

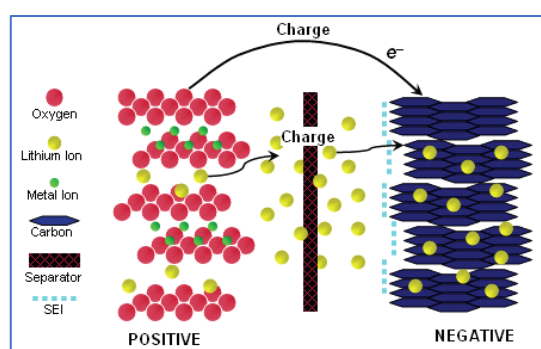
# Batteries for electrochemical energy storage

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## Introduction

Electrochemical energy storage in the form of rechargeable (secondary) batteries holds great potential in a range of applications, covering many aspects of the future needs for mobile and stationary energy storage. Relative to other storage technologies <sup>1</sup> like, e.g., thermal energy storage, electrochemical processes can operate isothermally and thereby avoid the Carnot limitations.

### Battery facts: Lithium ion (Li-ion) batteries



A rechargeable lithium battery cell consists of a positive and a negative electrode separated by an electrolyte and normally a separator membrane to avoid short-circuiting the battery cell. The charge is carried by lithium cations in the membrane and by electrons in the outer circuit.

Upon charge, electrons are moved from the positive to the negative electrode and upon discharge the process is reversed.

The positive electrode typically consists of a transition metal oxide (e.g.  $\text{LiCoO}_2$  (LCO),  $\text{LiMn}_2\text{O}_4$  (LMO)) or other transition metal compounds (e.g.,  $\text{LiFePO}_4$  (LFP)). The negative electrode is usually carbon (graphite) which may intercalate lithium up to  $\text{LiC}_6$ . One of the promising new anode materials is silicon, where more than four lithium atoms may be intercalated per silicon atom (3).

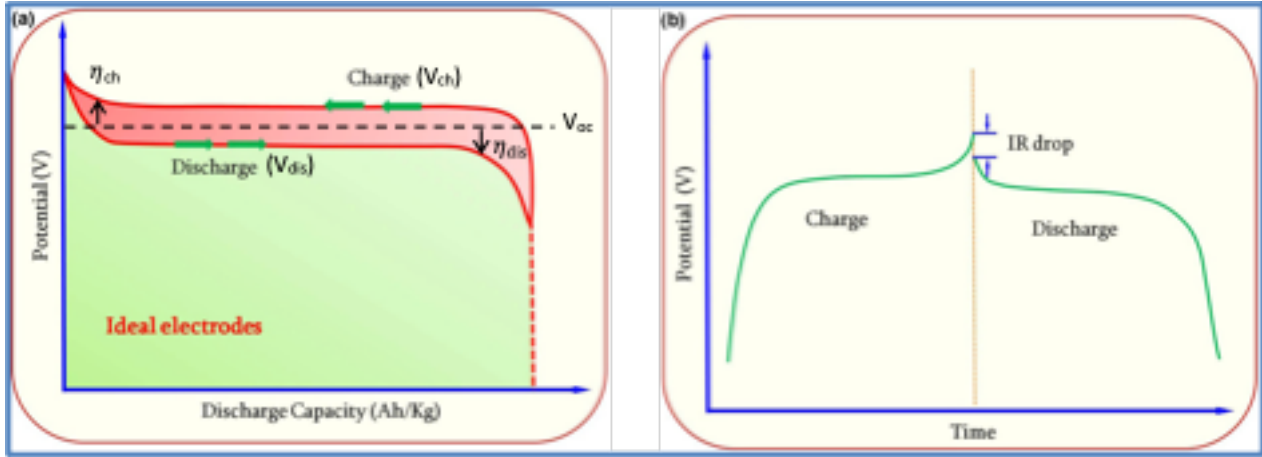
The potential applications for batteries range from portable consumer electronics such as mobile phones and laptops, over applications like electric scooters, battery electric vehicles (BEV), truck lifts, and boats and ferries, to large-scale grid-based applications for, e.g., short-term load balancing of fluctuating, renewable sources like wind and solar energy. In comparison, areas such as aviation, heavy-load, long-range transportation of goods, and seasonal energy storage require radical technological improvements and remain out of range of existing battery technologies. The diversity of the near term applications also place very different requirements and potential showstoppers on the batteries, e.g., in terms energy and power density, charge/discharge rates, durability, cycle and calendar life, price and safety <sup>2,3</sup>.

This chapter introduces the fundamental battery concepts and the specific needs and challenges of current and future battery technologies, focusing specifically on mobile and stationary applications. The general needs in a European and global context are very similar, and particular emphasis will be placed on the role of batteries in the energy sector and the related charge/discharge rates and efficiency, as well as durability and safety <sup>4</sup>. Fundamental materials challenges and development needs will be discussed for a number of specifically promising battery chemistries, specifically lithium-ion (Li-ion), all-solid-state batteries (ASSB), and beyond Li-ion such as multi-valent batteries, e.g., Mg-ion, metal-sulfur, and metal-air batteries. Particular focus will be placed on the current status and emerging battery chemistries and their role in future applications and integration in the energy infrastructure, and how novel AI-assisted

procedures for closed-loop optimization (CLO) and discovery of battery materials and cells can accelerate the development and performance of new batteries <sup>5</sup>.

## Battery Basics

A battery consists of one or more interconnected electrochemical cells, each giving a current ( $I$ ) at a voltage ( $V$ ) for a time  $\Delta t$ . The output current,  $I$ , and/or the time  $\Delta t$  to depletion of the stored energy in a battery can be increased by enlarging the area of the electrodes or connecting cells in parallel; the voltage  $V$  for a desired power  $P = IV$  by connecting cells in series <sup>6</sup>.



**Figure 1** (a) Schematic of potential hysteresis in an ideal electrode material's charge/discharge procedure. (b) Illustration of the potential drop in the interval between charge and discharge. Internal resistances chiefly induce the IR drop (reproduced from <sup>7</sup>).

The battery cell consists of two electrodes (see the battery facts box), the negative electrode (often referred to as the anode) and the positive electrode (cathode), separated by an electrolyte, which can be either a liquid or a solid, albeit solid–solid interfaces are generally more challenging unless the solid electrolyte is a polymer or the solid electrodes are thin <sup>8</sup>. The solid electrodes are (typically) separated by a liquid electrolyte which is kept apart by an electrolyte-permeable separator membrane.

The electrolyte conducts the ionic component of the chemical reaction between the negative and positive electrode, e.g., Li<sup>+</sup>, but it forces the electronic component to traverse an external circuit, where it does work (see battery facts). A rechargeable battery cell has reversible chemical reactions at the two electrodes <sup>6</sup>.

During discharge and charge, an internal battery resistance,  $R$ , to the ionic current  $I_i = I$  reduces the output voltage  $V_{dis}$  (discharge) from the open-circuit voltage  $V_{oc}$  by a polarization  $\eta = I_{dis}R$  and increases the voltage  $V_{ch}$  required to reverse the chemical reaction on charge by the overvoltage  $\eta_{ch} = I_{ch}R$ :

$$V_{dis} = V_{oc} - \eta_{dis}(q, I_{dis}) \quad (1)$$

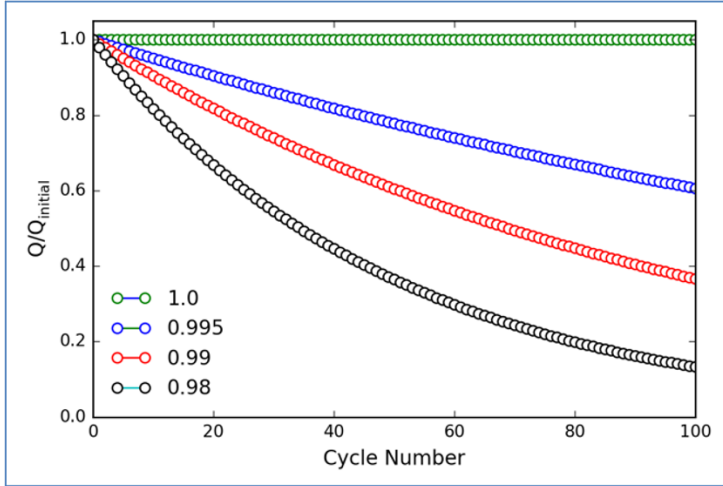
$$V_{ch} = V_{oc} + \eta_{ch}(q, I_{ch}) \quad (2)$$

Where  $q$  represents the state of charge and  $Q$  is the total charge per unit weight (Ah/kg) or per volume (Ah/L) transferred by the current  $I = dq/dt$  on discharge or charge (see **Figure 1**).  $Q(I)$  is referred to as the cell capacity for a given current  $I$ ;  $Q$  depends on  $I$  because the rate of transfer of ions across the electrode/electrolyte interfaces becomes diffusion-limited at high currents <sup>6</sup>.

Another critical aspect in assessing the performance of a secondary battery is its ability to retain capacity over multiple charge/discharge cycles. The percent Coulombic efficiency of a single cycle associated with a capacity fade is

$$100 \times (Q / Q_{\text{initial}}) \quad (3)$$

The cycle life is generally defined as the number of cycles until the capacity fades to 80% of its initial reversible value. As illustrated in **Figure 2**, only an extremely low capacity fade is acceptable for a battery to achieve a cycle life beyond 1000 charge-discharge cycles, which is requested for many commercial applications.



**Figure 2** The percent Coulombic efficiency as a function of the number of charge-discharge cycles.

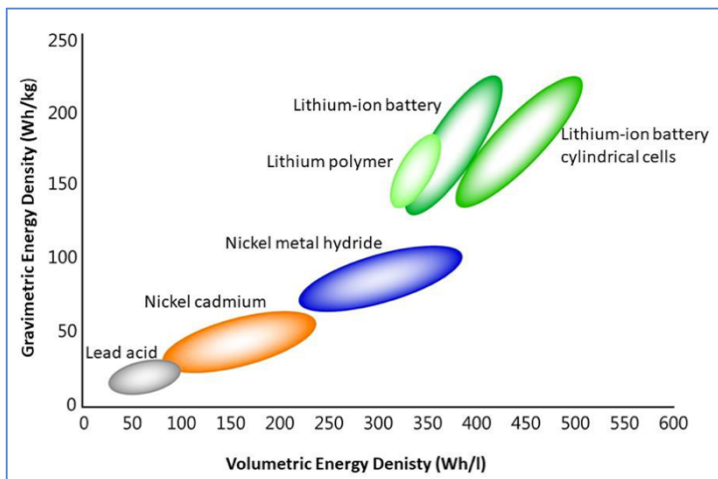
Additional figures of merit of a rechargeable battery cell, aside from safety and cost (discussed below), are its density (specific and volumetric) of stored energy and its output power  $P(q) = V(q)I_{\text{dis}}$  for a given discharge current. The stored energy is the product of the average voltage  $\langle V(q) \rangle$  and the capacity  $Q(I)$ . The open-circuit voltage  $V_{\text{oc}}$  of a cell is the difference between the electrochemical potentials  $\mu_{\text{A}}$  and  $\mu_{\text{C}}$  of the negative (anode) and positive (cathode) electrode:

$$V_{\text{OC}} = (\mu_{\text{A}} - \mu_{\text{C}})/e \quad (4)$$

The available energy stored in a fully charged cell depends on the discharge current  $I_{\text{dis}}$ ; it may be obtained by measuring the time  $\Delta t(I_{\text{dis}})$  for its complete discharge at a constant  $I_{\text{dis}} = dq/dt$ . The gravimetric energy density (Wh/kg or mWh/g) is dependent on  $I_{\text{dis}}$  through  $Q(I_{\text{dis}})$ . The volumetric energy density (Wh/L) is particularly interesting for portable devices and automotive applications <sup>6</sup>.

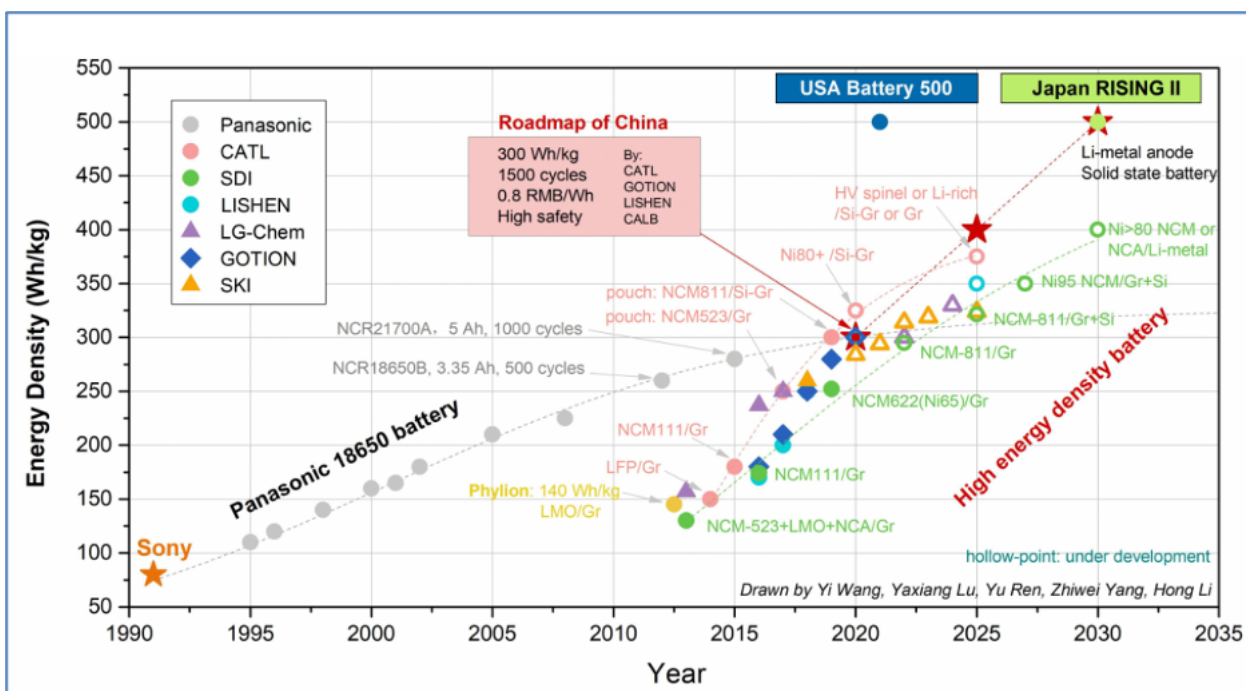
### Battery challenges for energy storage applications

Batteries play an essential role in developing a society based increasingly on sustainable energy. Present-day rechargeable lithium-ion (Li-ion) battery technology has been very successful since its development more than 30 years ago <sup>9</sup>, primarily due to the increased energy density compared to earlier battery chemistries like lead-acid, nickel-cadmium, and nickel-metal hydride batteries (Ni-MH), see **Figure 3**.



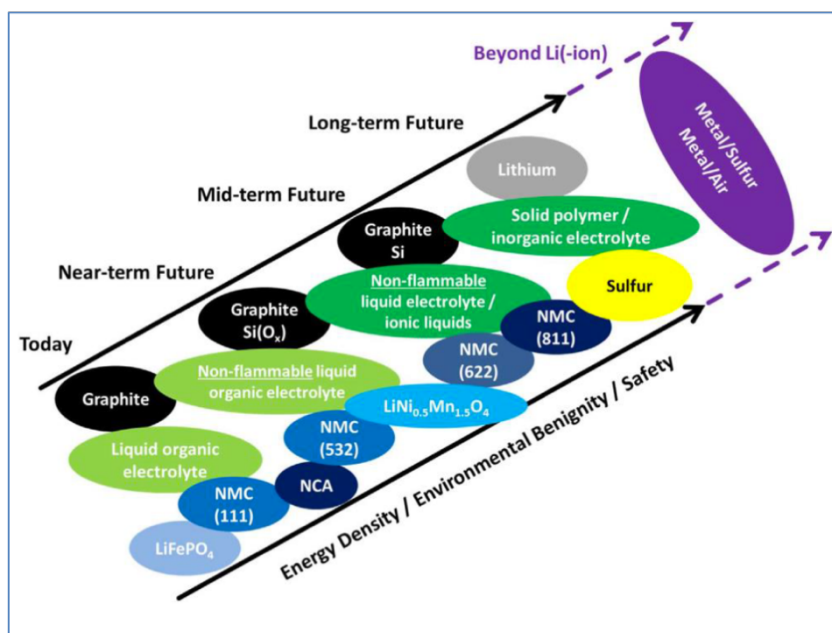
**Figure 3** Comparison of the different battery technologies regarding volumetric and gravimetric energy density <sup>3</sup>.

Since the commercialization of the lithium cobalt oxide (LCO) battery by SONY in 1991, the specific energy (Wh/kg) of Li-ion batteries (LIB) has increased from ~80 Wh/kg to around ~250 Wh/kg for state-of-the-art NMC (nickel manganese cobalt) and NCA (nickel cobalt aluminium) batteries, see **Figure 4**.



**Figure 4** Historical developments in the energy density for different lithium-ion batteries<sup>4</sup>.

While the energy density of LIB has increased by upwards of 4-5% per year on average over the last 30 years, there is still a strong need to develop new battery materials, chemistries, and cell designs to reach the growing demands from the automotive industry, in particular, e.g., NMC 811 in the mid-term, and lithium metal anodes and all-solid-state batteries in the long-term perspective, see **Figure 5**.



**Figure 5** Joint perspectives of automotive battery R&D in China, Europe, Germany, Japan, and the USA <sup>10</sup>.

The present-day LIB is fabricated in a discharged state, and it uses reversible Li extraction from an oxide host as the rechargeable positive electrode (cathode), and carbon or buffered spongy silicon as the negative electrode (anode). The capacity of the oxide host is limited to the reversible solid-solution range of Li in the cathode host structure operating on the redox energy of a single transition metal cation, albeit the recent advent of anionic redox in transition metal polyanionic cathodes may enhance the specific capacities <sup>11–13</sup>. Rechargeable LIBs capable of over 10,000 safe charge/discharge cycles at an acceptable rate, equivalent to >10-year operational life, have been achieved <sup>14</sup> and predictions have been made for Li-ion batteries for battery electric vehicles (BEV) capable of lasting 1–2 million miles <sup>15</sup>. Therefore, a fundamental challenge for the chemist and electrochemical engineer is to develop a strategy that will retain this cycle life at an acceptable rate in a safe and (more) affordable battery with a larger energy density than is realizable with current strategies.

Li-ion batteries are leading the market for consumer electronics, power applications, e.g., power tools and BEVs in particular. The most promising expanding markets for high power batteries are within e-mobility and transportation (specifically BEVs), and as intermittent storage facilities for renewable sources such as wind and solar energy, where short term storage and balancing (time-scales of seconds, minutes to hours) is a necessity due to their intermittent nature and inherent lack of correlation with user demand.

Large-scale battery plants are now being constructed, e.g., the 150MW/193.5MWh Tesla Li-ion battery (Hornsedale Power Reserve) alongside the Hornsdale wind farm in Australia (**Figure 6**), and the 200MW/800MWh Vanadium Redox Flow Battery (VRFB) currently under construction in Dalian, China (**Figure 7**) to provide additional power system reliability and continued cost savings to consumers.





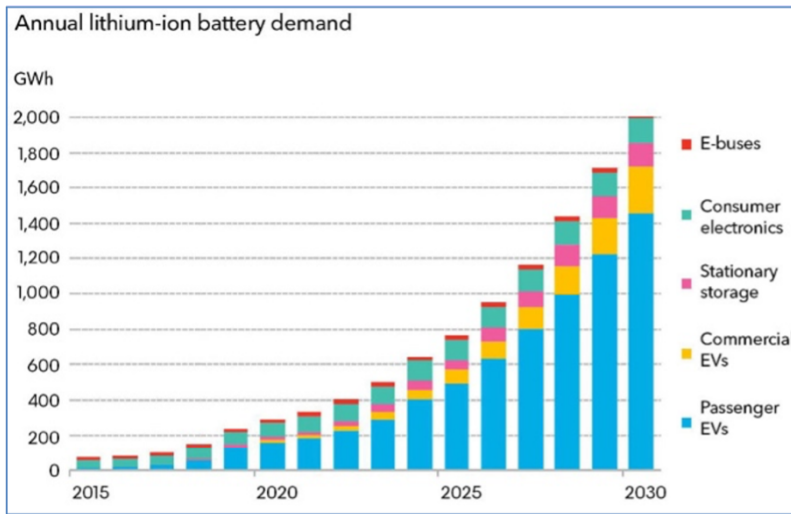
**Figure 6** The Tesla battery (Hornsdale Power Reserve) was built alongside the Hornsdale wind farm in Australia and upgraded in 2021 to 150MW/193.5MWh as the largest Lithium-ion battery globally (Teslarati).



**Figure 7** World's largest battery: 200MW/800MWh vanadium redox flow battery, Dalian, China (under construction).

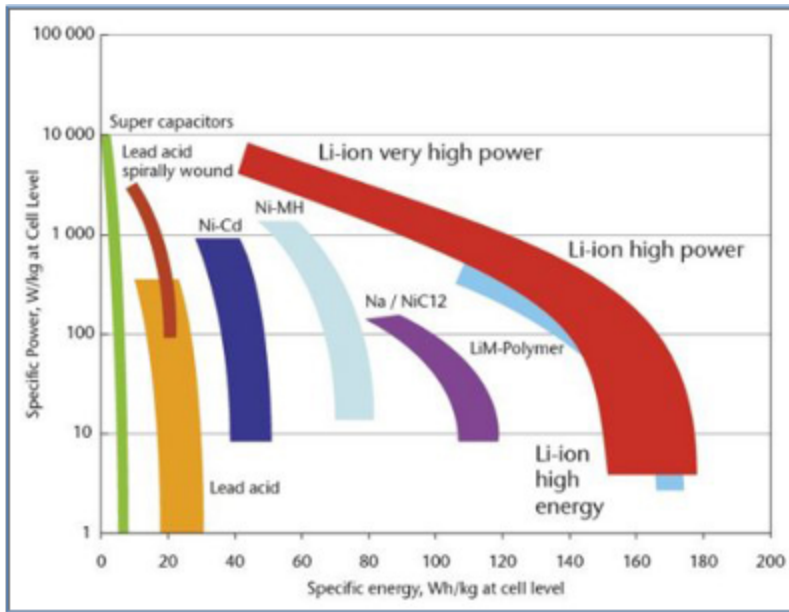
The use of batteries for passenger electric vehicles and electric transport in particular is expected to grow dramatically over the next decade and expectedly expand into applications like commercial EVs and stationary storage (**Figure 8**), creating a growing demand for specialized battery solutions like redox flow batteries (RFB). Li-ion based technologies are, however, expected to continue to dominate this market in the

foreseeable future <sup>16</sup>. The Li-ion chemistries are particularly well suited for moderate energy density applications and low-to-moderate power density requirements for typical portable applications and e-mobility.

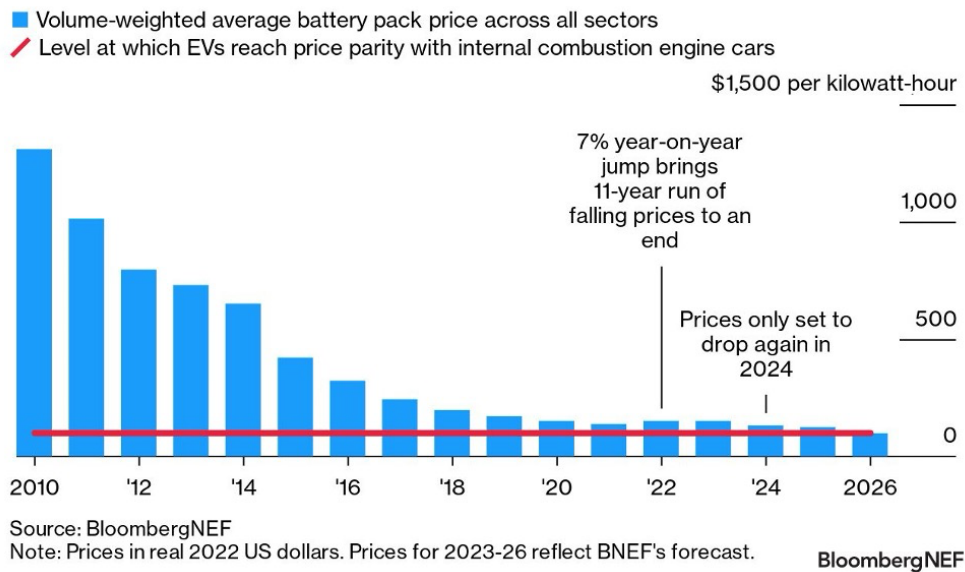


**Figure 8** Projected annual demand for lithium-ion batteries (Energycentral.com, 2020).

It is possible to make high power density (W/kg) lithium batteries, but the corresponding energy density (Wh/kg) typically decreases significantly when high current densities are needed (**Figure 9**). The concept “C-rate” refers to how many times per hour the battery capacity is discharged (or charged), e.g., 20 complete discharges per hour is a C-rate of 20, and one discharge per 5 hours is a C-rate of C/5. Discharge at higher current densities (or C-rates) causes the apparent capacity to decrease. Although lithium-ion batteries for transportation and e-mobility have become the largest market for Li-ion batteries internationally and will remain so for the foreseeable future (**Figure 8**), cost remains a key driver in this development. To achieve a successful large-scale implementation of battery technologies in the transportation sector, many fundamental challenges remain to be resolved, mainly related to the power density lifetime/durability and price <sup>10</sup>. The cost of LiB cells and packs has decreased by roughly 10-20% per year (**Figure 10**) over the last decade and is projected to drop below \$100/kWh before 2025. It is, however, important to note that this dramatic reduction has primarily resulted from the economy of scales rather than radical innovation, and that the curve has been flattening out in the last years; effectively plateauing at the end of 2021 due to supply bottlenecks, despite a resurgence of cheaper battery chemistries like lithium iron phosphate (LFP) in new BEVs like the Tesla Model 3. Continued investments in the development of low-cost, high energy and power-density batteries are needed to solve the future demands for the transportation sector and stationary storage applications.



**Figure 9** The specific power as a function of specific energy for a range of different battery chemistries (a Ragone plot). For all systems, a decrease in the energy density is observed when high currents are drawn, illustrating the challenges of optimizing both simultaneously <sup>3</sup>.



**Figure 10** Developments in pack and cell level cost for Li-ion batteries (Bloomberg, 2023) <sup>16</sup>.

BEVs may ultimately also play an important role in decentralized grid-scale storage as elements in the daily fluctuations of electricity consumption. However, technically and economically viable solutions still need to be developed. Significant efforts are currently being placed on improving the energy density, taking into account an increased awareness of the developmental needs in terms of reduced materials cost, reduced dependence on scarce materials, improved battery durability and cycle life, and safety <sup>1</sup>.

Large-scale battery solutions for, e.g., grid-scale storage in connection with intermittent sustainable energy sources, face quite different challenges than portable and mobile applications. Here, cost, volume, and fast charge/discharge rates are essential, as well as durability and low maintenance requirements. LIB



technologies face competition from alternate battery technologies such as the redox flow batteries discussed above <sup>17</sup>. Stabilizing supply/grid fluctuations on a second or sub-second scale requires high-speed and reversible energy storage with insignificant energy loss and high durability. The most significant potential for electrochemical storage in the future, sustainable energy infrastructure is probably in dealing with hourly and daily fluctuations due to variations in wind and solar power production.

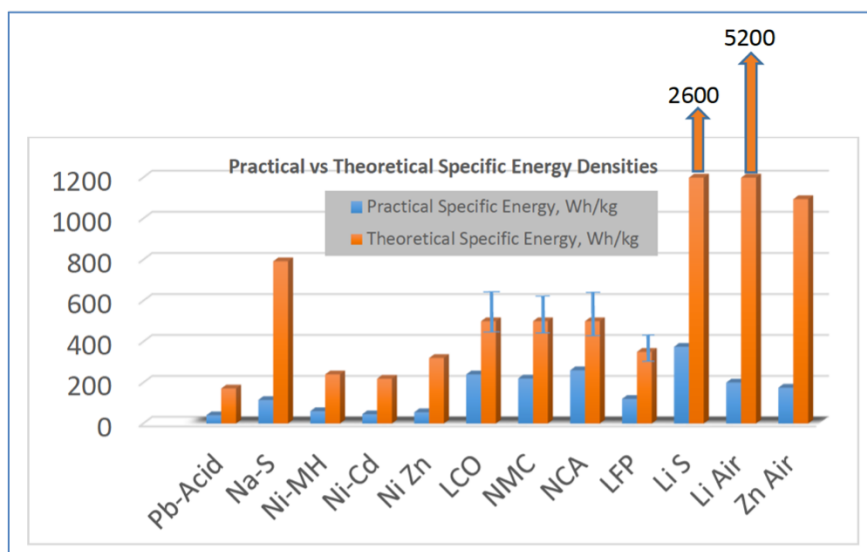
Commercial systems based on highly durable lithium batteries, with, e.g., lithium titanate oxide (LTO) negative electrodes, are already in operation as solutions for wind energy and solar power stations. However, the number of existing facilities is still limited.

## Technological and materials challenges

Lithium-based batteries still face significant challenges related to materials, durability, interfaces, raw materials cost, scalability, and production. An absolute key point for the massive introduction of Li-ion batteries in the transportation and energy sectors is to solve the significant challenges related to storage capacity, degradation, cyclability, stability, and safety issues concerning uncontrolled chemical reactions. To reach these objectives, it is particularly important to have a clear understanding of the battery interfaces' role in improving electrode materials and system performance.

As discussed above, one of the largest obstacles for large-scale use of today's LIBs is the price, mainly due to high materials production cost. Although continued cost reduction from mass production is foreseen, a significant reduction in materials price must still be achieved by increased research in alternative battery materials. Another challenge, which must be considered, is the use and availability of resources and the environmental impact/toxicity of the materials. Limited resources of certain key elements, e.g., cobalt, may lead to a shortage or increase in price <sup>18</sup>. The future batteries must be extensively based on abundant and reusable resources, which makes, e.g., LFP and manganese-based batteries very attractive from a resource and environmental perspective.

A number of different electrode materials and novel battery chemistries hold the potential to leap-frog the development of new batteries with substantially improved performance and/or cost, as discussed below (**Figure 11**).



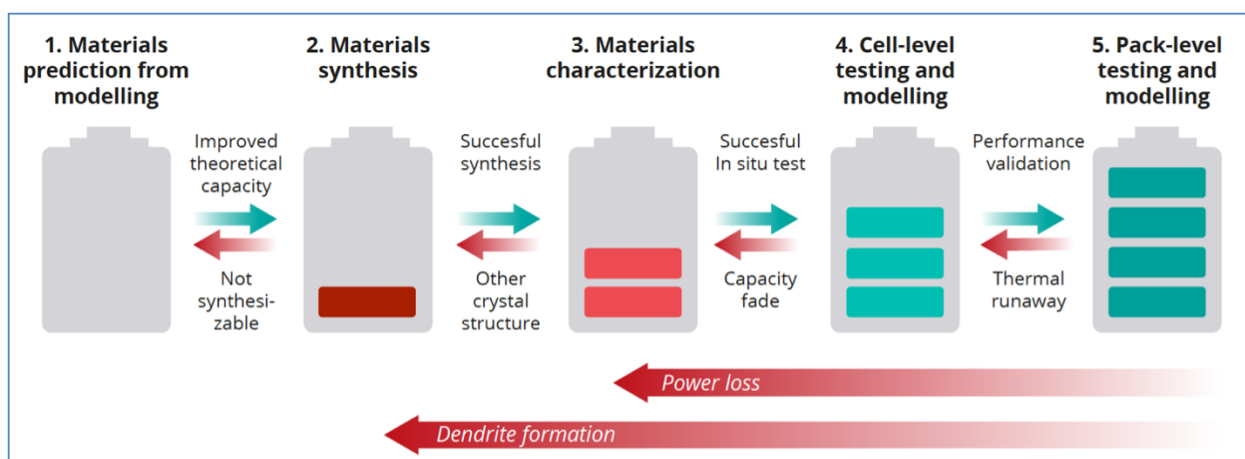
**Figure 11** Comparison between theoretical and practical energy densities for materials of major battery chemistries at the cell level.

The gravimetric (Wh/kg) and volumetric (Wh/L) energy densities should be improved, especially for future applications in non-passenger transportation, e.g., short-to-medium range heavy-duty transportation of goods <sup>19</sup>, where the batteries needed for achieving a competitive driving range are still too heavy and/or limits the accessible cargo space. While the energy density of LIBs is high compared to earlier battery technologies (**Figure 3**), it has only increased moderately over the last two decades. Promising high energy density materials include Ni-rich NMC (nickel manganese cobalt), Li-rich high voltage cathode materials, and silicon nanoparticles as anode materials (**Figure 5**). However, even an increase by a factor of two can only be achieved by a paradigm shift in the way lithium is stored in the materials. Emerging battery technologies for the next-generation energy storage solutions offer the potential of more than a two-fold increase in the energy density, e.g., lithium-air batteries <sup>20</sup>, lithium-sulfur batteries <sup>21</sup>, Mg-ion <sup>22</sup>, and Mg-S batteries <sup>12</sup> and other conversion type batteries such fluoride batteries <sup>23</sup>.

The power density naturally impacts the re-charging time for electric vehicles. It is, however, an even more critical parameter for energy storage in connection with intermittent renewable energy plants, where it is necessary to be able to accommodate large currents in and out of the battery with very low energy loss, without any significant decrease in capacity or lifetime, and without compromising safety. **Figure 9** shows the power density and specific energy for various electrochemical storage solutions; the highest power density is reached by super-capacitors, but with very low energy density. The energy density decreases with an increased specific power. It is possible with existing LIBs to achieve high power densities, but also here at the expense of energy density, i.e., when the battery is operated at high power densities, the available capacity decreases significantly.

The challenges related to improving the batteries are mainly associated with the materials and interface properties, as reflected in issues pertaining to the ionic and electronic transport, reactivity/degradation, stability, kinetic barriers, and phase mobility. To solve these challenges, a better understanding of the fundamental mechanisms at the atomic scale must be developed. This requires a dedicated effort, where experimental and theoretical efforts are combined, i.e., a synergy between computational chemistry, synthesis/electrode fabrication, and advanced structural/electrochemical characterization must be achieved.

The development of the Li-ion battery, for which Profs. John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino received the Nobel Prize in Chemistry 2019, took nearly 20 years from Stanley Whittingham's initial idea about intercalation in  $\text{TiS}_2$  in 1972 to the commercial Li-ion battery by Sony in 1991. A battery concept and architecture that has largely remained unchanged ever since and still relies on scarce materials like cobalt, nickel, and lithium. In a traditional sequential battery development process (**Figure 12**), each step of the discovery value chain is dependent upon the successful completion (green arrows) of the previous step(s). In contrast, failure (red arrows) sets the process back by one or more steps.



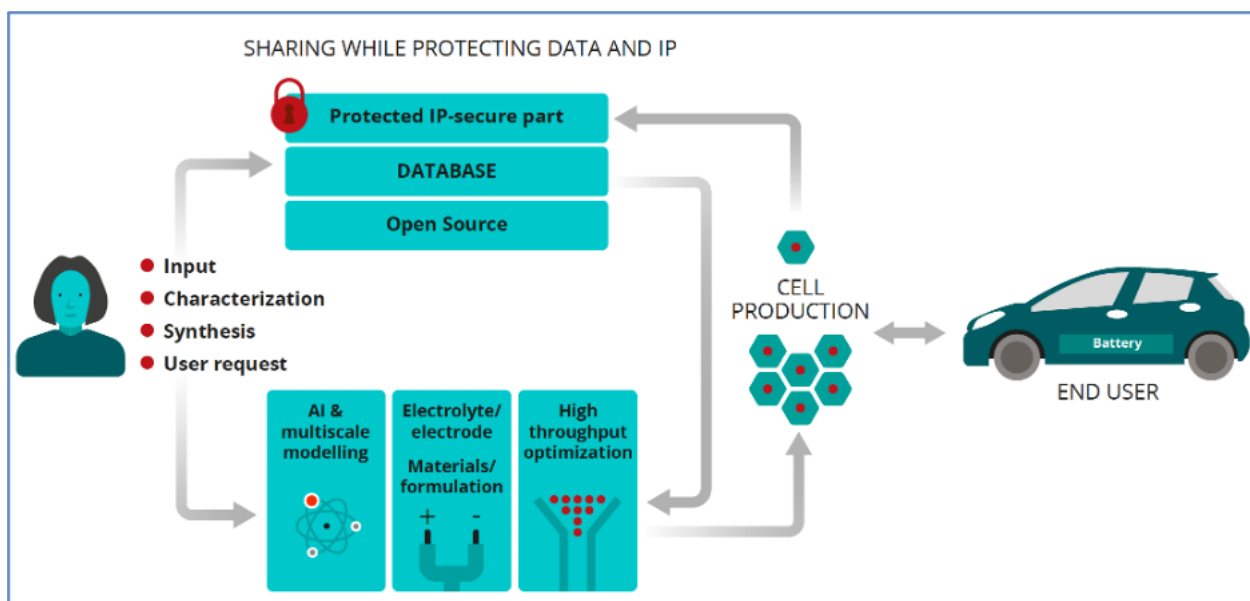
**Figure 12** A traditional sequential and Edisonian battery development process.

## AI accelerated battery discovery and development

Today, advanced materials account for nearly half of the manufacturing costs of clean energy technologies such as high-performance Li-ion batteries. This number is expected to reach eighty percent in the future. Relying on existing trial-and-error-based development processes, discovering novel high-performance battery materials and cell designs entails considerable effort, expense, and time – traditionally 10-20 years from initial discovery to commercialization. Historically, these innovation cycles rely on cost reduction by accelerated manufacturing and engineering rather than deployment of new “quantum leap” technologies.

Experience has shown that when developing new battery chemistries or introducing new functionalities into existing battery technology, interfaces hold the key to exploiting the full potential of the electrode materials and developing ultra-high performance, sustainable and smart batteries. Advanced materials are the foundation of nearly every clean energy innovation, particularly emerging battery technologies.

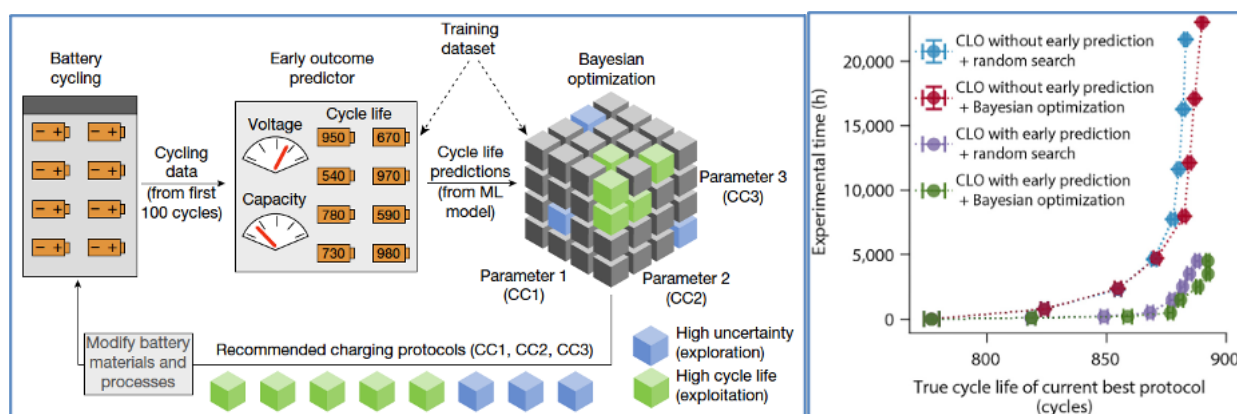
A new path for accelerated development of ultra-high performance, sustainable and smart batteries hinges on the development of radically faster and more energy- and cost-effective methods for battery discovery and manufacturing. In particular, methods utilizing automated/autonomous procedures, artificial intelligence (AI)<sup>24</sup>, and machine learning (ML)<sup>25</sup> to accelerate the discovery process through the creation of closed-loop optimization (CLO)<sup>5,26–28</sup> procedures. In CLO, new battery materials can be discovered and developed by utilizing data from all parts of the battery development and discovery cycle, spanning computer simulations over synthesis and characterization to end-user data, e.g., performance data from BEVs (**Figure 13**).



**Figure 13** A closed-loop materials discovery platform for accelerated battery development <sup>27</sup>.

ML and other data-driven approaches offer a promising gateway to leverage large datasets from computational and experimental investigations from various areas in science and engineering <sup>24</sup>. The large techno-economic and societal impact of rechargeable batteries as energy storage devices coupled with the inherent complexity of the electrochemical processes make batteries a perfect testbed for ML-accelerated materials optimization and innovation, as discussed in the following chapter. Computer-based simulation and prediction techniques such as atomic-scale simulations and machine/deep learning approaches play an ever-increasing role in searching for novel battery materials, components, and cell designs. While computational efforts have focused extensively on discovering and designing novel high-energy and high-power density materials, less attention has been paid to applying ML techniques to improve the manufacturing and performance of existing battery materials and cells.

By a combination of ML and high-throughput experiments in a CLO setup (see **Figure 14**) it has been demonstrated that it is possible to develop fast-charging strategies to enhance battery cycle life without a priori knowledge of the underlying physical mechanisms at play. This was done by creating an adaptive OED (optimal experimental design) approach to search for the current and voltage profiles in fast charging protocols that maximize battery cycle life, i.e., getting better performance out of existing battery cells <sup>25</sup>.



**Figure 14** Closed-loop optimization (CLO) of Li-ion battery cells for fast charging <sup>5,26</sup>.

## Understanding and controlling battery interfaces

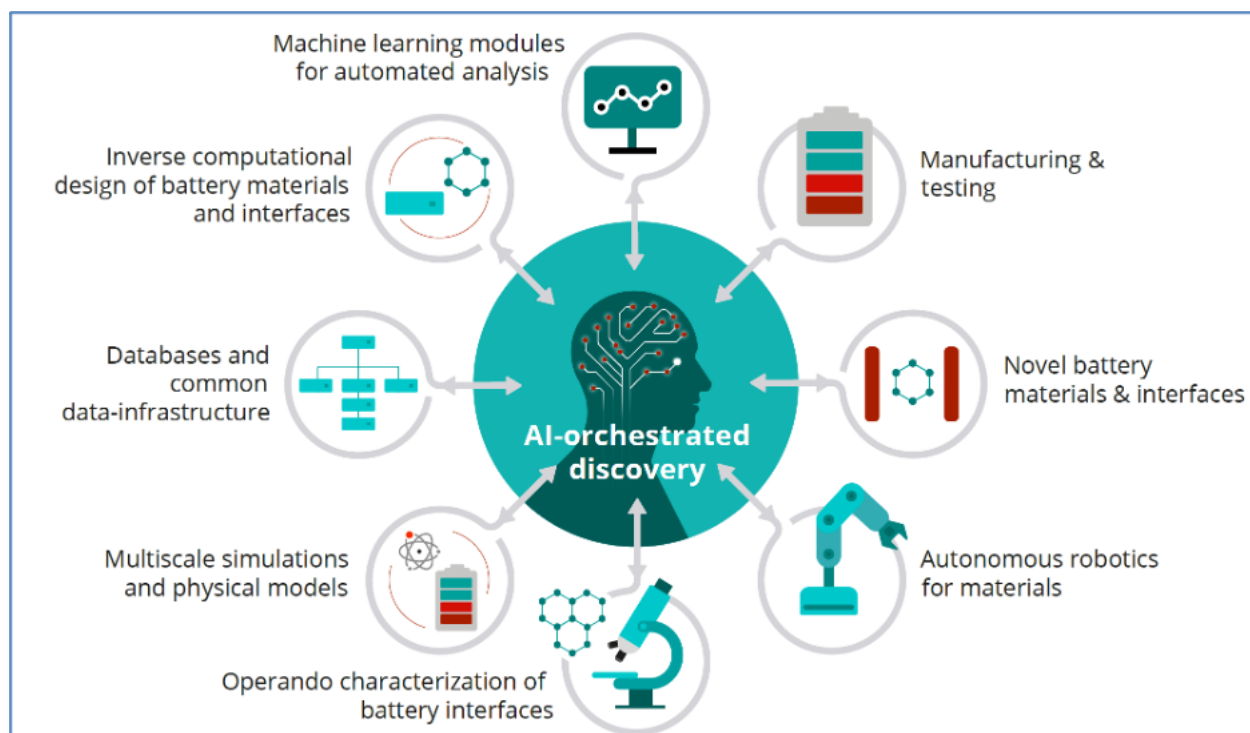
Essential performance metrics like battery safety, energy efficiency, and cycle stability are all dependent on the performance of the battery interfaces. The use of integrated computational design, materials synthesis, and *in situ* characterization is often needed to obtain a detailed understanding of the link between the fundamental mechanisms and the electrochemical performance, which can be used to develop future battery materials and technologies.

Batteries consist of a multitude of different interfaces and interphases, but few are as complex and pose as many challenges to the design of ultra-high performance batteries as the solid-electrolyte interphase (SEI) <sup>29</sup> [10.1002/admi.202101734] at the electrode-electrolyte interface. Therefore, particular emphasis must be placed on understanding and controlling these interphases, but the described methodology will be equally applicable to other battery interfaces and interphases. Proactive and dynamic control of the SEI formation and complex composition and morphology remains a “Grand Challenge” in battery research and development - a challenge in striking need of more advanced and versatile prediction and design techniques. Radically new approaches are needed to accelerate the discovery and development of ultra-high-performing and durable materials and interphases in rechargeable batteries.

The large-scale European research initiative BATTERY 2030+ ([www.battery2030.eu](http://www.battery2030.eu)) seeks “to reinvent the ways we invent batteries” by bringing together European strongholds to join forces in speeding up scientific discoveries, creating synergies, and avoiding over-redundant research. BATTERY 2030+ has a long-term focus, which is necessary to address the obstacles preventing current and future battery technologies from performing close to their theoretical limits while at the same time minimizing environmental impact and cutting down life-cycle carbon footprint <sup>4,30</sup>.

A core element in BATTERY is the project “BIG-MAP” or Battery Interface Genome (BIG) – Materials Acceleration Platform (MAP) initiative ([www.big-map.eu](http://www.big-map.eu)), in which AI will be utilized to drastically reduce the battery materials development cycle time. A central aspect will be developing a shared European data infrastructure capable of performing autonomous acquisition <sup>31</sup>, handling, and utilization of data from all domains of the battery development cycle <sup>32</sup>. Novel AI-based tools and physical models will be developed to utilize large amounts of data, with a strong emphasis on battery materials, interfaces, and interphases <sup>27</sup>(Figure 15).





**Figure 15** The closed-loop data and information flow diagram for autonomous AI-orchestrated battery discovery and development in BIG-MAP: Battery Interface Genome – Materials Acceleration Platform ([www.big-map.eu](http://www.big-map.eu)) project <sup>33</sup>.

A few examples of promising future battery technologies, e.g., metal-air and metal-sulfur battery solutions for high energy densities; conversion batteries; robust, low-cost batteries, e.g., sodium batteries; novel flow-type batteries, are presented below.

## Batteries for the future

It is essential to realize that different applications place very different demands on battery performance. For use in grid-scale storage, heavier batteries may be used compared to mobile applications (lower energy density), but high power density and long term stability (high number of charge/discharge cycles) is mandatory for the storage facility to be able to run for many years with minimum maintenance.

Therefore, the solutions to present-day and future challenges in battery research will depend specifically on the targeted applications. An absolute key point for the successful mass-introduction of Li-ion batteries in the transportation and energy sectors is to solve the significant challenges related to price, storage capacity, degradation, cyclability, stability, and safety issues concerning uncontrolled chemical reactions.

Perspectives and potential for high energy batteries: Presently, the energy density in lithium batteries is limited by the use of the transition metals, specifically the critical raw material (CRM) cobalt. The potential is determined on the positive electrode by a one-electron oxidation/reduction, e.g., of cobalt or iron, and on the negative electrode by the oxidation potential of lithium or a lithium compound. Future needs call for a significant increase in the energy density of batteries, but this can only be improved in a limited number of ways. These are currently under investigation, but the potential impact varies, as outlined below.

- 1) Use of lighter electrode materials: Novel battery chemistries without transition metals are under development where other reactions are utilized, e.g., the reaction of lithium with oxygen (lithium-air)<sup>20</sup> or sulfur (lithium-sulphur)<sup>21</sup>. (Potentially a factor of two or more in the energy density, see **Figure 11**).
- 2) Higher potentials (voltage) will give a higher energy density. Substantial research is put into developing high voltage cathode materials, with the potential approaching 5V<sup>34</sup>. However, large challenges with electrolyte stability, safety, and cyclability still have to be overcome. (Potentially a factor of 1.2-1.3 in energy density).
- 3) Transferring more than 1 electron per active transition metal atom could potentially increase the energy density, e.g., Mg-ion batteries<sup>22</sup> by using several oxidation states of iron or manganese, or utilization of anionic redox processes in the positive electrode. In addition, conversion type batteries involving, e.g., iron fluoride are of increasing interest<sup>35</sup>, as are other metal-air batteries such as zinc-air<sup>36</sup>. (Potentially a factor of 1.5-2.5 in energy density).
- 4) The use of thin solid electrolytes to create all-solid-state batteries (ASSB) may also improve the energy density, e.g., by enabling the use of metallic Li-anodes. Expected to be mass produced by Toyota and introduced in BEVs from 2027-28, but the cost should be reduced and the durability improved further<sup>37</sup>. (Potentially a factor of 1-1.5 in energy density).

High power batteries: The increasing demand for high power densities has led to intensified research into battery interfaces and the optimization of transport properties. Much of the power density limitation in batteries is caused by electronic and ionic transport issues in bulk and across interfaces<sup>38</sup>. Optimization of transport properties relies on knowledge of structure and defects in external and internal interfaces in the active electrodes and on reactions between solids and the electrolyte. In addition, nano-structuring of materials and 3D structuring of batteries is important for high-power operation<sup>39</sup>.

Low-energy-density and robust solutions: For grid-scale storage, land-based operational storage systems, and sea transport, the energy density is not as important. Here, alternative battery chemistries such as the redox flow batteries, e.g., vanadium in aqueous electrolyte solutions and cerium–zinc, are of interest<sup>40</sup>. In addition, the development of cheap and robust sodium batteries is of considerable interest<sup>41</sup>, but further developments are needed for both technologies.

## Perspectives on electrochemical storage in batteries

As outlined in this chapter, the use of battery technologies is expected to play an ever-increasing role in multiple levels of the future energy infrastructure:

- Electrification of the transportation sector will require safe, efficient, and inexpensive energy storage solutions that are fully scalable. Existing lithium-ion and next-generation batteries will continue to be a key factor in this development.

- Grid-scale storage for load balancing in connection with renewable energy sources may in part be based on electrochemical storage, but these technologies should also be fully scalable to deal with the TWh challenge.

Highly application-specific demands in terms of, e.g., energy/power density, charge/discharge rates, durability, and safety, as well as reduced cost do, however, dictate continued improvements in existing battery technologies and development of novel high-performance batteries, if sustainable battery solutions are going to become competitive for transportation and stationary applications. Naturally, an increasing focus on the development and use of automotive and large-scale batteries is seen internationally, and substantial investments in fundamental battery research, e.g., the BATTERY 2030+ initiative, materials development, and implementation of new battery technologies, are also needed to facilitate and enable the on-going transition to a society based on sustainable energy sources.

## Glossary

AI	Artificial Intelligence
ASSB	All-solid-state batteries
BIG-MAP	Battery Interface Genome – Materials Acceleration Platform
BMS	Battery Management System
CEI	Cathode Electrolyte Interface
CRM	Critical Raw Materials
Energy density	Energy per unit volume (Wh/l)
HPC	High Performance Computing
HTS	High-Throughput Screening
LFP	Lithium iron phosphate
LIB	Lithium ion Battery
LCO	Lithium Cobalt Oxide
LMO	Lithium Manganese Oxide
MAP	Material Acceleration Platform
ML	Machine Learning
NCA	Lithium nickel cobalt aluminum oxide
NMC $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$	Lithium nickel manganese cobalt oxide –
NMC 622	Lithium nickel manganese cobalt oxide – $\text{LiNi}_{0.6}\text{Mn}_{0.2}\text{Co}_{0.2}\text{O}_2$
NMC 811	Lithium nickel manganese cobalt oxide – $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$
Power density	Power per unit volume (W/l)
RFB	Redox Flow Batteries
SEI	Solid Electrolyte Interphase
SoC	State of Charge
Specific energy	Energy per unit mass (Wh/kg)
TWh	Terawatt hours

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