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Editorial to the Special Issue: How to Reinvent the Ways to Invent the Batteries of the Future – the Battery 2030+ Large-Scale Research Initiative Roadmap

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The demand for batteries is accelerating way beyond what was foreseen only a few years ago. This rapid transition towards a more electrified society is a crucial dimension of reaching a carbon-neutral economy as established in the strategies of the European Commission's (EC) green deal, the Fit for 55 package,[1] and the green recovery plans.[2] Batteries are a core technology to transform the energy sector, mainly for large-scale energy storage and the transportation sector, primarily for passenger and commercial EVs. Furthermore, batteries play a vital role in innovation and efficiency in a wide range of other sectors and industries with applications like portable electronics, including electric scooters, power tools, autonomous robotics, surveillance and delivery drones, aviation, medical devices, sensors, etc. However, ultra-high-performance batteries are needed to harvest the full potential of battery-powered innovation in these areas. Equally important is reaching significantly improved battery cost-performance ratios with longer life, enhanced reliability and safety, and more sustainable and scalable approaches using less critical raw materials. These are the batteries that can deliver capacities well above those of the highly successful lithium-ion batteries that are well-performing at a low cost today. To go beyond the state-of-the-art of this battery chemistry (article number 2102904), more sustainable, more scalable, and faster research approaches are required that simultaneously consider the need for novel materials and new concepts for faster exploration and screening and scaling-up of these (both experimentally and theoretically). At the same time, novel research approaches must also integrate the synthesizability, manufacturability, and recyclability of such batteries directly into the discovery and development process to reduce environmental footprint and cost. This is, in essence what this special issue is about. The scientific arguments comprising the Battery 2030+ Roadmap and the different parts of it are described in-depth, highlighting the challenges that need to be overcome for realizing the vision of developing the scientific insights and transformative research infrastructure that is needed to supply the future demand for sustainable, ultra-performant and smart batteries. And this is faster than ever before in scientific and industrial history. For this, new tools and platforms will be realized through the new digital era with artificial intelligence paired with high-throughput simulation, synthesis and characterization techniques are the foundation. The realization of a modular battery Materials Acceleration Platform (MAP) is an essential part of this strategy, as described in the roadmap (article number 2102785) and in this special issue (article number 2102702) (article number 2102638).

Globally, there is a range of battery roadmaps and strategic action plans, all more or less focusing on different chemistries and new battery concepts outlining both timelines and expectations in terms of performances. Among the most important

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ones for Europe is the SET-Plan action 7,[3] where different actions have been described for Europe to become more competitive in this sector. Since this was published in 2018, the ETIP Batteries Europe recently launched six different roadmaps along the full battery value chain,[4] describing the long-term expectations for future battery chemistries, which has a more updated view on the battery landscape compared to the earlier presented SET-Plan. The European battery partnership BEPA – Batt4EU, launched in 2021, has also published a strategic action plan.[5]

The Battery 2030+ roadmap takes a different approach[6] and aims at the development of data-assisted transformative tools and methodologies to accelerate the procedure of identifying and discovering novel battery materials, concepts, cell designs and smart functionalities. We are aware that for all these dimensions, we must consider and integrate manufacturability and recyclability from the start. By formulating a "chemistry neutral" approach we will rely on concepts like transfer learning and the modular nature of the MAP to open a new path to all kinds of ultra-high-performance batteries. This initiative can therefore be seen as an enabler of the emerging battery chemistries as described in the specials issue, as well as in other roadmaps.[7] The overarching concept and research idea is to **"reinvent the way we invent the batteries of the future"**.

The development of a chemistry-neutral toolkit of enabling technologies for novel battery materials and concepts emerges as the core of the roadmap effort (article number 2102694) (article number 2102698). This transformation can be reached only by realizing its long-term vision with a perspective even longer than ten years.

We are acutely aware that the ability to understand, control and design of battery interfaces will play a central role in the way forward (article number 2102687) (article number 2102678). Many unwanted side reactions are initiated and evolve at the different interfaces in batteries, affecting power and energy of the battery cell as well as life-time and safety. Careful consideration of these aspects is particularly important for new battery chemistries with higher energy content than for lithium-ion batteries. To accommodate the characteristics of different chemistries, the tools for the digitalization of large amounts of data must be employed to fully exploit the potential of machine learning and artificial intelligence to invent novel materials and better engineer interfaces to increase the life of demanding new chemistries (article number 2102698) (article number 2102652).

By introducing sensors and smart functionalities directly into the battery cells, quality, reliability, lifetime, and safety can be improved while complex reactions can be accommodated at low cost, without hampering manufacturing or recycling processes. This will be particularly important to enhance the competitiveness of more unstable (future) chemistries in terms of stability with today's lithium-ion batteries. Battery 2030+ addresses these challenges in an ambitious long-term vision paired with novel ideas on how to introduce self-healing components into the battery cell design (article number 2102652).

Sensors have for some time been utilized in battery packs for monitoring global reactions like temperature variations, pressure, etc. Introducing sensors into a battery cell takes the smartness further by pinpointing details in degradation of interfaces, hot-spots for thermal runaway and long-term degradation processes. In its vision on sensor development, the Battery 2030+ roadmap addresses the challenge to stop these processes preemptively, i.e., before they have reached a level beyond repair, by leveraging the generative deep learning spatio-temporal models described in the Battery Interface Genome (BIG) part of the roadmap and this special issue (article number 2102785). A smart sensing system could furthermore support future efficient recycling and repurposing. In this special issue, the state-of-the-art and the prospects of batters sensing will be discussed.

Self-healing is studied in many fields beyond batteries. We envision that approaches developed for drug-delivery could be repurposed for batteries as well. Here, the "drug substance" is encapsulated into a host structure and released by either an external or an internal stimulus. The external stimulus could be triggered by a sensor positioned within the battery cell detecting the onset of a degradation mechanism. The internal ones could be a chemical reacting at a certain potential, from mechanical variations in particle expansion or contraction. Other internal stimuli could be functional groups anchored on the electrode surface, or multi-layered components of molecules that can react when electrode particle cracks due to long-term cycling or prevent degradation of the electrolyte. Examples of what these self-healing components could be for batteries will be described in this special issue (article number 2102652).

Is it possible to define long-term research strategies at the fundamental level that also includes applied activities such as battery cell manufacturing and recycling? Our profound answer to this is yes! In two papers (article number 2102696) (article number 2102917) we share our view on how digitalization tools and smart battery functionalization can be beneficial, and even necessary for the development of cost-effective and low carbon-dioxide emission processes to increase the efficiency, sustainability and the recoverability or recycling of the batteries.

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Conflict of Interest

The authors declare no conflict of interest.

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