps, ECS Trans. 64 (2015) 131–145, https://doi.org/10.1149/06422.0131ECST/XML.
[50] Y. Bai, N. Muralidharan, Y.K. Sun, S. Passerini, M. Stanley Whittingham, I. Belharouak, Energy and environmental aspects in recycling lithium-ion batteries: concept of battery identity global passport, Mater. Today 41 (2020) 304–315, https://doi.org/10.1016/J.MATTOD.2020.09.001.
[51] M. Ahuis, A. Aluzoun, M. Keppeler, S. Melzig, A. Kwade, Direct recycling of lithium-ion battery production scrap – solvent-based recovery and reuse of anode and cathode coating materials, J. Power Sources 593 (2024) 233995, https://doi.org/10.1016/J.JPOWSOUR.2023.233995.
[52] M. Vaccari, F. Parlanti, F.M. Manni, M. Orefice, F. Mathieux, G. Pannocchia, L. Tognotti, A. Bertei, Assessing performance in lithium-ion batteries recycling processes: a quantitative modeling perspective, Resour. Conserv. Recycl. 206 (2024) 107643, https://doi.org/10.1016/J.RESCONREC.2024.107643.
[53] M. Wasesa, T. Hidayat, D.T. Andariesta, M.G. Natha, A.K. Attazahri, M. A. Afrianto, M.Z. Mubarok, Z. Zulhan, U.S. Putro, Economic and environmental assessments of an integrated lithium-ion battery waste recycling supply chain: a hybrid simulation approach, J. Clean. Prod. 379 (2022) 134625, https://doi.org/10.1016/J.JCLEPRO.2022.134625.
[54] M. Rinne, H. Elomaa, A. Porvali, M. Lundström, Simulation-based life cycle assessment for hydrometallurgical recycling of mixed LIB and NiMH waste, Resour. Conserv. Recycl. 170 (2021) 105586, https://doi.org/10.1016/J.RESCONREC.2021.105586.
[55] S. Blömeke, C. Scheller, F. Cerdas, C. Thies, R. Hachenberger, M. Gonter, C. Herrmann, T.S. Spengler, Material and energy flow analysis for environmental and economic impact assessment of industrial recycling routes for lithium-ion traction batteries, J. Clean. Prod. 377 (2022) 134344, https://doi.org/10.1016/J.JCLEPRO.2022.134344.
[56] V. Nguyen-Tien, Q. Dai, G.D.J. Harper, P.A. Anderson, R.J.R. Elliott, Optimising the geospatial configuration of a future lithium ion battery recycling industry in the transition to electric vehicles and a circular economy, Appl. Energy 321 (2022) 119230, https://doi.org/10.1016/J.APENERGY.2022.119230.
[57] M.F. Niri, K. Liu, G. Apachitei, L.R. Ramirez, M. Lain, D. Widanage, J. Marco, Machine learning for optimised and clean Li-ion battery manufacturing: revealing the dependency between electrode and cell characteristics, J. Clean. Prod. 324 (2021) 129272, https://doi.org/10.1016/J.JCLEPRO.2021.129272.
[58] M.A. Filz, S. Gellrich, A. Turetskyy, J. Wessel, C. Herrmann, S. Thiede, Virtual quality gates in manufacturing systems: framework, implementation and potential, J. Manuf. Mater. Process. 4 (2020) 106, https://doi.org/10.3390/JMMP4040106, 2020, Vol. 4, Page 106.
[59] International Organization for Standardization, Quality Management Systems — Requirements, ISO Standard No. 9001:2015-11, 2015.
[60] A. Turetskyy, J. Wessel, C. Herrmann, S. Thiede, Data-driven cyber-physical system for quality gates in lithium-ion battery cell manufacturing, Procedia CIRP 93 (2020) 168–173, https://doi.org/10.1016/J.PROCIR.2020.03.077.
[61] S. Stock, S. Pohlmann, F.J. Günter, L. Hille, J. Hagemeister, G. Reinhart, Early quality classification and prediction of battery cycle life in production using machine learning, J. Energy Storage 50 (2022) 104144, https://doi.org/10.1016/J.EST.2022.104144.
[62] E. Rohkohl, M. Schönemann, Y. Bodrov, C. Herrmann, Multi-criteria and real-time control of continuous battery cell production steps using deep learning, Adv. Indust. Manuf. Eng. 6 (2023) 100108, https://doi.org/10.1016/J.AIME.2022.100108.
[63] H.J. Kim, T.N.V. Krishna, K. Zeb, V. Rajangam, C.V.V. Muralee Gopi, S. Sambasivam, K.V.G. Raghavendra, I.M. Obaidat, A comprehensive review of Li-ion battery materials and their recycling techniques, Electronics 9 (2020) 1161, https://doi.org/10.3390/ELECTRONICS9071161, 2020, Vol. 9, Page 1161.
[64] A. Naumann, S. Süß, M. Mennenga, C. Herrmann, Towards an integrated control system for a scrap-free circular production of lithium-ion batteries, Procedia CIRP 120 (2023) 297–302, https://doi.org/10.1016/J.PROCIR.2023.08.053.
[65] S.P. Stier, X. Xu, L. Gold, M. Möckel, Ontology-based battery production dataspace and its interweaving with artificial intelligence-empowered data analytics, Energy Technol. 12 (2024) 2301305, https://doi.org/10.1002/ENTE.202301305.
[66] Battery Lab Factory, Technische Universität Braunschweig, ViPro: development of virtual production systems in battery cell production for cross-process production control, in: , 2024. https://www.tu-braunschweig.de/en/blb/research/projects/vipro. (Accessed 10 June 2024) (accessed June 10, 2024).
[67] RWTH Aachen University, DataBatt, in: , 2024. https://www.pem.rwth-aachen.de/cms/pem/forschung/projekte/vergangene-forschungsprojekte/~simnu/databatt/?lidx=1 (accessed June 10, 2024).
[68] S.P. Stier, General-Process-Ontology/ontology: v0.2.0 (v0.2.0), Zenodo, 2023, https://doi.org/10.5281/zenodo.7799527.
[69] S. Clark, F.L. Bleken, S. Stier, E. Flores, C.W. Andersen, M. Marcinek, A. Szczesna-Chrzan, M. Gaberscek, M.R. Palacin, M. Uhrin, J. Friis, Toward a unified description of battery data, Adv. Energy Mater. 12 (2022) 2102702, https://doi.org/10.1002/AENM.202102702.
[70] A.A. Franco, A. Rucci, D. Brandell, C. Frayret, M. Gaberscek, P. Jankowski, P. Johansson, Boosting rechargeable batteries R&D by multiscale modeling: myth or reality? Chem. Rev. 119 (2019) 4569–4627, https://doi.org/10.1021/acs.chemrev.8b00239.
[71] T. Lombardo, J.B. Hoock, E.N. Primo, A.C. Ngandjong, M. Duquesnoy, A. A. Franco, Accelerated optimization methods for force-field parametrization in battery electrode manufacturing modeling, Batter Supercaps 3 (2020) 721–730, https://doi.org/10.1002/BATT.202000049.
[72] A.A. Franco, ERC ARTISTIC project, in: , 2024. https://www.erc-artistic.eu/ (accessed June 30, 2024).
[73] J. Xu, A.C. Ngandjong, C. Liu, F.M. Zanotto, O. Arcelus, A. Demortière, A. A. Franco, Lithium ion battery electrode manufacturing model accounting for 3D realistic shapes of active material particles, J. Power Sources 554 (2023) 232294, https://doi.org/10.1016/J.JPOWSOUR.2022.232294.
[74] T. Lombardo, A.C. Ngandjong, A. Belhcen, A.A. Franco, Carbon-binder migration: a three-dimensional drying model for lithium-ion battery electrodes, Energy Storage Mater. 43 (2021) 337–347, https://doi.org/10.1016/J.ENSM.2021.09.015.
[75] A. Shodiev, M. Chouchane, M. Gaberscek, O. Arcelus, J. Xu, H. Oularbi, J. Yu, J. Li, M. Morcrette, A.A. Franco, Deconvoluting the benefits of porosity distribution in layered electrodes on the electrochemical performance of Li-ion batteries, Energy Storage Mater. 47 (2022) 462–471, https://doi.org/10.1016/J.ENSM.2022.01.058.
[76] C. Liu, O. Arcelus, T. Lombardo, H. Oularbi, A.A. Franco, Towards a 3D-resolved model of Si/Graphite composite electrodes from manufacturing simulations, J. Power Sources 512 (2021), https://doi.org/10.1016/j.jpowsour.2021.230486.
[77] D. Weitze, F.M. Zanotto, D.Z. Dominguez, A.A. Franco, Simulating solid-state battery cathode manufacturing via wet-processing with resolved active material geometries, Energy Storage Mater. 73 (2024) 103747, https://doi.org/10.1016/J.ENSM.2024.103747.
[78] M. Alabdali, F.M. Zanotto, M. Duquesnoy, A.K. Hatz, D. Ma, J. Auvergniot, V. Viallet, V. Seznec, A.A. Franco, Three-dimensional physical modeling of the wet manufacturing process of solid-state battery electrodes, J. Power Sources 580 (2023) 233427, https://doi.org/10.1016/J.JPOWSOUR.2023.233427.
[79] S. Pinilla, F.M. Zanotto, D.Z. Dominguez, T. García, A.A. Franco, Carbon-Binder-Domain porosity extraction through lithium-ion battery electrode impedance data, Energy Storage Mater. (2024) 103818, https://doi.org/10.1016/J.ENSM.2024.103818.

[80] T. Lombardo, M. Duquesnoy, H. El-Bouysidy, F. Årén, A. Gallo-Bueno, P. B. Jørgensen, A. Bhowmik, A. Demortière, E. Ayerbe, F. Alcaide, M. Reynaud, J. Carrasco, A. Grimaud, C. Zhang, T. Vegge, P. Johansson, A.A. Franco, Artificial intelligence applied to battery research: hype or reality? Chem. Rev. 122 (2022) 10899–10969, https://doi.org/10.1021/acs.chemrev.1c00108.

[81] M. Duquesnoy, I. Boyano, L. Ganborena, P. Cereijo, E. Ayerbe, A.A. Franco, Machine learning-based assessment of the impact of the manufacturing process on battery electrode heterogeneity, Energy AI 5 (2021) 100090, https://doi.org/10.1016/J.EGYAI.2021.100090.

[82] A. Shodiev, M. Duquesnoy, O. Arcelus, M. Chouchane, J. Li, A.A. Franco, Machine learning 3D-resolved prediction of electrolyte infiltration in battery porous electrodes, J. Power Sources 511 (2021) 230384, https://doi.org/10.1016/J.JPOWSOUR.2021.230384.

[83] D.E. Galvez-Aranda, T. Le Dinh, U. Vijay, F.M. Zanotto, A.A. Franco, Time-dependent deep learning manufacturing process model for battery electrode microstructure prediction, Adv. Energy Mater. 14 (2024) 2400376, https://doi.org/10.1002/AENM.202400376.

[84] M. Duquesnoy, C. Liu, D.Z. Dominguez, V. Kumar, E. Ayerbe, A.A. Franco, Machine learning-assisted multi-objective optimization of battery manufacturing from synthetic data generated by physics-based simulations, Energy Storage Mater. 56 (2023) 50–61, https://doi.org/10.1016/J.ENSM.2022.12.040.

[85] U. Vijay, D.E. Galvez-Aranda, F.M. Zanotto, T. Le-Dinh, M. Alabdali, M. Asch, A. A. Franco, A hybrid modelling approach coupling physics-based simulation and deep learning for battery electrode manufacturing simulations, Energy Storage Mater. (2024) 103883, https://doi.org/10.1016/J.ENSM.2024.103883.

[86] L. Yu, Y. Bai, B. Polzin, I. Belharouak, Unlocking the value of recycling scrap from Li-ion battery manufacturing: challenges and outlook, J. Power Sources 593 (2024) 233955, https://doi.org/10.1016/J.JPOWSOUR.2023.233955.

[87] D. Song, X. Wang, H. Nie, H. Shi, D. Wang, F. Guo, X. Shi, L. Zhang, Heat treatment of LiCoO2 recovered from cathode scraps with solvent method, J. Power Sources 249 (2014) 137–141, https://doi.org/10.1016/J.JPOWSOUR.2013.10.062.

[88] X. Zhang, Y. Xie, H. Cao, F. Nawaz, Y. Zhang, A novel process for recycling and resynthesizing LiNi1/3Co1/3Mn1/3O2 from the cathode scraps intended for lithium-ion batteries, Waste Manag. 34 (2014) 1715–1724, https://doi.org/10.1016/J.WASMAN.2014.05.023.

[89] Y. Guo, C. Guo, P. Huang, Q. Han, F. Wang, H. Zhang, H. Liu, Y.C. Cao, Y. Yao, Y. Huang, Rejuvenating LiNi0.5Co0.2Mn0.3O2 cathode directly from battery scraps, eScience 3 (2023) 100091, https://doi.org/10.1016/J.ESCI.2023.100091.

[90] N.A. Peppas, J.C. Wu, E.D. von Meerwall, Mathematical modeling and experimental characterization of polymer dissolution, Macromolecules 27 (1994) 5626–5638, https://doi.org/10.1021/ma00098a017.

[91] K. Yu, H. Yang, B.H. Dao, Q. Shi, C.M. Yakacki, Dissolution of covalent adaptable network polymers in organic solvent, J. Mech. Phys. Solid. 109 (2017) 78–94, https://doi.org/10.1016/J.JMPS.2017.08.006.

[92] R. Denolf, J. Hogie, F.L. Figueira, I. Mertens, T. De Somer, D.R. D'hooge, R. Hoogenboom, S. De Meester, Constructing and validating ternary phase diagrams as basis for polymer dissolution recycling, J. Mol. Liq. 387 (2023) 122630, https://doi.org/10.1016/J.MOLLIQ.2023.122630.

[93] W. Zhang, E.D. Gomez, S.T. Milner, Predicting flory-huggins χ from simulations, Phys. Rev. Lett. 119 (2017) 017801, https://doi.org/10.1103/PHYSREVLETT.119.017801/.

[94] P. Zhou, K.L. Sánchez-Rivera, G.W. Huber, R.C. Van Lehn, Computational approach for rapidly predicting temperature-dependent polymer solubilities using molecular-scale models, ChemSusChem 14 (2021) 4307–4316, https://doi.org/10.1002/CSSC.202101137.

[95] P. Zhou, J. Yu, K.L. Sánchez-Rivera, G.W. Huber, R.C. Van Lehn, Large-scale computational polymer solubility predictions and applications to dissolution-based plastic recycling, Green Chem. 25 (2023) 4402–4414, https://doi.org/10.1039/D3GC00404J.

[96] X. Yin, A. Opara, H. Du, J.D. Miller, Molecular dynamics simulations of metal–cyanide complexes: fundamental considerations in gold hydrometallurgy, Hydrometallurgy 106 (2011) 64–70, https://doi.org/10.1016/J.HYDROMET.2010.12.004.

[97] M.G. Muraleedharan, R. Herz-Thyhsen, J.C. Dewey, J.P. Kaszuba, A.C.T. van Duin, Understanding the chemistry of cation leaching in illite/water interfacial system using reactive molecular dynamics simulations and hydrothermal experiments, Acta Mater. 186 (2020) 564–574, https://doi.org/10.1016/J.ACTAMAT.2019.12.059.

[98] A.K. Chew, S. Jiang, W. Zhang, V.M. Zavala, R.C. Van Lehn, Fast predictions of liquid-phase acid-catalyzed reaction rates using molecular dynamics simulations and convolutional neural networks, Chem. Sci. 11 (2020) 12464–12476, https://doi.org/10.1039/D0SC03261A.

[99] T. Song, K. Jiang, J. Zhou, D. Wang, N. Xu, Y. Feng, CFD modelling of gas–liquid flow in an industrial scale gas-stirred leaching tank, Int. J. Miner. Process. 142 (2015) 63–72, https://doi.org/10.1016/J.MINPRO.2015.01.005.

[100] R. Zhou, N. Yang, J. Li, A conceptual model for analyzing particle effects on gas-liquid flows in slurry bubble columns, Powder Technol. 365 (2020) 28–38, https://doi.org/10.1016/J.POWTEC.2019.03.025.

[101] F. Ahmadi, M. Ebrahimian, R.S. Sanders, S. Ghaemi, Particle image and tracking velocimetry of solid-liquid turbulence in a horizontal channel flow, Int. J. Multiphas. Flow 112 (2019) 83–99, https://doi.org/10.1016/J.IJMULTIPHASEFLOW.2018.12.007.

[102] J.S. Newman, C.W. Tobias, Theoretical analysis of current distribution in porous electrodes, J. Electrochem. Soc. 109 (1962) 1183, https://doi.org/10.1149/1.2425269.

[103] T. Fuller, M. Doyle, J. Newman, Modeling of galvanostatic charge and discharge, J. Electrochem. Soc. 140 (1993), https://doi.org/10.1149/1.2221597.

[104] T.F. Fuller, M. Doyle, J. Newman, Simulation and Optimization of the Dual Lithium Ion Insertion Cell, J. Electrochem. Soc 141 (1994). https://doi.org/10.1149/1.2054684.

[105] F. Brosa Planella, W. Ai, A.M. Boyce, A. Ghosh, I. Korotkin, S. Sahu, V. Sulzer, R. Timms, T.G. Tranter, M. Zyskin, S.J. Cooper, J.S. Edge, J.M. Foster, M. Marinescu, B. Wu, G. Richardson, A continuum of physics-based lithium-ion battery models reviewed, Progress in Energy 4 (2022) 042003, https://doi.org/10.1088/2516-1083/AC7D31.

[106] C. Liu, T. Lombardo, J. Xu, A.C. Ngandjong, A.A. Franco, An experimentally-validated 3D electrochemical model revealing electrode manufacturing parameters' effects on battery performance, Energy Storage Mater. 54 (2023) 156–163, https://doi.org/10.1016/J.ENSM.2022.10.035.

[107] J.M. Reniers, G. Mulder, D.A. Howey, Review and performance comparison of mechanical-chemical degradation models for lithium-ion batteries, J. Electrochem. Soc. 166 (2019) 3189–3200, https://doi.org/10.1149/2.0281914jes.

[108] R. Mehta, A. Gupta, Mathematical modelling of electrochemical, thermal and degradation processes in lithium-ion cells—a comprehensive review, Renew. Sustain. Energy Rev. 192 (2024) 114264, https://doi.org/10.1016/J.RSER.2023.114264.

[109] X. Han, Z. Wang, Z. Wei, A novel approach for health management online-monitoring of lithium-ion batteries based on model-data fusion, Appl. Energy 302 (2021) 117511, https://doi.org/10.1016/J.APENERGY.2021.117511.

[110] Regulation (EU) 2023/1542 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL, Concerning Batteries and Waste Batteries, Official Journal of the European Union, 2023.

[111] S. Jung, Mathematical model of lithium-ion batteries with blended-electrode system, J. Power Sources 264 (2014) 184–194, https://doi.org/10.1016/J.JPOWSOUR.2014.04.072.

[112] M. Petit, E. Calas, J. Bernard, A simplified electrochemical model for modelling Li-ion batteries comprising blend and bidispersed electrodes for high power applications, J. Power Sources 479 (2020) 228766, https://doi.org/10.1016/J.JPOWSOUR.2020.228766.

[113] D. Beck, M. Dubarry, Electrode blending simulations using the mechanistic degradation modes modeling approach, Batteries 10 (2024) 159, https://doi.org/10.3390/BATTERIES10050159, 2024, Vol. 10, Page 159.

[114] Understand Comsol, Design, and optimize battery systems, battery design module, in: , 2024. https://www.comsol.com/battery-design-module. (Accessed 31 July 2024).

[115] Siemens, Simcenter Battery Design Studio Software, Simcenter fluids and thermal simulation, in: , 2024. https://plm.sw.siemens.com/en-US/simcenter/fluids-thermal-simulation/battery-design-studio/. (Accessed 20 July 2024).

[116] Mathworks, Developing battery systems with simulink and Simscape, MathWorks, in: , 2024. https://www.mathworks.com/campaigns/offers/next/battery-systems-white-paper.html. (Accessed 31 July 2024).

[117] Y. Liu, B. Guo, X. Zou, Y. Li, S. Shi, Machine learning assisted materials design and discovery for rechargeable batteries, Energy Storage Mater. 31 (2020) 434–450, https://doi.org/10.1016/J.ENSM.2020.06.033.

[118] B.R. Chen, C.M. Walker, S. Kim, M.R. Kunz, T.R. Tanim, E.J. Dufek, Battery aging mode identification across NMC compositions and designs using machine learning, Joule 6 (2022) 2776–2793, https://doi.org/10.1016/J.JOULE.2022.10.016.

[119] Y. Lu, C.Z. Zhao, J.Q. Huang, Q. Zhang, The timescale identification decoupling complicated kinetic processes in lithium batteries, Joule 6 (2022) 1172–1198, https://doi.org/10.1016/J.JOULE.2022.05.005.

[120] Y. Zhang, Q. Tang, Y. Zhang, J. Wang, U. Stimming, A.A. Lee, Identifying degradation patterns of lithium ion batteries from impedance spectroscopy using machine learning, Nat. Commun. 11 (2020) 1–6, https://doi.org/10.1038/s41467-020-15235-7, 2020 11:1.

[121] K.A. Severson, P.M. Attia, N. Jin, N. Perkins, B. Jiang, Z. Yang, M.H. Chen, M. Aykol, P.K. Herring, D. Fraggedakis, M.Z. Bazant, S.J. Harris, W.C. Chueh, R. D. Braatz, Data-driven prediction of battery cycle life before capacity degradation, Nat. Energy 4 (2019) 383–391, https://doi.org/10.1038/s41560-019-0356-8, 2019 4:5.

[122] X. Hu, L. Xu, X. Lin, M. Pecht, Battery lifetime prognostics, Joule 4 (2020) 310–346, https://doi.org/10.1016/J.JOULE.2019.11.018.

[123] S. Fu, S. Tao, H. Fan, K. He, X. Liu, Y. Tao, J. Zuo, X. Zhang, Y. Wang, Y. Sun, Data-driven capacity estimation for lithium-ion batteries with feature matching based transfer learning method, Appl. Energy 353 (2024) 121991, https://doi.org/10.1016/J.APENERGY.2023.121991.

[124] P.K. Jones, U. Stimming, A.A. Lee, Impedance-based forecasting of lithium-ion battery performance amid uneven usage, Nat. Commun. 13 (2022) 1–9, https://doi.org/10.1038/s41467-022-32422-w, 2022 13:1.

[125] M.F. Ng, J. Zhao, Q. Yan, G.J. Conduit, Z.W. Seh, Predicting the state of charge and health of batteries using data-driven machine learning, Nat. Mach. Intell. 2 (2020) 161–170, https://doi.org/10.1038/s42256-020-0156-7, 2020 2:3.

[126] S. Haghi, M.F.V. Hidalgo, M.F. Niri, R. Daub, J. Marco, Machine learning in lithium-ion battery cell production: a comprehensive mapping study, Batter Supercaps 6 (2023), https://doi.org/10.1002/batt.202300046.

[127] V. Meunier, M. Leal De Souza, M. Morcrette, A. Grimaud, Design of workflows for crosstalk detection and lifetime deviation onset in Li-ion batteries, Joule 7 (2023) 42–56, https://doi.org/10.1016/J.JOULE.2022.12.004.

[128] C. Lv, X. Zhou, L. Zhong, C. Yan, M. Srinivasan, W. Seh, C. Liu, H. Pan, S. Li, Y. Wen, Q. Yan, C. Lv, L. Zhong, C. Yan, M. Srinivasan, S. Li, Q. Yan, X. Zhou,

Y. Wen, Z.W. Seh, C. Liu, H. Pan, Machine learning: an advanced platform for materials development and state prediction in lithium-ion batteries, Adv. Mater. 34 (2022) 2101474, https://doi.org/10.1002/ADMA.202101474.
[129] B. Jiang, W.E. Gent, F. Mohr, S. Das, M.D. Berliner, M. Forsuelo, H. Zhao, P. M. Attia, A. Grover, P.K. Herring, M.Z. Bazant, S.J. Harris, S. Ermon, W.C. Chueh, R.D. Braatz, Bayesian learning for rapid prediction of lithium-ion battery-cycling protocols, Joule 5 (2021) 3187–3203, https://doi.org/10.1016/J.JOULE.2021.10.010.
[130] P.M. Attia, A. Grover, N. Jin, K.A. Severson, T.M. Markov, Y.H. Liao, M.H. Chen, B. Cheong, N. Perkins, Z. Yang, P.K. Herring, M. Aykol, S.J. Harris, R.D. Braatz, S. Ermon, W.C. Chueh, Closed-loop optimization of fast-charging protocols for batteries with machine learning, Nature 578 (2020) 397–402, https://doi.org/10.1038/s41586-020-1994-5, 2020 578:7795.
[131] L.H. Rieger, E. Flores, K.F. Nielsen, P. Norby, E. Ayerbe, O. Winther, T. Vegge, A. Bhowmik, Uncertainty-aware and explainable machine learning for early prediction of battery degradation trajectory, Digital Discovery 2 (2023) 112–122, https://doi.org/10.1039/D2DD00067A.
[132] S.J. Harris, M.M. Noack, Statistical and machine learning-based durability-testing strategies for energy storage, Joule 7 (2023) 920–934, https://doi.org/10.1016/J.JOULE.2023.03.008.
[133] A. Weng, P. Mohtat, P.M. Attia, V. Sulzer, S. Lee, G. Less, A. Stefanopoulou, Predicting the impact of formation protocols on battery lifetime immediately after manufacturing, Joule 5 (2021) 2971–2992, https://doi.org/10.1016/J.JOULE.2021.09.015.
[134] G. Harper, R. Sommerville, E. Kendrick, L. Driscoll, P. Slater, R. Stolkin, A. Walton, P. Christensen, O. Heidrich, S. Lambert, A. Abbott, K. Ryder, L. Gaines, P. Anderson, Recycling lithium-ion batteries from electric vehicles, Nature 575 (2019) 75–86, https://doi.org/10.1038/s41586-019-1682-5.
[135] N. Dawson-Elli, S.B. Lee, M. Pathak, K. Mitra, V.R. Subramanian, Data science approaches for electrochemical engineers: an introduction through surrogate model development for lithium-ion batteries, J. Electrochem. Soc. 165 (2018) A1–A15, https://doi.org/10.1149/2.1391714JES.
[136] W. Li, J. Zhang, F. Ringbeck, D. Jöst, L. Zhang, Z. Wei, D.U. Sauer, Physics-informed neural networks for electrode-level state estimation in lithium-ion batteries, J. Power Sources 506 (2021) 230034, https://doi.org/10.1016/J.JPOWSOUR.2021.230034.
[137] A. Marcato, J.E. Santos, C. Liu, G. Boccardo, D. Marchisio, A.A. Franco, Modeling the 4D discharge of lithium-ion batteries with a multiscale time-dependent deep learning framework, Energy Storage Mater. 63 (2023), https://doi.org/10.1016/j.ensm.2023.102927.
[138] P.J. Weddle, S. Kim, B.R. Chen, Z. Yi, P. Gasper, A.M. Colclasure, K. Smith, K. L. Gering, T.R. Tanim, E.J. Dufek, Battery state-of-health diagnostics during fast cycling using physics-informed deep-learning, J. Power Sources 585 (2023) 233582, https://doi.org/10.1016/J.JPOWSOUR.2023.233582.
[139] S. Navidi, A. Thelen, T. Li, C. Hu, Physics-informed machine learning for battery degradation diagnostics: a comparison of state-of-the-art methods, Energy Storage Mater. 68 (2024) 103343, https://doi.org/10.1016/J.ENSM.2024.103343.
[140] G.E. Karniadakis, I.G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, L. Yang, Physics-informed machine learning, Nat. Reviews Phys. (2021) 422–440, https://doi.org/10.1038/s42254-021-00314-5, 2021 3:6 3.
[141] M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, J. Comput. Phys. 378 (2019) 686–707, https://doi.org/10.1016/J.JCP.2018.10.045.
[142] R.G. Nascimento, M. Corbetta, C.S. Kulkarni, F.A.C. Viana, Hybrid physics-informed neural networks for lithium-ion battery modeling and prognosis, J. Power Sources 513 (2021) 230526, https://doi.org/10.1016/J.JPOWSOUR.2021.230526.
[143] Z. Xu, Y. Guo, J.H. Saleh, A physics-informed dynamic deep autoencoder for accurate state-of-health prediction of lithium-ion battery, Neural Comput. Appl. 34 (2022) 15997–16017, https://doi.org/10.1007/S00521-022-07291-5/TABLES/8.
[144] S. Kohtz, Y. Xu, Z. Zheng, P. Wang, Physics-informed machine learning model for battery state of health prognostics using partial charging segments, Mech. Syst. Signal Process. 172 (2022) 109002, https://doi.org/10.1016/J.YMSSP.2022.109002.
[145] A. Thelen, Y.H. Lui, S. Shen, S. Laflamme, S. Hu, H. Ye, C. Hu, Integrating physics-based modeling and machine learning for degradation diagnostics of lithium-ion batteries, Energy Storage Mater. 50 (2022) 668–695, https://doi.org/10.1016/J.ENSM.2022.05.047.
[146] J. Shi, A. Rivera, D. Wu, Battery health management using physics-informed machine learning: online degradation modeling and remaining useful life prediction, Mech. Syst. Signal Process. 179 (2022) 109347, https://doi.org/10.1016/J.YMSSP.2022.109347.
[147] H. Tu, S. Moura, Y. Wang, H. Fang, Integrating physics-based modeling with machine learning for lithium-ion batteries, Appl. Energy 329 (2023) 120289, https://doi.org/10.1016/J.APENERGY.2022.120289.
[148] L. Ma, J. Tian, T. Zhang, Q. Guo, C. Hu, Accurate and efficient remaining useful life prediction of batteries enabled by physics-informed machine learning, J. Energy Chem. 91 (2024) 512–521, https://doi.org/10.1016/J.JECHEM.2023.12.043.
[149] T. Hofmann, J. Hamar, M. Rogge, C. Zoerr, S. Erhard, J.P. Schmidt, Physics-informed neural networks for state of health estimation in lithium-ion batteries, J. Electrochem. Soc. 170 (2023) 090524, https://doi.org/10.1149/1945-7111/ACF0EF.
[150] Y. Wang, C. Xiong, Y. Wang, P. Xu, C. Ju, J. Shi, G. Yang, J. Chu, Temperature state prediction for lithium-ion batteries based on improved physics informed neural networks, J. Energy Storage 73 (2023) 108863, https://doi.org/10.1016/J.EST.2023.108863.
[151] J. Xia, Q. Shi, H. Li, M. Zhou, K. Jiang, K. Wang, A novel sorting method for liquid metal batteries based on deep learning and sequential features, J. Energy Storage 64 (2023) 107093, https://doi.org/10.1016/J.EST.2023.107093.
[152] J. Neumann, M. Petranikova, M. Meeus, J.D. Gamarra, R. Younesi, M. Winter, S. Nowak, Recycling of lithium-ion batteries—current state of the art, circular economy, and next generation recycling, Adv. Energy Mater. 12 (2022) 2102917, https://doi.org/10.1002/AENM.202102917.
[153] Z. Zhou, A. Ran, S. Chen, X. Zhang, G. Wei, B. Li, F. Kang, X. Zhou, H. Sun, A fast screening framework for second-life batteries based on an improved bisecting K-means algorithm combined with fast pulse test, J. Energy Storage 31 (2020) 101739, https://doi.org/10.1016/J.EST.2020.101739.
[154] R. Sommerville, J. Shaw-Stewart, V. Goodship, N. Rowson, E. Kendrick, A review of physical processes used in the safe recycling of lithium ion batteries, Sustain. Mater. Technol. 25 (2020) e00197, https://doi.org/10.1016/J.SUSMAT.2020.E00197.
[155] E.L. Schneider, C.T. Oliveira, R.M. Brito, C.F. Malfatti, Classification of discarded NiMH and Li-Ion batteries and reuse of the cells still in operational conditions in prototypes, J. Power Sources 262 (2014) 1–9, https://doi.org/10.1016/J.JPOWSOUR.2014.03.095.
[156] R. Xiong, Y. Pan, W. Shen, H. Li, F. Sun, Lithium-ion battery aging mechanisms and diagnosis method for automotive applications: recent advances and perspectives, Renew. Sustain. Energy Rev. 131 (2020) 110048, https://doi.org/10.1016/J.RSER.2020.110048.
[157] C. Pastor-Fernández, T.F. Yu, W.D. Widanage, J. Marco, Critical review of non-invasive diagnosis techniques for quantification of degradation modes in lithium-ion batteries, Renew. Sustain. Energy Rev. 109 (2019) 138–159, https://doi.org/10.1016/J.RSER.2019.03.060.
[158] Y. Shen, B. Zou, Z. Zhang, M. Xu, S. Wang, Q. Li, H. Li, M. Zhou, K. Jiang, K. Wang, In situ detection of lithium-ion batteries by ultrasonic technologies, Energy Storage Mater. 62 (2023) 102915, https://doi.org/10.1016/J.ENSM.2023.102915.
[159] J. Hou, W. Wu, L. Li, X. Tong, R. Hu, W. Wu, W. Cai, H. Wang, Estimation of remaining capacity of lithium-ion batteries based on X-ray computed tomography, J. Energy Storage 55 (2022) 105369, https://doi.org/10.1016/J.EST.2022.105369.
[160] X. Lai, D. Qiao, Y. Zheng, M. Ouyang, X. Han, L. Zhou, A rapid screening and regrouping approach based on neural networks for large-scale retired lithium-ion cells in second-use applications, J. Clean. Prod. 213 (2019) 776–791, https://doi.org/10.1016/J.JCLEPRO.2018.12.210.
[161] P. Zhou, Z. He, T. Han, X. Li, X. Lai, L. Yan, T. Lv, J. Xie, Y. Zheng, A rapid classification method of the retired LiCoxNiyMn1−x−yO2 batteries for electric vehicles, Energy Rep. 6 (2020) 672–683, https://doi.org/10.1016/J.EGYR.2020.03.013.
[162] S. Tao, H. Liu, C. Sun, H. Ji, G. Ji, Z. Han, R. Gao, J. Ma, R. Ma, Y. Chen, S. Fu, Y. Wang, Y. Sun, Y. Rong, X. Zhang, G. Zhou, H. Sun, Collaborative and privacy-preserving retired battery sorting for profitable direct recycling via federated machine learning, Nat. Commun. 14 (2023) 1–14, https://doi.org/10.1038/s41467-023-43883-y, 2023 14:1.
[163] G. Wei, Y. Liu, B. Jiao, N. Chang, M. Wu, G. Liu, X. Lin, X.F. Weng, J. Chen, L. Zhang, C. Zhu, G. Wang, P. Xu, J. Di, Q. Li, Direct recycling of spent Li-ion batteries: challenges and opportunities toward practical applications, iScience 26 (2023) 107676, https://doi.org/10.1016/J.ISCI.2023.107676.
[164] Y. Lu, M. Maftouni, T. Yang, P. Zheng, D. Young, Z.J. Kong, Z. Li, A novel disassembly process of end-of-life lithium-ion batteries enhanced by online sensing and machine learning techniques, J. Intell. Manuf. 34 (2023) 2463–2475, https://doi.org/10.1007/S10845-022-01936-X/FIGURES/10.
[165] K. Meng, G. Xu, X. Peng, K. Youcef-Toumi, J. Li, Intelligent disassembly of electric-vehicle batteries: a forward-looking overview, Resour. Conserv. Recycl. 182 (2022) 106207, https://doi.org/10.1016/J.RESCONREC.2022.106207.
[166] A. Hogan, E. Blomqvist, M. Cochez, C. D'Amato, G. De Melo, C. Gutierrez, S. Kirrane, J.E.L. Gayo, R. Navigli, S. Neumaier, A.C.N. Ngomo, A. Polleres, S. M. Rashid, A. Rula, L. Schmelzeisen, J. Sequeda, S. Staab, A. Zimmermann, Knowledge Graphs, ACM Comput. Surv. 54 (2021), https://doi.org/10.1145/3447772.
[167] J. Wang, J. Huang, R. Li, J. Wang, J. Huang, R. Li, Knowledge graph construction of end-of-life electric vehicle batteries for robotic disassembly, Appl. Sci. 13 (2023) 13153, https://doi.org/10.3390/APP132413153, 2023, Vol. 13, Page 13153.
[168] J. Piątek, S. Afyon, T.M. Budnyak, S. Budnyk, M.H. Sipponen, A. Slabon, Sustainable Li-ion batteries: chemistry and recycling, Adv. Energy Mater. 11 (2021) 2003456, https://doi.org/10.1002/AENM.202003456.
[169] B. Niu, X. Wang, Z. Xu, Application of machine learning to guide efficient metal leaching from spent lithium-ion batteries and comprehensively reveal the process parameter influences, J. Clean. Prod. 410 (2023) 137188, https://doi.org/10.1016/J.JCLEPRO.2023.137188.
[170] R.P. Sheth, N.S. Ranawat, A. Chakraborty, R.P. Mishra, M. Khandelwal, The lithium-ion battery recycling process from a circular economy perspective—a review and future directions, Energies 16 (2023) 3228, https://doi.org/10.3390/EN16073228, 2023, Vol. 16, Page 3228.
[171] F. Punt, S. Doose, A.C. Böttcher, S. Breitung-Faes, A. Kwade, Modeling and flow sheet simulation of selected mechanical recycling processes for Li-ion batteries, Chem. Ing. Tech. 95 (2023) 59–67, https://doi.org/10.1002/CITE.202200156.

[172] K. Richa, C.W. Babbitt, G. Gaustad, Eco-efficiency analysis of a lithium-ion battery waste hierarchy inspired by circular economy, J. Ind. Ecol. 21 (2017) 715–730, https://doi.org/10.1111/JIEC.12607.
[173] J.R. Castillo-Sánchez, K. Oishi, L. St-Germain, D. Ait-Amer, J.P. Harvey, The power of computational thermochemistry in high-temperature process design and optimization: Part 1 — unit operations, Calphad 82 (2023) 102593, https://doi.org/10.1016/J.CALPHAD.2023.102593.
[174] CIRPASS, Project results. https://cirpassproject.eu/project-results/, 2024. (Accessed 20 July 2024).
[175] Hereon, Harmonization of advanced materials ecosystems serving strategic innovation markets to pave the way to a Digital Materials & Product Passport: DigiPass. https://www.hereon.de/about_us/eu_projects/horizon_europe/key/113621/index.php.en, 2024. (Accessed 20 July 2024).
[176] Battery Pass, The Value of the EU Battery Passport, Version 0.9 - an exploratory assessment of economic, environmental and social benefits, in: , 2024. https://thebatterypass.eu/assets/images/value-assessment/pdf/2024_BatteryPassport_Value_Assessment.pdf. (Accessed 31 August 2024).
[177] S. Stier, Battery-Value-Chain-Ontology/ontology: v0.3.0. Zenodo. https://doi.org/10.5281/zenodo.7799522, 2023.
[178] S.P. Stier, A. Räder, L. Gold, M.A. Popp, A. Triol, Linked data schema repositories for interoperable data spaces, in: 19th International Conference on Semantic Systems (SEMANTiCS 2023), Zenodo, 2023, https://doi.org/10.5281/zenodo.10528692.
[179] European Commission, CORDIS - EU research results, European Commission (n.d.). https://cordis.europa.eu/search/en (accessed July 1, 2024).
[180] Agence Nationale de la Recherche, Résultats de recherche de projets financés: "batterie et recyclage," Agence Nationale de La Recherche (n.d.). https://anr.fr/fr/projets-finances-et-impact/projets-finances/resultats-de-votre-recherche/?q=batterie+et+recyclage&id=1959&L=0 (accessed July 1, 2024).
[181] Batterieforum Deutschland, BecoSearch: Project Map, (n.d.). https://becosearch.com/projects/maplist (accessed July 5, 2024).
[182] Centro para el Desarrollo Tecnológico y la Innovación, Proyectos Aprobados, (n.d.). https://www.cdti.es/proyectos-aprobados (accessed July 15, 2024).
[183] UK Research and Innovation, Innovate UK funded projects since 2004, (n.d.). https://ukri.org/publications/innovate-uk-funded-projects-since-2004/(accessed July 20, 2024).
[184] A. Hassan, S.A. Khan, R. Li, W. Su, X. Zhou, M. Wang, B. Wang, Second-life batteries: a review on power grid applications, degradation mechanisms, and power electronics interface architectures, Batteries 9 (2023) 571, https://doi.org/10.3390/BATTERIES9120571, 2023, Vol. 9, Page 571.
[185] M. Slattery, J. Dunn, A. Kendall, Transportation of electric vehicle lithium-ion batteries at end-of-life: a literature review, Resour. Conserv. Recycl. 174 (2021), https://doi.org/10.1016/j.resconrec.2021.105755.
[186] LiPLANET, LiPLANET Pilot Lines,, 2024, p. 2024. https://liplanet.eu/pilot-lines/. (Accessed 31 August 2024).