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doi.org/10.1002/batt.202400385

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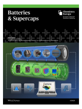

The ARTISTIC Battery Manufacturing Digitalization Initiative: From Fundamental Research to Industrialization

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Our ARTISTIC project was born in 2018 to improve the efficiency of lithium-ion battery cell manufacturing process through computational modelling, allowing the research and development of new digital tools to accelerate the optimization of this process. Thanks to the development and use of innovative numerical models, machine learning algorithms and virtual and mixed reality tools, we could significantly advance the understanding of manufacturing/battery cell performance relationships. However, scientific research by itself is not enough to bring innovations into practical applications for society. The creation of spin-offs or start-ups can ease the transition from research to application, since it allows scaling up the research outputs into products or services ready-to-use by the customers. In this Concept, we discuss the benefits of this transition, we introduce the research findings obtained in the last years within the framework of our ARTISTIC project, and our actions to move from our research to industrial products.

Introduction

Lithium-ion batteries (LIBs) are the most common type of rechargeable battery used in portable electronic devices, such as smartphones, laptops and tablets, thanks to their high energy density, low self-discharge rate and long lifespan.[1–3] LIBs have revolutionized the energy storage industry, being also essential for the development and adoption of electric vehicles, which offer a more sustainable alternative to traditional gasoline-powered cars.[4-5] Furthermore, LIBs have been also considered for storing energy generated from renewable sources such as solar and wind power.[6-8] However, although LIBs are a critical component for the continued progress of sustainable energy solutions, they still have room for improvement in terms of cost and recharging time reduction, energy density and lifetime enhancement. Therefore, it is still necessary to work on the optimization of LIBs designing and manufacturing.[9]

Scientific experiments and computational simulations are equally important in the development of the next generation of LIBs to overcome the current challenges. While scientific experiments can provide direct measurements with relevant information about LIB cell performance as a function of the chosen electrode materials and manufacturing parameters, computational simulations can help to predict and understand different phenomena that cannot be easily explored by experiments. One major interest of computational simulations is their ability to analyze simultaneously (in the case of multiscale approaches) processes occurring at multiple length and time scales. Some examples of physics-based simulation methods used in battery research include first-principles calculations,[—10-13] molecular dynamics (MD)[—14-16] and the finite element method (FEM).[17-18] Computational simulations have been shown to be particularly interesting in inspiring experimentalists about the battery materials to synthesize.[19] Researchers are also using computer simulations to study the charge transport mechanisms, the degradation phenomena, and to improve battery cell design.[—20-22] During three decades, there has been many efforts towards the development of more and more relevant physics-based computational models describing the complexity of battery cells, and LIBs in particular. However, given the multi-physics characteristic of a LIB cell, this task is quite challenging due to three main factors: first, making sure that all the relevant physics is included in a computational model for the purpose for which the model is designed for, second, finding ways to solve the underlying mathematical description of those physics, and third to find efficient ways to calibrate the model and validate experimentally its results.[23] In this context, the ARTISTIC project[24] was born in 2018, funded by the European Research Council (ERC), under the Horizon 2020 program, to develop new computational tools for the optimization of LIB cell manufacturing processes. The project, led by Professor

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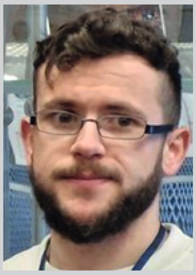
Alejandro A. Franco from Université de Picardie Jules-Verne (UPJV),[25] was enriched by fruitful interactions with external industrial actors. By providing insightful predictions of the performance of LIB electrodes and cells as a function of the manufacturing process parameters, the ARTISTIC project significantly advanced the understanding of the manufacturing/performance relationships, a crucial aspect to tackle while intending to further optimize LIB cells. Thanks to the development of new computational tools for the optimization of the electrode and the cell manufacturing processes, new predictive methods were developed, guiding the production of LIB electrodes with the desired microstructure. Therefore, it was possible to reach an improved understanding of the factors that affect the LIB cell performance. Consequently, one can say that the ARTISTIC project has introduced a novel methodology with strong potential to accelerate LIB cell manufacturing process optimization.

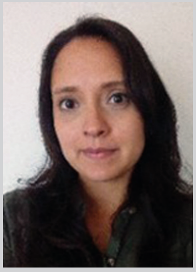
The ARTISTIC project has developed a significant number of new methods, techniques and algorithms for the optimization of the LIB electrode and cell manufacturing process at the machinery level, with models later extended by us to the simulation of the manufacturing process of Sodium Ion and Solid State Battery electrodes.[–26-28] Physics-based numerical models, Machine Learning (ML) algorithms, computational



Dr. Javier F. Troncoso worked as Research Engineer in Prof. Alejandro A. Franco's group (Université de Picardie Jules Verne -UPJV-, Amiens, France). Javier holds a PhD in Computational Physics Applied to Materials Science from Queen's University Belfast. He has worked as a postdoctoral researcher at EMPA, in Switzerland, and then at UPJV under the supervision of Alejandro. He also has work experience as a software developer in data science at GFT Technologies.

Dr. Franco M. Zanotto was a postdoctoral researcher working in Prof. Alejandro A. Franco's group (Université de Picardie Jules Verne, Amiens, France). Franco obtained a PhD in Chemistry from Universidad Nacional de Cordoba, Argentina, in 2019 and worked as a postdoctoral scholar at Florida State University. He was part of the Horizon Europe PULSELION project. Working mainly in computational modelling, his interests include molecular and granular dynamics, electrochemical processes, charge transfer, mass transport, and chemical kinetics.

Dr. Diego E. Galvez-Aranda is a postdoctoral researcher working in Prof. Alejandro A. Franco's group (Université de Picardie Jules Verne, Amiens, France). Diego holds a PhD in Electrical Engineering from Texas A&M University, US. He worked as a postdoctoral researcher in the Chemical Engineering Department at Texas A&M. His experience involves the development of advanced deep learning models to simulate the operation principles of electrochemical energy materials and interfaces. Additionally, he has a computational modelling background including methods such as molecular dynamics, ab-initio molecular dynamics and DFT calculations to study different electrolyte-electrode interfaces.



Diana Zapata Dominguez holds a Ph.D. in physics applied to the characterization of Lithium Ion Batteries (LIBs) from the University of Grenoble Alpes. She has been working on characterizing and optimizing positive and negative electrodes for LIBs since her master's degree. Her postdoctoral work in Prof. Alejandro A. Franco's group (Université de Picardie Jules Verne, Amiens, France) involved the experimental validation and confrontation of the manufacturing process models in LIBs developed by the ERC-funded ARTISTIC project members. She contributed on the fabrication process for LIBs and its implementation in tools developed in virtual and mixed reality for advancing the training and education on LIB technologies.

Lucie Denisart holds a Master's degree in ergonomics from the University of Lorraine and has work experience at the Biomedical Research Institute for the Armed Forces (IRBA, Brétigny sur Orge). She has skills that allow her to implement an effective and systemic ergonomic approach. She worked as ergonomist engineer in Prof. Alejandro A. Franco's group (Université de Picardie Jules Verne, Amiens, France) where she used her skills related to user experience, such as the implementation of a user-centered design approach, collection of needs or realization of user tests.

Prof. Dr. Alejandro A. Franco is a Full Professor at the Université de Picardie Jules Verne (Amiens, France) and an Honorary Member of the Institut Universitaire de France. Prof. Franco is recipient of two ERC grants (ARTISTIC and SMARTISTIC projects) focusing on battery manufacturing digitalization. In 2019, he was honored with the French Prize for Pedagogy Innovation for his utilization of Virtual Reality in teaching battery sciences. He is the recipient of the 2024 Battery Division M. Stanley Whittingham Mid-Career Award of the Electrochemical Society (ECS). He coordinates the Erasmus+ i-MESC (Interdisciplinarity in Materials for Energy Storage and Conversion) International MSc. Programme. He is co-founder of the start-up under creation mentioned in this Concept.

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optimization algorithms, and Mixed and Virtual Reality tools are some of the employed techniques in the development of the ARTISTIC-produced digital solutions. The developed physics-based numerical models can predict electrode microstructure as a function of the chosen manufacturing parameters, and cell performance as a function of the predicted microstructure of the electrodes, all this with 3D spatial resolution at the mesoscale and as a function of time. The developed ML algorithms can predict the electrode and cell manufacturing/performance relationships considering experimental and simulation data. The developed computational optimization algorithms can find the optimal electrode and cell design as well as the set of manufacturing process parameters to adopt for given target properties and performance. Mixed and Virtual Reality tools, we developed on the acquired knowledge, can be used to train new battery pilot line operators and to analyze experimental and simulation results data in an immersive and interactive way. These findings have the potential to make batteries, and LIBs in particular, more affordable, efficient and reliable, boosting battery research and the development of new battery designs and manufacturing strategies. Additionally, the project compiled an experimental database, from its own experimental work by using the battery prototyping line available in our laboratory, that serves to calibrate and validate our computational physics-based models and to train our ML algorithms, as well as to guide battery researchers and operators while they are training themselves in the manufacturing process. The combination of experimental data with physics-based and ML models in the ARTISTIC project has contributed to the development of a pioneering digital model (and until some extent a digital shadow) of battery cell manufacturing. Figure 1 displays the concept of digital models, shadows and twins used in this Concept. In a digital model, the data flow is manual, between the physical object and its digital counterpart (digital object). In the digital shadow, the data is collected automatically from the physical object and send automatically into its digital counterpart. The outcome from the digital object serves to manually adjust its physical counterpart. The digital object is a virtual replica of the battery manufacturing process allowing the simulation of different steps, predicting *e.g.* the resulting electrode properties and the associated electrochemical performance. In a digital twin, there is an automated bidirectional data flow between the physical object and its digital counterpart. Most of the work published about battery manufacturing is nowadays focused on digital models, much less about digital shadows, and digital twins have just started to emerge in the chemistry field with the concept of autonomous labs for materials synthesis.[29] However, regarding the latter, to the best of our knowledge, not yet for battery manufacturing.

We can picture four stages in the development chain of rechargeable batteries: laboratory, prototyping, pilot line and factory (see Figure 2). The laboratory scale consists of developing proof of concept of a cell, demonstrating its feasibility to use materials synthetized at the lab scale using specific electrodes and/or electrolyte formulations. Associated electrochemical characterizations are typically carried out in coin cells. At the lab scale, the degree of variability of manufacturing and testing parameters is generally very high as most of the operations are manual.

The prototyping scale consists of scaling up the lab proof of concept cell into an industrial format (*e.g.* 18650 or pouch cell), and it is the stage where the manufacturing process (*e.g.* electrodes formulations, coating speeds, calendering degree) is optimized. Depending on the battery prototyping line, there can be as many as 20 semi-manual activities in the preparation of the electrodes (premixing, mixing, coating, drying and calendering) and of the cells (filling, sealing, formation and tab welding, degassing and resealing for pouch and cylindrical cells). There can be also more than 50 manual activities (*e.g.* transporting and adding active material, carbon powder, binder and solvent, transporting the slurry pots and the electrodes, operating each of the processing machines associated to each of the semi-manual activities, visual inspection of the outcomes

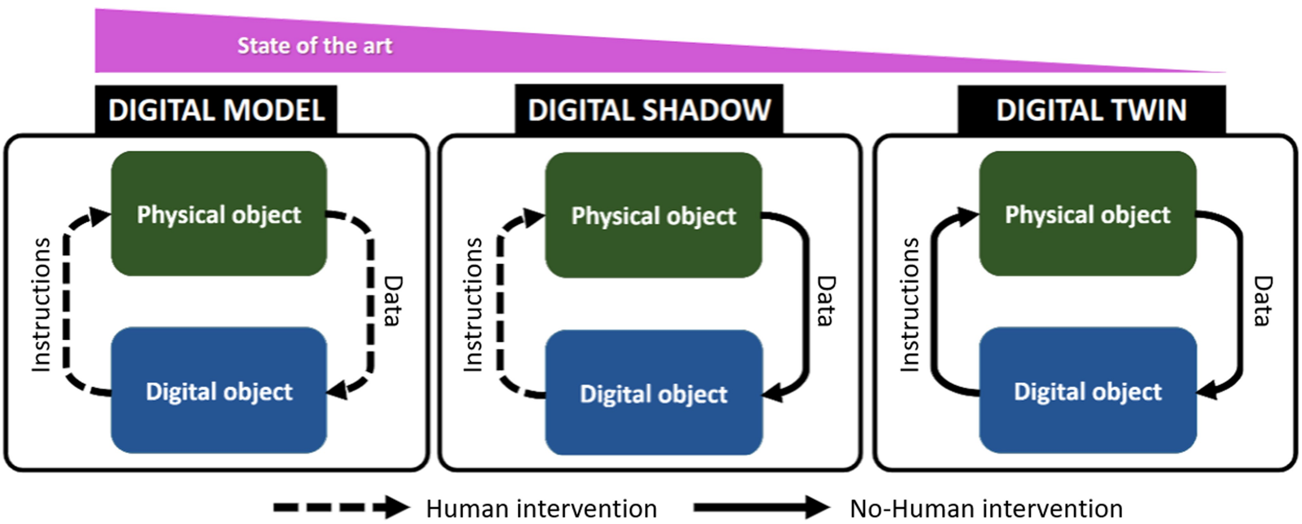

Figure 1. Definition of digital models, digital shadows and digital twins used in this Concept. A digital twin implies a fully automated data exchange between the physical and digital objects, as opposed to a digital model, in which the data exchange is manual.

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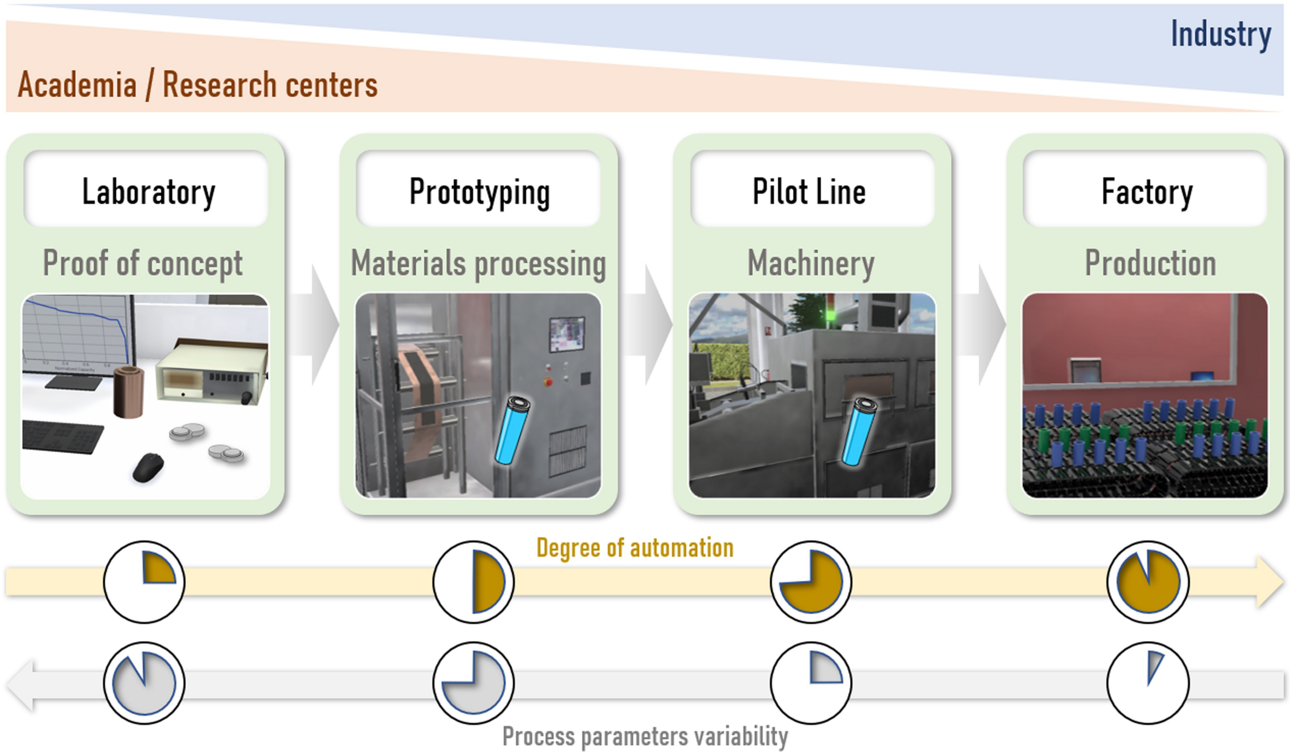

Figure 2. Degree of automation and process parameters variability in the four stages of a battery development process: Laboratory, Prototyping, Pilot Line, and Factory. The triangles on the top indicate the predominance (activity volume) of each of the stages in academia/research centers (which decreases from left to right) and in industry (which increases from left to right).

for each of the semi-manual steps, electrode cutting, electrode-separator alignment during the cell assembly, and tab welding). Consequently, there is less, but still significant, parameters variability, partly due to the search of manufacturing parameters to maximize cell performance. This can lead to high scrap rates.

The pilot line stage mimics, at reduced scale, the factory operation. The optimized manufacturing process at the prototyping scale is transferred into the pilot line to check the feasibility of battery cell mass production and to fine tune the automation of the machinery. The variability degree of manufacturing is here much less since the primary goal is to check the mass production feasibility with the optimized manufacturing parameters at the prototyping scale. The factory stage is where the cells mass production occurs. At the factory stage the process is fully automated and its parameters are not intended to change. Our ARTISTIC initiative proposes a software platform for inverse designing the machinery parameters (*e.g.* coater speed, drying rate, calender pressure) under scenarios where there exists a significant variability of these parameters, like in prototyping and pilot line stages. However, it can also be applied at the factory scale as a tool to track data and establish a powerful digital backbone or digital twin.

In this Concept, we discuss the addition of an industrialization dimension at the heart of the ARTISTIC software to accelerate the development of its technological innovations and meet the market challenges in the battery sector.

The ARTISTIC Project

The ARTISTIC project was a highly innovative and multidisciplinary scientific project born in 2018 that aimed to optimize the manufacturing process of rechargeable battery technologies by using computational modeling. The project developed pioneering physics-based numerical models calibrated and validated against experimental results to improve the understanding of the impact of manufacturing process parameters on the final properties of LIB electrodes and cell's properties and ML tools to automate and optimize the electrodes and cells manufacturing process.

During its implementation, the ARTISTIC project was committed to Open Science for the advancement of scientific research, by making results and research methods available to the public to accelerate the pace of innovation in battery research and development. The ARTISTIC findings are public through its website[24] and through Prof. Alejandro A. Franco's research group website,[25] providing access to all the articles published since 2018.

In order to allow users to use some of our models, we released the ARTISTIC Online Calculator in 2020.[24, 30] This is a web platform that offers a user-friendly interface to simulate the manufacturing process of LIB electrodes in three dimensions. The ARTISTIC Online Calculator is a valuable tool for researchers and engineers who are working on improving the performance of LIBs and can be used to study the effects of different parameters on the performance of the electrodes. This

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information can be used to design new electrodes that are more efficient and have a longer lifespan. The ARTISTIC Online Calculator has aroused the interest of more than 1500 users (*ca.* 50% from industry) since the opening of the first version in 2020.

Additionally, the ARTISTIC project supported also our strong commitment to train the next generation of battery researchers, producing a series of educational resources to teach about battery manufacturing processes. The project has organized a series of free webinars since 2020 (4 editions, with 2600+ participants worldwide) committed to presenting and exchanging about the project results with the community.[24] Furthermore, the project released two online serious games that allow players to navigate electrode microstructures and manufacture LIB cells.[31,32] We believe that the practices applied within the ARTISTIC project are a good example of how to promote and share the scientific data, methods and results in a way that is free, accessible, and reusable. In the next sub-sections, we review the methods developed in the ARTISTIC project, together with a description of some of the findings obtained thanks to them.

Physics-based Models

Physics-based models can be seen as interpretations of specific aspects or processes from the real world. Physics-based models, implicitly or explicitly, consider a set of assumptions, dictating the physical processes that are considered in such interpretation. Typically, these physical processes are described by well-known mathematical equations, which are solved numerically to obtain a physics-based simulation. Different physical equations can be applied to a wide range of systems, as they incorporate specific parameters that can capture effects of material properties and/or of manufacturing conditions. Therefore, even if they are validated using a limited set of experimental measurements, they have the potential for extrapolation and do not require a large amount of data to be effective. Additionally, they aim to reproduce the behavior of the real system based on the consideration of real physical processes. As a result, they can reveal insights and relationships between events with a diversity of spatial and temporal resolutions, offering a complementary understanding of the real process to what experimental characterization techniques can deliver.

In the battery research context, physics-based models are applied in performance prediction, ageing processes, and, in recent years, in manufacturing, with the ARTISTIC project having offered a pioneering contribution for the latter. While in terms of basic research, physics-based models are useful to understand the physical processes involved in each of the manufacturing stages, their interest in the industry sector is mainly to optimize parameters faster. One of the main objectives of industry is to obtain the manufacturing conditions that maximize the battery cell performance and safety, while minimizing cost and environmental impact, among other variables of interest. Ideally, physics-based models could be used to screen parameters without the need of high-throughput experiments, saving materials and time (see Figure 3). It is important to mention that all the physics-based models must be calibrated and validated by experimental data: in fact, parameterization of the models is a crucial step in its development. Therefore, we explain more about how this validation process is executed for our ARTISTIC physics-based models in the next sub-section: Model Parametrization and Experimental Validation. One possible limitation of a physics-based model is its use in a real-time application. The computational cost associated with these models, if they are resolved with spatial 3D-resolution and as a function of time, can be still order of magnitudes greater than real-time processes. As an example, our initial generation of ARTISTIC models for physics-based electrode manufacturing simulation needed, in average, 2–3 days to be completed in our university supercomputer using 28 cores with each core consisting of a dual-processor Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40 GHz 128 GB of memory. Therefore, the research activity behind the development of physical models can also include the search of methods to decrease their computational time to get close to a real-time application, for example through the optimization of the parallelization of the codes solving the models across the supercomputer nodes.

Since LIB cells manufacturing and operation involve complex processes, combining simultaneously various physical phenomena, the development of a model requires the integration of several kinds of physics-based approaches communicating to each other through the different manufacturing stages. In the ARTISTIC project, a novel multi-physics model to describe the whole electrode manufacturing chain (slurry preparation, solvent evaporation and calendering) has been introduced by us (see Figure 4).[33-35] We consider an electrode slurry as composed by discrete particles (granular model) using MD-like methods such as Corse-Grained Molecular Dynamics (CGMD) and the Discrete Element Method (DEM).[35] Solid particles, such as those of the active material (AM) can be considered individually or made of primary particles to account for deformation or cracking.[36,37] The granular or coarse grained approach also allows to describe solvent, soluble components

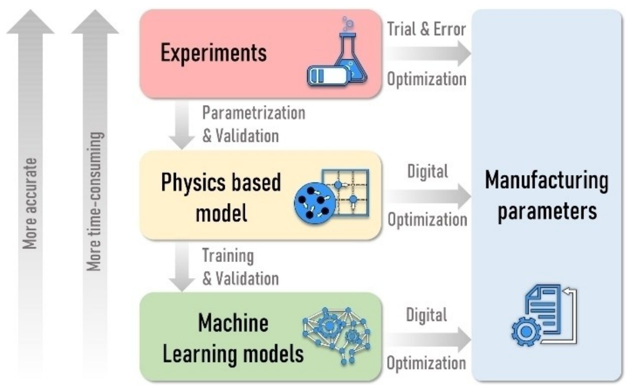

Figure 3. The three approaches adopted in our ARTISTIC initiative to determine an appropriate set of manufacturing parameters that optimizes a LIB electrode or cell.

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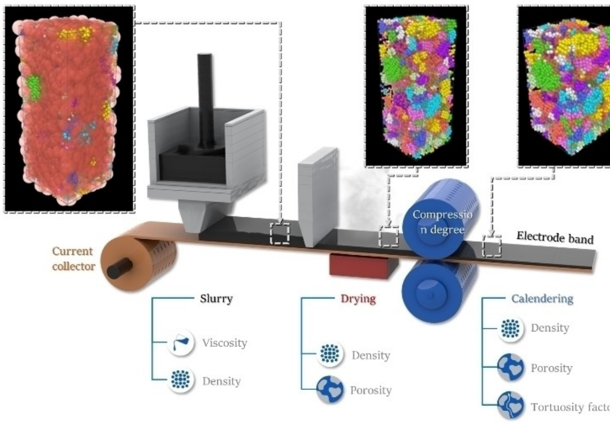

Figure 4. The ARTISTIC granular models for electrode slurry, drying and calendering, where some of the parameters used for their calibration and validation are indicated.

such as binder, and well-distributed nanometric particles such as carbon black, as a single entity, also in the form of particles. This approach has been proven to be general enough to be successfully adapted to different electrode chemistries.[26-28, 34, 38]

Additionally, another phenomenon studied in the ARTISTIC project is the electrolyte infiltration during the LIB cell manufacturing. We use the Lattice Boltzmann Method (LBM) which is a computational fluid dynamics technique that simulates fluid flow by discretizing the Boltzmann equation, describing the statistical behavior of particles in a fluid. LBM transforms complex fluid dynamics problems into manageable lattice operations, making it particularly effective for multiscale simulations, multiphase flows, and fluid-structure interactions. LBM accurately reproduces the behavior predicted by the Navier-Stokes equation. It is particularly well suited to describe liquid movement within porous networks. Regarding our application to study electrolyte infiltration, two main outputs can be obtained from our LBM simulations. The first one is the saturation curves, which allow the comparison between infiltration times for different electrode microstructures assessing the impact of manufacturing parameters on the required infiltration time. The second one is the local electrolyte distribution at each point within the pore network at the end of the process, allowing to identify sections that remain filled with air due to pores poorly interconnected to the others for example. Such undesired incomplete infiltration process effectively reduces the cell electrochemical performance and therefore is of high interest in the manufacturing process. The LBM has been used in the ARTISTIC project to perform electrolyte infiltration simulations in single electrodes and in representative sections of full cells,[39] to train ML tools for the generation of surrogate models,[40] and to analyze the effect on infiltration kinetics of having LIB cell electrodes composed of several layers of varying structural parameters.[41]

Another important phenomena studied in the ARTISTIC projects are the effects of manufacturing parameters on electrode performance,[35] mechanical effects,[38] and the benefits of having multi-layered electrodes with varying porosity.[42] In that sense, the ARTISTIC project developed several continuum models using the FEM method, since its versatility in solving a wide range of physical equations and its capability to describe irregular geometries. Therefore, FEM has revealed for us ideal for the simulation of electrochemical performance of the virtually manufactured electrodes (generated by the CGMD and DEM simulations and virtually infiltrated or not by LBM simulations). This process must explicitly consider mathematical descriptions of the electrochemical reaction kinetics (and eventually electrochemical double-layer formation) at the interface between AM and electrolyte, lithium diffusion in the AM, electronic transport in both AM and Carbon Binder Domain (CBD), electronic transfer between the AM and CBD, and lithium-ion transport in the electrolyte. As our electrochemical models are intended to describe the phenomena primarily at the mesoscale (*e.g.* volumes of $100\times100\times100\ \mu m^3$), the temporal and 3D space dependence at the micrometer scale is considered by meshing the electrode microstructures obtained in the previous manufacturing steps, without the need for assumptions related to particle size distributions, porosity, tortuosity factors and contact areas.[42] Additionally, the FEM has also been applied by us to simulate electrochemical impedance spectroscopy experiments under symmetric cell conditions -experiments typically used to extract the electrode tortuosity factor-.[42,43]

Physics-based models are a powerful tool when high-throughput experimentation is inaccessible, cost-prohibitive, or time consuming. Therefore, in this context, physics-based models are a core factor in the development of a digital twin.[44, 45] However, the main obstacle to the use of these models in digital twins is their above-mentioned computational cost. This prevents them from being used in completely autonomous loops that would respond in real-time to automatically extracted experimental data. One possible solution for overcoming this cost, besides the use of purely data-driven ML models or the use of further optimized High Performance Computing parallelization schemes, is the creation of surrogate models. ML-based models can be trained using physics-based modeling results, allowing them to bypass them entirely and further accelerating the optimization process. In this approach, demonstrated also by us, a large amount of physics-based simulations is recorded and used as training data for ML models.[1] While the production of data and training can be in some cases time-consuming, the resulting model is much quicker, being more suitable for real-time applications. Conversely, the disadvantage of this process is the limited extrapolation capability of the resulting ML surrogate models. The derivation of deep-learning surrogate models, mimicking the particle dynamics predicted by the physics based simulations, as demonstrated by us in a recent publication, offers both physical-awareness and computational speed for the manufacturing simulations.[46] This approach that we have proposed gives the promise to be a game changer towards the direct implementation of physics-based modeling approaches in digital twins.

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Model Parametrization and Experimental Validation

In order to validate scientific results it is crucial to design rigorous experimental protocols. An adequate experimental validation of a model is necessary to be able to affirm that it has been well tuned and is able to replicate the phenomena observed in experiments. The design of experimental strategies depends on the study objective and the model's complexity. For physics-based models, the validation approach is implemented by adjusting or comparing directly (by superposition) the modeling results with the the experimental data.[42,47,48] For data-driven (ML) model conception and validation, it is necessary to consider an extensive quantity of data to foster a satisfactory predictive accuracy.[45] While some models are more feasible to be validated or parametrized, others require more complicated setups. For instance, models to predict the risk of battery cell failure require to consider situations outside the box: consequently, they require complex strategies for conceiving experiments.[49]

For extracting experimental data relevant for computational models development, a wide diversity of characterization methods exist.[50,51] Typical experimental techniques for a model development that we use to build our manufacturing and performance models include Scanning Electron Microscopy (SEM), particle size analyzers and Computer Tomography.[—33,35-37] In addition, densimeter, electronic mass balance, thickness gauge, and porosimeter are employed for tuning the electrode manufacturing models for achieving correct output electrodes characteristics, such as density, mass loading, thickness, and porosity.[35] Conductivity of the electrolyte and of the electrode, both needed in our performance models, can be assessed by using the voltage response from a DC current.[52] Electrochemical techniques such as electrochemical impedance spectroscopy, galvanostatic intermittent titration technique (GITT), potentiostatic intermittent titration technique (PITT) and galvanostatic cycling with potential limitations help us to validate the tortuosity factor of our predicted electrode microstructures, to inform our electrochemical models with open circuit voltage, diffusion coefficients, and calibrate them for correct cell capacity, energy, and power densities.[43,53,54] Additional techniques, such as rheometry and micro-indentation can be used to calibrate and validate our electrode slurry and calendering models, through the experimental viscosity vs. shear-rate curves and electrode mechanical properties (elasticity and plasticity), respectively.[33,35]

Within our ARTISTIC project, our physics-based models are calibrated and validated against experimental results obtained at different manufacturing process steps. For instance, the CGMD-calculated 3D slurry microstructure model is parametrized and validated by experimental slurry viscosities and densities for different active material chemistries, particle sizes, formulations and solid contents. An example is provided in Figure 5 for slurries made of NMC111, carbon black, PVdF binder and NMP as solvent. Despite some minor deviations occurring at low shear rate, we can observe a significant similarity between the model and experimental data, demonstrating the capacity of the model to capture the influence of formulation and solid content on the slurry viscosities for different shear rates.[33]

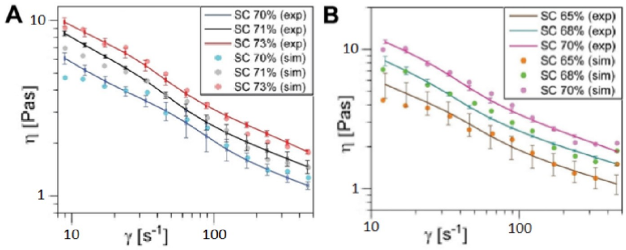

Figure 5. Viscosity vs. shear rate plot for slurries made of (A) 96:2:2 weight % and (B) 95:2.5:2.5 weight % of NMC, carbon black, and PVdF, for different solid contents. The lines and dots represent the experimental and simulated results, respectively. The error bars correspond to the experimental results. Figure adapted from Ref.[33]

Additionally, the CGMD and DEM predicted dried and calendered electrode microstructures are calibrated and validated by comparing properties such as the electrode porosity (Figure 6b) using the mass, density, and thickness of the virtual and real electrodes, their tortuosity factors, their electrical conductivities, etc. The mechanical properties (arising from micro-indentation experiments and simulations) can be also used: in Figure 6a an example is shown with almost equivalent curves with a small standard deviation.[35,36]

Regarding the electrochemical behavior of electrodes, several 4D (time + 3 spatial dimensions) electrochemical models, using the electrode microstructures virtually generated by our manufacturing process model, have been developed in the ARTISTIC project to capture the (de)lithiation and charge transport dynamics of electrodes in half, full and symmetric cells. For the latter (for example) the model predicts the electrochemical impedance spectra in NMC porous cathodes with a trend (in terms of influence of electrode formulations) that compare very well against *in house* experimental results.[43] We have, for example, studied the impedance response and the inter-phase conductivity relations after electrodes calendering.

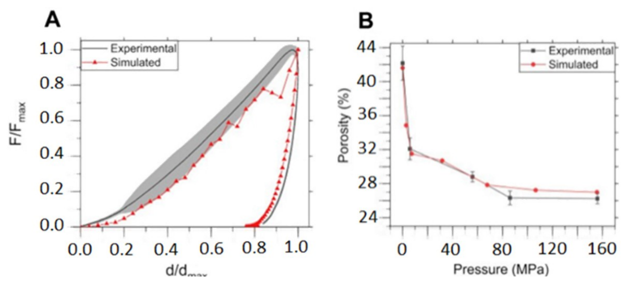

Figure 6. Comparison between the experimental and simulated data (black and red line, respectively) for A) the mechanical validation of our model from a micro indentation curve. Force and displacement of the micro-indentation were normalized relative to the maximal force(F)/displacement(d). B) Modeling/experiment comparison of the evolution of the electrode porosity as a function of the applied calendering pressure. Figure adapted from Ref.[35]

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Our 4D model considers different electrode components electronic conductivities, ion diffusion/conduction within the pores, giving explanations of the experimentally observed deviations from the 45° slope in the Nyquist plots.[—43,55-57]

Finally, we have used experimental electrochemical performances to validate our 4D-resolved electrochemical models, *e.g.* for different electrode formulations and calendering degrees (see Figure 7).[54] This model demonstrates that an effective carbon and binder distribution within the electrode greatly influences the conductive electronic network, allowing full electrode utilization. Our electrochemical model, informed with the electrode microstructures predicted by our manufacturing simulator, showed good agreement with the experimental data for the different cathode formulations, calendering degrees, and C-rates.

It is worth to mention that, in general in a physical model, it is difficult to know the minimum amount of experimental data needed for its appropriate validation. Depending on the goal of the model, and how robust one wants the model to be, we can define a suitable amount of data to validate it. As an example, we can define model robustness when it is able to replicate more than one parameter simultaneously, like porosity and tortuosity factor. If a model is only able to predict one parameter is less robust, but still useful depending on its application. In general, the required amount of experimental data should be enough to capture the nature of the phenomena we want to model. For example, in the experiment described in Figure 5, the calculated viscosities for 13 shear rates per solid content (SC), are experimentally validated. In that case, we consider that the chosen 13 points are enough to cover the trend displayed by the viscosity vs. shear-rate curve, and the range of shear-rate values of interest.

Thanks to the complete validation and parametrization of models through experimental results, simulation models could ensure the optimal microstructure or electrochemical performance parameter set. Additionally, simulation models also contribute to understand the experimental results by physics-based rationalization. In addition, experiments can help to determine the impact of input parameters on the model outputs and prioritize the optimization or use of parameters. The capability of our research group to have direct access to the battery prototyping line of the French Network on Electrochemical Energy Storage (RS2E)[58] -located in the same building- has been very positive towards the development of reliable and physical-sound manufacturing and electrochemical battery cell models.

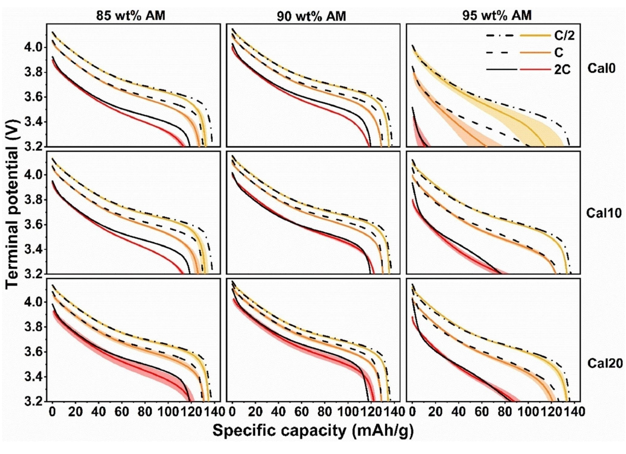

Figure 7. Comparison between the experimental and simulated results for the discharges at 0.5, 1, and 2 C (yellow, orange, and red colored against black lines, respectively) for the corresponding formulations and calendering degrees (see columns and rows, respectively). Figure adapted from Ref.[54]

Machine Learning

ML algorithms have the ability to learn patterns from data without being explicitly programmed.[45] In supervised learning, algorithms are trained with a given set of labelled data and learn how to map the input to the output values by minimizing the error between the predicted and the actual output. In unsupervised learning, the model is provided with un-labelled data in which it looks for hidden or underlying patterns. Supervised learning can be used in classification and forecasting problems, and unsupervised learning can be used for tasks such as clustering and dimensionality reduction, which makes ML a rapidly growing field with a wide range of applications. In Chemistry and in Physics, ML algorithms have been proven to be a magnificent tool for the prediction of material properties,[59,60] the modelling of chemical reactions,[61] the analysis of experimental and simulation data[62] or the application of reverse engineering.[63,64] High-throughput experimentation (HTE) allows the execution of large numbers of experiments in parallel while requiring less effort per experiment when compared to traditional means of experimentation. Even though, HTE by itself, it can be seen as a quicker trial & error approach, when combined with ML techniques has the potential to speed up and improve exploration and optimization processes.[65,66]

ML has become increasingly important in the battery field due to its ability to handle multidimensional datasets.[1,11,—67-71] ML has emerged as a powerful tool to simplify complex problems at a less expensive computational cost. However, the lack of reliable experimental or simulation datasets restricts the number of ML algorithms that can be efficiently applied, despite the numerous initiatives to expand battery data.[68] As a consequence, the use of ML in the battery field is still in progress and is a promising tool that can contribute significantly to the next generation of batteries.

In this scenario, the ARTISTIC project has explored and implemented the use of ML algorithms in the modelling development of battery manufacturing process, reducing waste and increasing efficiency. Some of the pioneering applications we developed in the ARTISTIC project are the design and development of optimization algorithms of manufacturing variables[1,72] and the prediction of the impact of manufacturing parameters on electrode properties.[34,46,73] LIBs and their manufacturing process are complex and therefore entail unique challenges to the applications of ML.[45] As the battery industry and research, and consequently, their resulting battery data, continue to grow, the importance of ML will only increase. With

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its ability to optimize manufacturing processes and improve battery performance, as we demonstrated in the ARTISTIC project, we believe that our ML models can be important tools for manufacturers looking to stay competitive in this rapidly evolving field.

In the ARTISTIC project, several ML methods have been applied for first time to improve the knowledge of battery cell manufacturing: for example, k-means, Support Vector Machine, Decision Tree, neural networks and Gaussian Naïve Bayes for the prediction of electrode properties based on the slurry formulation and coating conditions, Sure Independent Screening and Sparsifying Operator (SISSO) to track the effect of manufacturing processes over a wide array of mesoscale electrode properties.

We applied text-mining techniques to facilitate the process of reviewing the literature published in the battery field[—74-76] and compared the performance of different ML algorithms to uncover the interdependencies between manufacturing parameters and final electrode properties.[73,77-79] Additionally, we also used ML techniques to parametrize computational models at the mesoscale[33,34, 72] predicting electrode properties.[1,35] Figure 8 describes how our Bayesian multi-objective optimization technique works to predict which manufacturing parameters to adopt in order to reach optimal textural and performance properties of LIB electrodes and cells.[1,72] Consequently, the ARTISTIC project has shown that ML can be used to improve the performance of battery cells in a significant number of ways, with a special focus on inverse design, *i.e.* at predicting which machinery manufacturing parameters to adopt to reach electrodes or cells with desired properties.

Within the ARTISTIC project, we have also generated an extensive database containing a broad range of experimental and simulation data. This database contains information about numerous experiments and simulations with different chemistry formulations and parameter choices. Data is the foundation of ML, since more high-quality data generally leads to better ML models. To ensure the accuracy and reliability of this database, we employed rigorous data collection and preparation methods, and the data was then cleaned and pre-processed to remove inconsistencies or errors. We store our data in a structured database. For example, correlation matrices can be used to identify and visualize interdependencies (Figure 9). Pearson correlation coefficients always range between −1 and 1 and the sign of the coefficient indicates the direction of the relationship, with a positive value meaning that the variables change together in the same direction, while a negative value means they change together in opposite directions. A Pearson correlation coefficient of zero means that there is no linear relationship between the variables. In Figure 9, the variables represent different used materials in the formulation of experiments. White fields mean that the two materials have never been used together in a same experiment.

Mixed and Virtual Reality

Mixed Reality (MR) is a technology that overlies interactive holograms in the real environment. By wearing a MR headset, *e.g.* the HoloLens 2 from Microsoft, the user can interact with both virtual and real objects in real time, as we can see in

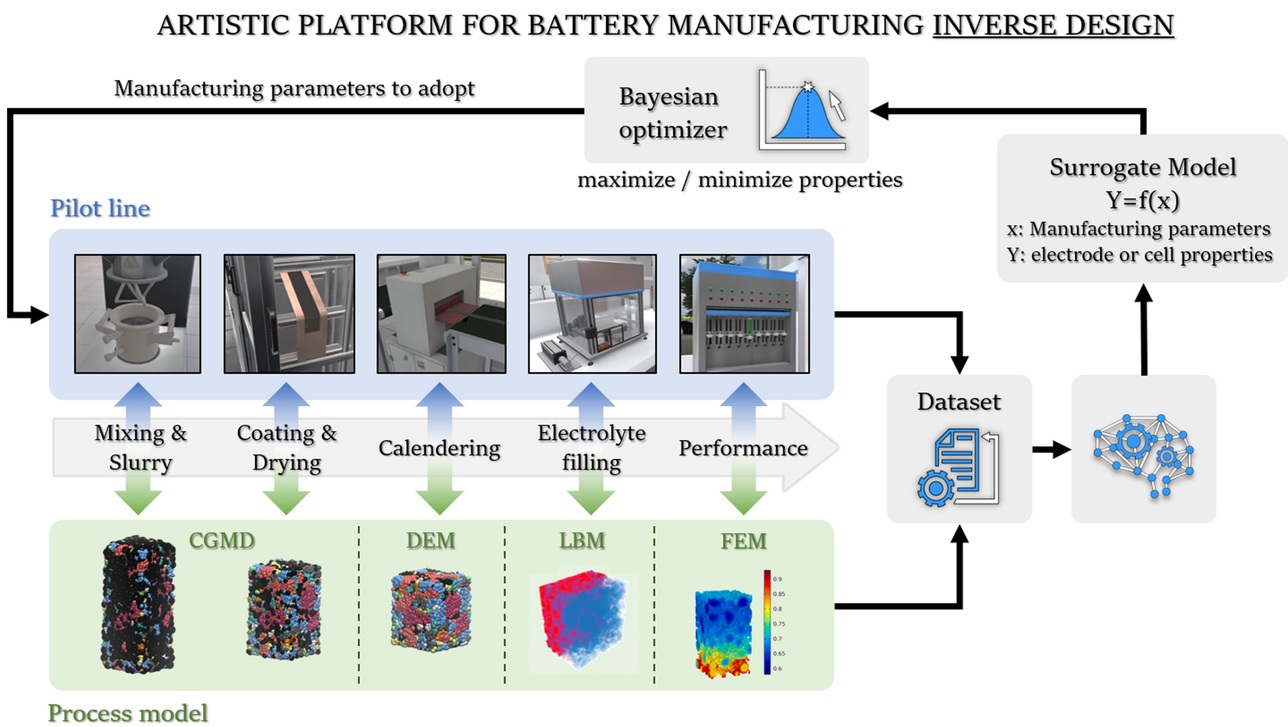

Figure 8. Scheme representing how Bayesian optimization techniques were used in the ARTISTIC project to optimize battery manufacturing process parameters. Synthetic data (produced by the physics-based manufacturing modeling chain) and experimental data was used to train surrogate models, and then Bayesian optimizers were used to determine the best input parameters that optimize output battery properties. Read Ref.[1] for more information.

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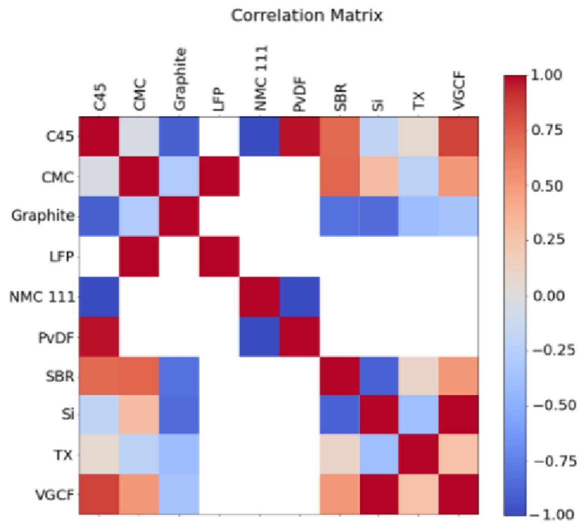

Figure 9. Example of Correlation Matrix for some of the materials used in the formulations investigated in the ARTISTIC project.

Figure 10, MR frees up the hands users and can enhance the environment by implementing useful information to help decision-making in real time.

MR has strong potential, particularly in the field of activity assistance and training. For example, it can make possible to observe and advise technicians on their activities directly in the place of work to increase productivity, particularly for complex tasks.[80] In our viewpoint, this technology has also tremendous potential to be used to allow users to consult data and provide feedback, which is very important for assisting technicians and engineers in prototyping or pilot lines. As shown in other application domains, the user can use this technology to access information about some work in progress.[81] It also helps reducing the number of people involved in critical tasks.[82]

We have developed a novel training and assistance tool for the manufacturing of LIB electrodes using MR.[83] This tool allows the user to enter, by interacting with holographic panels, useful information (*e.g.* formulation, manufactured electrode thickness) in a database and then keep track of his/her ongoing experiments right in the place of work. This allows the user to be more efficient in his/her scientific work. At the same time, it was essential to develop a user-friendly system, intuitive interfaces and avoid typical inconveniences associated with immersive technologies, *e.g.* simulation sickness and cognitive load. As part of the ARTISTIC project, the associated SMARTISTIC project (also funded by the European Research Council) and the STARS project (funded by CNRS), we performed a number of ergonomic studies to gather information about how the device is used in real-life situations, in order to design a tool that corresponds to real-life activity in the experimental lab. As part of the user tests, we investigated the device's usability, simulation sickness and cognitive workload.

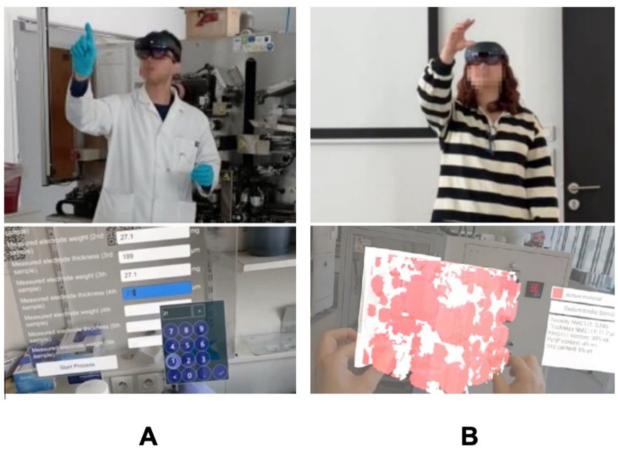

Figure 10. One of our lab researchers is using our Mixed Reality tool with HoloLens glasses while he is performing an experiment. He can inform, by interacting with a holographic notebook, about the experiment he is doing, and this directly in the place of work. B. Trainee using our Mixed Reality tool in HoloLens to learn about LIB electrode microstructures.

We asked several professionals (engineers and students) to manufacture electrodes assisted by our Mixed Reality application in HoloLens 2. We found that users of the device were satisfied and enthusiastic about using it and they showed no symptoms of simulation sickness. For detailed investigations on the usability of our Mixed Reality tools, the readers are invited to consult our previous papers.[83,84] Thus, during this work, we led the use of MR technologies in the battery field, and introduced this technology to facilitate data collection. At the same time, we worked on the development of a training feature,[83] supported on textual holographic panels, being aware that, in the battery industry, gigafactories present a huge demand for skilled and operational labor, and the successful implementation and production of gigafactories in Europe depends on the ability of countries to supply sufficient skilled labor. With this training module, we aim to train lab technicians and researchers in the realization of experiments, regardless of their previous experience.

Virtual Reality (VR) is a computer-generated technology to simulate and/or recreate an interactive three-dimensional environment thanks to the use of special electronic equipment, such as headsets, gloves, and motion sensors. We developed training tools based on VR and on the coupling between VR and MR that provide MSc. students with digital immersive and semi-immersive environments to learn some of the theoretical fundamentals of the battery manufacturing process.[32,84] Thanks to these tools, users can learn about the main machinery parameters involved in a battery manufacturing process without an intensive need for external supervisors and in a safe environment, thus optimizing resources.

Open Science and Industrialization

Battery experts generate a very significant amount of experimental and simulation data, which is critical for a deeper understanding of the physical, chemical and electrochemical processes and for advancing the technology. However, this data should be properly reported[76] and processed to minimize errors and guarantee the reproducibility of the findings, as well as for their correct interpretation. The appropriate planning,

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collection and storage of this data are crucial for the validation of results and to increase the impact and visibility of the findings. The right data preservation is also essential to enable its future use in ML applications. The Data Science field is in continuous growth, with new ML algorithms and techniques being developed regularly, so, in other words, data preservation can make possible the application of future methods able to provide information that is still unknown today.

As scientific research is data-driven, progress in scientific knowledge becomes intimately tightened to data availability, and this data, in modern science, is often stored in digital format, which makes its redistribution easier. By sharing data and the computer programs used in its analysis, other researchers can verify one's findings to catch potential experimental or computational errors, determine the generalizability of the results to different systems or extend the knowledge of the scientific community by further post-processing. However, the lack of infrastructure to store large datasets and the lack of time and resources for training about good practices can make permanent data storage and sharing difficult, resulting in shortage of robust databases. This problem can be worsened by the lack of widely accepted regulations and standards that promote a common understanding of how information should be stored, for, *e.g.*, promoting the widespread use of certain files and data formats. Furthermore, strict confidentiality rules in companies or research centers do not promote the free publication of scientific data, limit the guidance to the academia researchers towards pertinent studies and, at the same time, making the possession of data a comparative advantage that only the privileged owners can and should exploit. However, these confidentiality restrictions can be overcome through collaborative approaches between industry and academia, in which respective researchers share their private data to boost research.

It is evident that collaborative approaches between research centers or academic labs and industries can boost technological innovation and progress in the battery field. This collaboration can help to bring together different perspectives and expertise, which can result in new ideas and solutions and can provide the needed resources and experience to move from research to development. Figure 2 shows the main differences between industrial factories and research labs. As we can see, labs incorporate a lower degree of automation due to the large parameter space studied since their activities aim to develop new research lines (out of predefined parameter spaces) and proof of concepts, while factories are close to market and focus in already known processes, so both provide complementary knowledge.

The commercialization of products arising from ideas and research performed in universities through industrial partners or start-ups created for that purpose can accelerate and improve progress and innovation,[85] and make research findings reach society in an effective and efficient way.[86,87] Start-ups and companies have a higher experience in development and commercialization. They also typically have greater resources to produce shorter-term technological innovations and near-term social impacts. Thanks to this, they can help make research findings reach society more quickly, as they are motivated to get their products and services to market as fast as possible.

In this scenario, it can be noticed that public research centers and industries have different policies regarding Intellectual Property (IP) practices. While research centers can make scientific research, data and methodology openly accessible to all to promote transparency and collaboration, industrial actors usually prioritize proprietary research and profit, leading to restricted access to scientific findings to avoid potential conflicts of interest or favor competitors. However, although open science fosters great trust, collaborative approaches and inspiration towards new ideas, it can also produce a loss of competitive advantage, thus discouraging investing. For example, if companies anticipate that research findings by a potential academic collaborator will be freely accessible to competitors, it might happen that they may be less willing to allocate resources to establish a partnership with it, reducing overall investment in scientific advancement and, consequently, economic development. Therefore, while Open Science needs to be promoted in research labs, it is not common in private organizations, but this still promotes innovation through competition.

In the battery industry, there is a significant need for fundamental research that addresses the challenge of understanding the complex mechanisms occurring during the battery cell manufacturing process. For this purpose, there is the need to implement strategies to perform experiments and numerical physics-based simulations in a synergistic manner, and exploit this data through ML algorithms for accelerating the optimization. Therefore, the production of extensive databases and the development and application of robust and modern ML algorithms is the right way to accelerate the optimization and automation of the battery manufacturing process. In this context, databases and workflows to exploit experimental and simulation data can provide industry with a valuable resource to develop new products and services or improve existing ones.[88] However, the lack of a standardized methodologies can lead to inconsistencies that make data comparison and model validation challenging in this scenario but, in this Concept, we recommend the adoption of standardized data collection and reporting protocols across laboratories. This could include agreed-upon formats for data presentation, detailed documentation of experimental conditions or the common use of materials or techniques.

Additionally, the right application of ML algorithms through already developed, optimized and documented software solutions can help industry at reducing production scrap rates and consequently production costs. Thanks to this, research centers and industries could have direct, fast and guided access to results arising from fundamental research, thus increasing its impact on society. Governments and universities have been promoting and stimulating economic activities arising from fundamental research.[89] This can be done by licensing IP to businesses, which can then use the new technologies to develop new products and services, by creating start-ups that commercialize the results of the research that has been done, by providing consulting services to businesses and govern-

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ments or by training the next generation of scientists and engineers. Thus, the transfer of knowledge obtained from scientific research to industrial partners or companies is increasing, and it is not an exception in the battery field, in which many companies have been created in the last years from fundamental research in universities. These start-ups work on the development of the next generation of batteries by using new chemistries and formulations. However, it is important for the battery industry to receive offers of digital tools that can accelerate the optimization of their battery manufacturing processes, from the lab to the factory. In this direction and based on the research outcomes of our unique ARTISTIC initiative, a new start-up company is being created to help with this problem, with more information to be released soon. This new start-up will aim at commercializing a software product to help with the acceleration of the optimization of the battery manufacturing process and the training of new technicians, operators and researchers.

In order to succeed in making the transition from scientific research to industry, it is necessary to change the scientific mindset. While in scientific research, the focus is on discovery and understanding, in industry, the focus is on development and commercialization and making economic profit from it to compensate for all efforts. Therefore, when transitioning to the industry, the new focus will have to be on the customers, and all objectives and milestones should be defined to meet the needs of potential or existing customers. This means that it is necessary to understand their main points and concerns, as well as the existing solutions that try to address them. As a consequence, new start-ups should conduct in-depth studies to evaluate their possibilities in the market and the way they organize their business. Figure 11 shows a summary of the path to move from fundamental research to commercialization.

The preparation of a solid business model and market study is essential. A business model is a plan that summarizes how the start-up will make money and includes details about the value proposition that the start-up can offer to its potential customers, the characteristics of the potential target customers, the channels to reach customers and the interactions with them. Additionally, important financial details about all the revenue streams and future costs will also be analyzed and key resources, activities and partnerships will be defined to guarantee that the start-up can deliver its value proposition. The business model is a valuable document for planning, decision-making, and communication, which requires all co-founders to converge in all critical ideas and define together future steps. Similarly, a market study is a piece of research aimed at understanding the target market, especially the needs, locations and expectations of potential clients, identifying the competition and their strengths and weaknesses, and the trends in the market. This information is crucial to set realistic goals and develop products and services that meet the needs of potential clients more effectively. However, the business environment and market are not static and can change, so it is still also important to be prepared for it and be able to adapt the work to meet these changes.

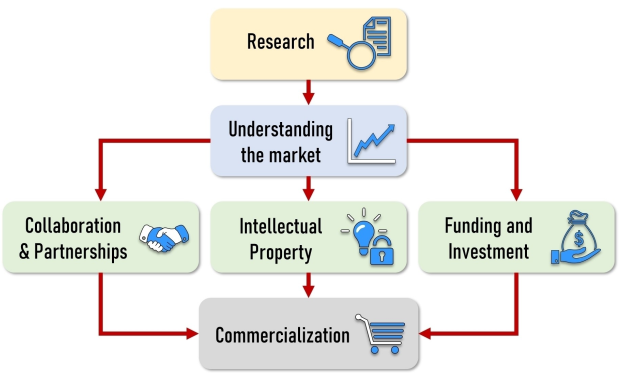

Figure 11. Scheme summarizing the needed actions to move from fundamental research to commercialization. First, it is necessary to produce scientific results, and then they have to be turned into some product or service. The next step is to search for collaborators and funding to increase the resources and accelerate the development and file patents or register licenses to protect the product before its commercialization.

Once the business plan and market studies are well defined, it is necessary to secure funding to conduct additional Research and Development (R&D). Furthermore, when and where needed, increase the number of team members and develop the product or service to bring it to market. Funding can come from a variety of sources, including personal savings, loans, grants, and investments. Depending on the country in which the start-up will have its headquarters, there will be a different number of organisms, including both public and private institutions, willing to offer investment. In the case of private institutions, they might ask for a part of equity in exchange. Thus, once the problem is well defined, the goals are set, the team is built and the resources are already available, it is possible to implement the final work needed to bring the results from scientific research to market and society. Additionally, collaborations and partnerships can also play an important role in the transition to commercialization, since they can provide valuable experience to the teams, increase the resources and mitigate risks. Finally, it is also important to protect the products or services before their commercialization, so negotiations on IP are essential, and patents or other licenses filed for their protection become mandatory. A similar path to all this is the one we are currently following to bring the ARTISTIC initiative results into the market and respond, in the most efficient manner, to the interest that we have received from the industry sector.

Conclusions

Within the ARTISTIC research project, we developed dozens of novel simulation models and ML algorithms as well as innovative VR/MR experiences to provide insight into the physicochemical phenomena occurring during battery cell manufacturing process at different length and time scales. The ARTISTIC project produced proof of concept software to reduce the time and cost of battery cells development while improving their performance and reliability, in particular thanks to physics-based manufacturing process modeling and ML. For instance, in

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the ARTISTIC project, we developed, calibrated and experimentally validated 3D digital physics-based models capable of simulating the manufacturing processes of battery electrodes, and ML models and multi-objective optimization algorithms to predict the influence of electrode manufacturing parameters on battery cell properties and the manufacturing parameters to be adopted in order to have electrodes with optimal properties. We also used MR and VR technologies to facilitate training and data exploration in our lab, being the first research group to bring these technologies to the battery field. However, although our scientific findings have demonstrated the strong potential to push battery development to the next level, they are not yet able to do it by themselves and a strong interaction with software engineering and battery industry is needed, in order to turn these scientific findings into commercial products or services that meet specific needs in the market and industry. This transition from fundamental research to commercialization is a complex and challenging process, and researchers are not usually prepared for it, so they have to be trained and/or surround themselves with the right industry and business people to perform together all needed actions. For this transition, it is necessary to perform market and business studies to understand the market dynamics and the potential demand for the new product or service arising from research results. It is also necessary to protect the product with licenses and patents and search for collaborators to increase resources, and for funding in order to accelerate R&D strategies. Thus, it is necessary to constitute a talented team with complementary profiles, such as engineers, business persons and lawyers. As indicated in this Concept, it is important to promote collaborations between public research centers and private companies or start-ups. Although sometimes it can be difficult to find a good balance between the protection of IP and the need to publish research findings, the development of IP agreements defining the ownership, the management and the use of IP can satisfy both sides. These agreements can include terms for delayed publications, allowing companies time to secure IP protection before research results are made public. This approach ensures that the company's competitive interests are guaranteed while still enabling academic researchers to fulfill their publication goals. In our laboratory, we are working in this direction to commercialize our innovative ARTISTIC digital tools and facilitate industrial actors the access to our knowledge and experience to promote their activities and push the battery technology progress forward. More information about the start-up that we are creating for this will be disclosed soon.

Acknowledgements

A.A.F. and J.F.T. acknowledge the European Research Council for the funding support through the ERC Proof-of-Concept grant No. 101069244 (SMARTISTIC project). A.A.F., L.D. and J.F.T. deeply acknowledge the CNRS INNOVATION RISE programme for the support. A.A.F. and F.M.Z. acknowledge the European Union's Horizon Europe research and innovation programme under grant agreement No. 101069686 (PULSELiON). A.A.F. and D. E. G. acknowledge the funding support of the French National Research Agency under the France 2030 program (Grant ANR-22-PEBA-0002, PEPR project "BATMAN"). A.A.F. and D.Z.D. deeply acknowledge the European Union's Horizon 2020 research and innovation program for the funding support through the European Research Council (grant agreement 772873 ARTISTIC project). A. A. F. and L. D. deeply acknowledge the Programme Maturation of CNRS and CNRS Innovation for the funding support of the STARS project. The authors acknowledge Dr. Francisco Fernandez, Utkarsh Vijay and Soorya Saranavan, from Prof. Franco's group, for useful discussions. A.A.F. acknowledges the Institut Universitaire de France for the support.

Conflict of Interests

The authors declare no conflict of interest.

Keywords: Rechargeable batteries · Manufacturing · Digital twins · Computational modeling · Artificial intelligence · Start-up

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Manuscript received: June 14, 2024
Revised manuscript received: September 6, 2024
Accepted manuscript online: September 12, 2024
Version of record online: November 28, 2024

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