



BATTERIES EUROPE

Development
of reporting
methodologies

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INTRODUCTION

The launch of the Batteries Europe technology platform on June 25, 2019 established the setting for the creation of a Strategic Research Agenda (SRA) on batteries. The SRA aims at providing a clear framework for European battery research and propose future actions required to continue supporting and promoting both competitiveness and sustainability in the European battery industry through research.

In this context, a global knowledge and understanding of the existing battery technologies and performance is an essential requirement. However, the benchmarking and comparison of different battery technologies are greatly hampered by the lack of a common reporting methodology. To address this deficit, the WGs of the Batteries Europe, led by WG 1 “New and Emerging technologies”, have initiated the development of such common reporting methodologies guidelines.

This document provides the basis for the development of homogenized performance metrics and a transparent reporting methodology, which are necessary for the reliable benchmarking of various battery chemistries. Furthermore, such performance metrics facilitates the identification of new promising materials and cell technologies whilst highlighting areas for further improvement.

For a successful implementation, the suggested reporting methodology needs to be adopted by a majority of scientists and implemented in all EU funded battery-related projects for monitoring the progress beyond the state-of-the-art. In addition, the reporting guidelines could, for example, be recommended as a requirement for publications originating from the EU funding in scientific journals^[1].

Editors and Board members of several high-level scientific journals are also members of several WGs within Batteries Europe. They could greatly assist in the implementation of such a recommendation. This would result in setting up the “gold standard” for scientific reports of battery chemistry developments in Europe and would set a trend for a worldwide implementation beyond Europe.

Whilst this development will not have an immediate impact, it will set a best practice for results’ reporting and will reduce the occurrence of “overly optimistic” claims often occurring in the field of battery research^a.

^a *Thomas Edison himself said: “Just as soon as a man gets working on the secondary battery it brings out his latent capacity for lying”, The Electrician (London) Feb. 17, 1883, p. 329.*



1 Context

The EU SET Plan (Strategic Energy Technology Plan) has identified batteries as one of the key technologies necessary for the energy transition and has proposed in Action 7 a classification of the current and future cell chemistries which would enable the EU to become competitive in the global battery market to serve local electromobility and stationary storage^[2].

The optimised lithium-ion battery (LIB) cells of generation-1 through generation-3a (Fig. 1) represent the current core technologies for electric vehicle (EVs) and for stationary energy storage. These generations, and incremental improvements to them, are expected to remain the chemistries of choice for the nearest future considering the time typically required to move the technology from R&D on battery materials to large scale production^[3].

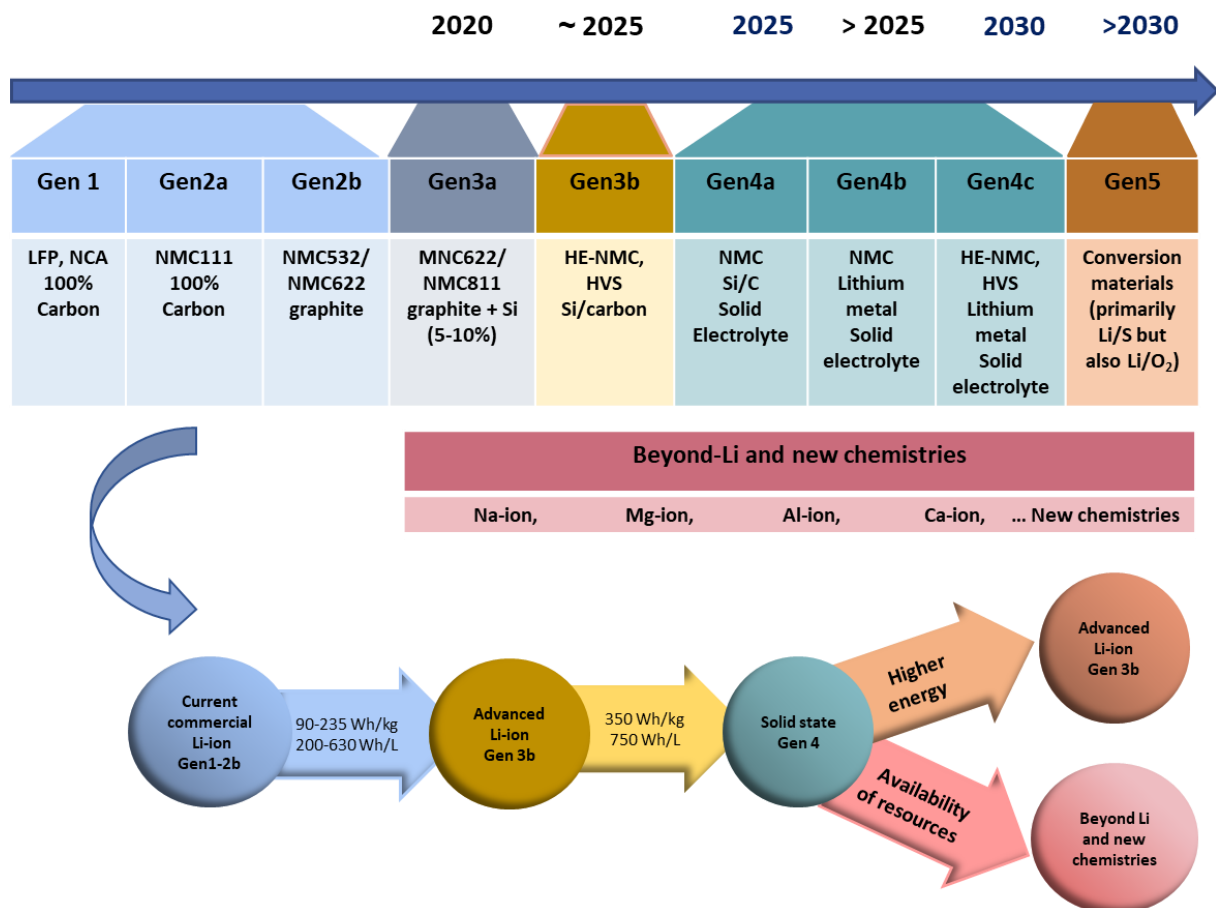


Figure 1. Today’s view on LIB cell chemistries and future beyond-Li and new chemistry cell technologies. Adapted from [2,4]

Present lithium based battery research (Gen 1 to 3a) focuses on incremental improvements in the energy density of Li-ion cells^[5]. The next leap can be



reached utilizing Li-metal anodes^[6] and there is plenty of room for innovation in future cell technologies or “next generation” chemistries^[7] for which important environmental benefits are expected, and which are currently at an early stage of development in the lab. Indeed, whilst energy density is one of the main Key Performance Indicators (KPIs) to be considered for EV applications, where LIBs will dominate the market for the next 10-15 years^[3], a growing variety of applications with different requirements have accelerated the research towards alternative chemistries potentially able to satisfy the requirements of a market diversification. The next-generation (non-lithium) chemistries also include sodium^[8], magnesium^[9], aluminium^[10], zinc^[11] and calcium-based^[12] systems as well as innovative redox flow systems^[13], where safety, cost, manufacturability, sustainability and dependency on raw critical materials play a fundamental role.

KPIs and characteristics are generally defined at a specific level, such as cell, module, pack or system level.

These scales are defined as follows:

- Cell level: an electrochemical device composed of three main components, *i.e.*, positive (cathode) and negative (anode) electrode and an electrolyte media (liquid-separator, solid, hybrid) and passive components such as current collectors and cell packaging).
- Module level: a single unit constituted by a group of cells connected in series or parallel.
- Pack level: a group of cells, a module, or a group of modules including auxiliary systems (mechanical support, thermal management, and electronic control).
- System level: a battery management system is integrated at the pack level.

In order to homogenize battery results and data including new and emerging technologies, this document principally refers to characteristic and performance metrics at the cell level, including its constituent components.

Within the frame of new and emerging technologies, continuous advances in electrode materials, electrolytes, functionalized separators, auxiliary inactive components (e.g., insulators, elastomers,) and cell designs are reported. Various electrochemical techniques and experimental conditions, different cell components and cell setups are used to characterize novel battery materials or any other components of interest, ultimately making accurate comparison of results from different studies extremely challenging. Furthermore, “inappropriate” selection of the cell components and/or



measurement conditions, often occurring in scientific literature, can lead to results, whose interpretation is very difficult^[14]. The general guidelines for treating new chemistries would help in this case to make right design of experiment for getting results allowing clear explanation.

In this context the peer reviewing process plays a key role. Indeed, expert reviewers called to proof the scientific appropriateness of a new manuscript have the duty and responsibility to accurately and consciously devote their knowledge, attention and time to this fundamental step.

In addition, it is worth mentioning, that in the last decades there has been a rush to publish results and the number of publications is growing exponentially. The number of scientific papers that have been retracted or present poor-quality science has increased accordingly, and this induces a lack of reproducibility of reported data, and low transparency in reporting methodology. The poor quality of the results has led to a loss of confidence in reported data and impact of the research performed^[15,16]. Thus, it is of uttermost importance that every step of the peer-review process is carefully done by all the members of the reviewing system, including authors themselves, editorial offices and reviewers. Ideally, a further step towards transparency would be a second level review process available post-publication, i.e., an online, open access review system assessing the accountability of the published work^[17].

Only a call to transparency and open science will enable the identification of the most promising research results and will prevent unnecessary time and effort being spent following misleading trails.

In addition, results reported in scientific literature as outstanding for new battery materials and device performances are often measured under conditions which are not transferrable to practical applications. Besides the basic cell design/structure and details on the cell components, cell performance strongly depends on the environmental conditions under which they are tested. Thus, all results should refer to consistent experimental conditions for accurate comparisons and reproducibility. Not only should the tests provide reproducible and useful data sets, but they are also required to enable a direct comparison between cell chemistries.

All of the above suggests the urgent need for the assessment of tools for benchmarking cell chemistries enabling performance comparison and their evolution over cell life.



1.1 Challenges when comparing results: illustrative examples

Reporting methodologies are essential for accurate comparisons and reproducibility. Thus, all results should refer to consistent experimental conditions.

Not only should the test conditions provide a reproducible and useful data set, but they are also required to enable a direct comparison between cell chemistries.

In this section, a summary of the most common misleading reporting practices found in the literature is given.

Before presenting some examples, some general remarks are highlighted below.

1 – Undefined and varying environmental test conditions: Beside the basic cell design/structure and details on the cell component characteristics, the cell performance strongly depends on the environmental conditions under which they are tested. Therefore, any environmental conditions that might influence the test results need to be reported, temperature being the most obvious one.

2 – Unrealistic and widely variable cell test parameters: Frequently, the theoretical KPIs evaluation is made irrespective of a feasible cell design or required ancillaries. Also, they are evaluated in tests not representing realistic operation conditions such as: ultra-low electrode areal loadings, excessive electrolyte and/or counter electrode, very low Coulombic, Voltaic and energy efficiency, very short cycle life.

3 – Undefined implications of materials structure: Materials with hierarchical nano- and sub-micro-structures have rather low density, resulting in low cell volumetric energy density. Additionally, they may require high electrolyte loadings to fill the porosity leading to higher costs and weight. This often goes unreported.

4 - For Metal-air battery cells the weight of the discharged cell should be considered for the gravimetric energy calculation. Especially for these cells, non-planar current collectors are frequently employed, which volume and mass should be included in the evaluation of the KPIs.

5 - If the electrolyte plays a role in the electrochemical reactions, its volume and weight should always be considered in the KPIs evaluation.

In the following sections we identify the specific challenges associated with benchmarking cell chemistries.



Challenge 1: Comparing results within the same cell chemistry

Inappropriately selected experimental conditions may result in confusing and/or misleading conclusions.

Undefined and varying environmental test conditions: the cell performance is known to strongly depend on the environmental conditions under which the cell is tested. Temperature for instance being the most obvious one. Detailed information about test conditions should always be given.

Unrealistic and widely variable cell composition: For example, an unrealistic excess of active and inactive components (electrolyte, carbon additive and binder, etc.) used in a given cell can substantially increase its cycle life.

Implications of undefined materials structure: Improved performance may arise from differences in the structure and morphology of the materials used. It is fundamental to report all the material properties to properly compare the results.

Challenge 2: Comparing different cell chemistries

Frequently, new emerging technologies are compared with mature commercial cell technologies, which are very well defined and use very realistic parameters. However, the same parameters cannot be easily applied to new and emerging technologies, making the comparison very challenging and leading to unrealistic conclusions.

One example demonstrating this difficulty is the comparison of the specific gravimetric capacity obtained for two different cell chemistries, such as lithium-ion and lithium-air cells.

The capacity of lithium-air cells is often reported per unit mass of the carbon “electrode” (acting as substrate for deposition of discharge product), not including the weight of the discharged product lithium oxide or lithium peroxide. This is substantially different from the lithium-ion cell case, in which the capacity is reported per mass of the discharge electrochemically active material.

In addition, the carbon “electrode” used in lithium-air systems generally present a very high porosity exceeding that of the discharged product and the porosity needed for the electrolyte to penetrate the electrode (about 30% in typical lithium-ion battery type electrodes). Moreover, the discharge products have much lower density than the typical lithium-ion cathode material. So overall, the energy density of the positive electrodes for lithium-air cells is expected to be substantially lower than that of Li-ion cells affecting the energy density (overall low active material density and large amount of electrolyte in the electrode pores). Nonetheless, all these aspects



are rarely taken into account and the reported energy density values of lithium-air system are generally exceeding those reported for lithium-ion cells when investigated at a lab scale level.

Other important examples of battery chemistries that often create difficulties in benchmarking cell performances are represented by silicon anodes and sulphur cathodes, respectively.

Challenge 3: extrapolating lab scale data to industrial scale

Lab scale testing conditions are often not directly applicable to industrial requirements. Here are two examples demonstrating why better protocols will be needed to ensure a sound evaluation of lab scale data.

Example 1: Enormous efforts have been devoted to identifying strategies to tackle the issues affecting the lithium-sulfur cell technology. Some of the proposed solutions might be useful; however, test conditions are not applicable to industry or are built on metrics that are not relevant or are misleading for practical applications.

For practical lithium-sulfur cells to reach an energy density $>500 \text{ Wh.kg}^{-1}$, the mass loading of sulfur must be at least in the range of $\sim 7\text{--}8 \text{ mg cm}^{-2}$. Such high mass loadings require thick sulfur electrodes ($>300 \mu\text{m}$). This leads, however, to serious polarization across the electrode due to rather long electronic and ionic paths through the electrode. Additionally, the metallic lithium anode capacity should be close to stoichiometry and a limited electrolyte volume should be employed. All these parameters are rarely adopted in lab-scale research cells, in which the sulfur cathode is tested with low mass loadings, high Li excess and unclear amount of electrolyte. Regrettably, the excellent performance and cyclability of low mass loading sulfur electrodes proven at lab-scale, cannot directly be transferred to a commercially viable system.

Example 2: Another interesting example is offered by hierarchically nanostructured electrodes, which generally present low tap density, making them unlikely to meet volumetric energy density demands for practical applications. However, for practical implementation high areal loading and tap density are crucial parameters to be considered. Nonetheless calendaring the electrode to increase the density, results in destroying hierarchical architectures leading to the loss of electrochemical performance.

Therefore, a direct comparison of results obtained at the lab scale and reported in literature for hierarchically nanostructured electrodes with a



mature technology which implies compromises, such as commercial lithium-ion cells, can be misleading. This is especially true for data reported in half cells where excess electrolyte and counter electrode are frequently used.

2 Classification of cell technologies

Over the years, cell technologies have been classified according to different requirements and characteristics.

The main classification arises from the reversibility of the conversion processes from chemical into electrical energy. Following this approach, non-rechargeable cells are defined as primary cells, while rechargeable cells are classified as secondary cells. However, this simple classification is already showing some limitations. For example, commercial Zn-air batteries are primary batteries, secondary (electrically rechargeable) zinc-air batteries are still under development. However, they can also be mechanically recharged (by adding more zinc once it is consumed) which adds extra confusion if not properly described.

A plethora of classifications have been proposed which so far are based on the electrolyte used (e.g., aqueous vs. non-aqueous), the chemistry (e.g. lithium-ion and post lithium chemistries) or according to their final application and expected performance requirements (e.g., high energy vs. high power), just to mention a few examples.

In order to maintain full neutrality with respect to the existing and new and emerging cell chemistries, in this report we restrict the classification to the structure of the fundamental unit, i.e., the cell.

A clear comparison between different cell technologies is facilitated by firstly defining the cell structure and consequently identifying the main constituents and characteristics.

All rechargeable cell chemistries can be split in two large families: closed cells and open cells. Different cell structures are in turn defined by the electrode nature. The many different types of existing and new and emerging cell chemistries can be identified in one of the cell configurations reported in Figure 2.



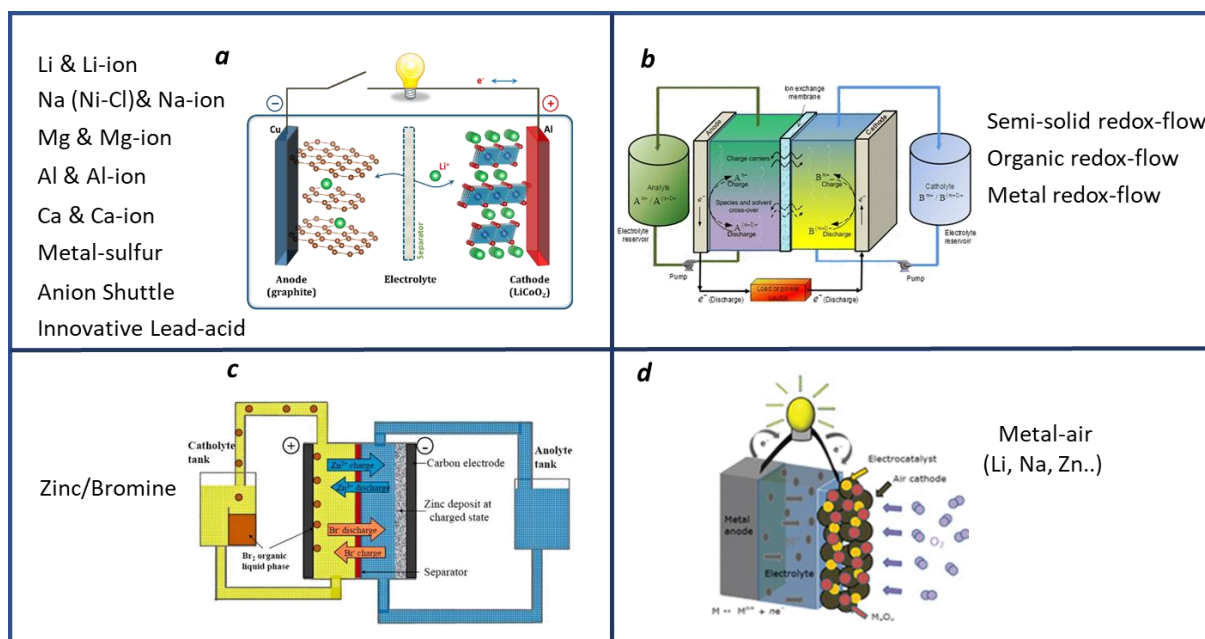


Figure 2. Architectures of existing and new and emerging cell chemistries. (a) Closed system, solid active materials; adapted from [18] (b) Closed system, liquid active materials; adapted from [19]. (c) Closed system, solid and liquid active materials; adapted from [20]. (d) Semi-open system, solid active materials; adapted from [21].

Looking more carefully at the various cell architectures it is possible to identify cells for which maximum energy storage is fixed by, at least, one electrode, i.e., Figure 2 a, c and d. For example, even though Zn-Air cells are open to the environment on one side, their energy storage capacity is limited by the total amount of zinc that is present inside the cell, while air is in endless supply. In these type of cells Energy and Power are bound because the amounts of reactants cannot be changed freely.

On the other hand, in some flow cells (see Figure 2 b) stored energy in the form of dissolved ions in the catholyte and anolyte. These can be stored outside of the electrochemical cell. Thus, the energy storage capability of flow cells depends on the size of the reservoirs storing the solutions. In these systems, the cell itself does not represent a limit to the energy storage capacity, but rather a limit to the power performance. This architecture enables independent power modulation upon changing the cell design and energy modulation by changing the size of the tanks.

Among the various flow-cell systems, Zn-Br batteries do not offer however the above-mentioned advantage. Indeed, Zn-Br cells can store bromine/bromide species in an external reservoir, but the zinc is plated on the electrode inside the converter. Thus, in Zn-Br batteries, the energy storage capacity is determined by the maximum amount of zinc that can be deposited by the surface area of negative electrode (Figure 2 c).



Similarly, metal-air cell chemistries are in general limited by the metal electrode even if oxygen is provided by air external to the cell (Figure 2 d).

Considering the different cell architectures, in this report we propose to divide all electrochemical cells into two main groups according to their capability to enable independent scaling of delivered power and energy. This concept is illustrated in Figure 3.

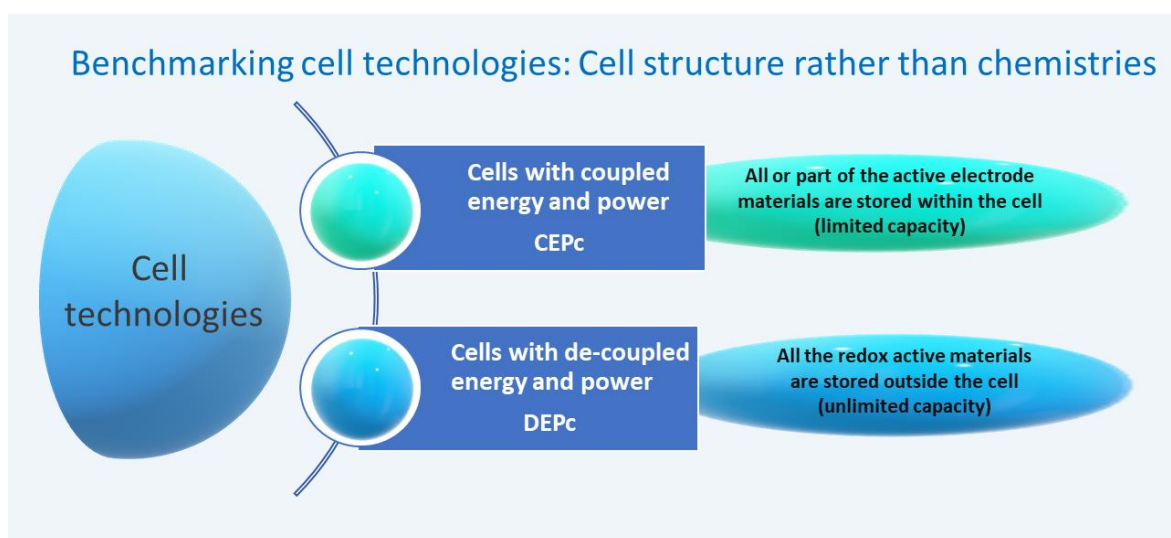


Figure 3. Cell classification according to the architecture and redox active materials configuration.

Cells in which at least one electrochemically active component is contained within the cell itself (e.g., lithium-ion or Zn-Br batteries), exhibit power and energy capabilities which are limited by the at least one of the electrodes. These types of cells are referred to as **CEPc** because their energy and power are coupled.

On the other hand, cells where all the electrochemically active materials are stored outside of the cell (e.g., conventional redox flow cells) are referred to as **DEPc**.

According to such classification, the main new emerging technologies can be grouped as follows:

Coupled Energy and power cells (CEPc)	Li & Li-ion, Na & Na-ion, K & K-ion, Mg & Mg-ion, Ca & Ca-ion, Al & Al-ion, Innovative Lead-acid, Innovative Zn & Zn-ion, Metal-sulphur, Metal-air, Anion Shuttle, Metal redox flow
Decoupled Energy and power cells (DEPc)	Metal-ion redox-flow, Organic redox-flow, Semi-solid redox-flow



This classification enables a direct comparison among cell technologies within the same class, although the direct comparison between CEPs and DEPs system is not trivial.

3 Reporting requirements; EU and national projects

A list of the most relevant parameters (or Key Performance Indicators, KPIs) to identify the performance of a battery cell include:

- Energy density of the cell (volumetric and gravimetric)
- Charge/discharge rate capability and characteristics for CEPc and power density vs. current density characteristics for DEPC
- Coulombic efficiency and Energy efficiency at operating condition.
- Cycle-life (degradation and aging phenomena)
- Shelf-life (degradation and aging phenomena)
- Operating temperature / back pressure (for metal-air)
- Technology readiness level (TRL)
- Preliminary materials and cell costs

Generally, only a few specific targets on performance, cost and sustainability are defined for each specific call depending on the foreseen application.

However, the use by projects of narrower KPI-sets, KPIs taken in isolation and/or ill-defined KPIs can sometimes result in amazing but false extrapolations.

For example, the “self-discharge” KPI has rarely been included in recent calls, although it is an extremely important parameter to qualify the energy efficiency or energy density of a certain cell chemistry.

The result of incompletely defined KPIs or incompletely selected KPI-sets can lead to overly optimistic results or conclusions, even if theoretically correct. This can induce wrong expectations and subsequent decisions, whether it be from EU and governmental agencies, industry or the general public.

For example, the theoretical energy of a “new” chemistry is often compared with the practical performance of an existing chemistry. This overly optimistic comparison is amongst the easiest to spot, but others are more subtle. Reporting the gravimetric performance of nanostructured materials without giving their tap density for example, ignoring the weight or volume



of other active component (*e.g.*, conducting graphite, binders, *etc.*) when needed in large amounts, or neglecting the weight and volume contribution of the electrolyte for a certain chemistry where it is an active component, will certainly mislead readers not skilled in the field. An extensive list is out of the scope of this report, but interested readers can refer to a few specific publications^[1,14,22-26].

Another point in argumentation is the fact that, often, materials are required to simultaneously present high energy and power capabilities. These two KPIs are known to be usually in conflict with each other because their optimization requires different cell designs (lower loadings can provide more power for example).

4 Reporting requirements in Scientific journals

To create a common ground for reporting research results related to batteries in scientific papers, several scientific publications and editorials have recently been made^[24-26]. The editorial board of Journal of Power Sources recently published a comprehensive document entitled "Good practice guide for papers on batteries for the Journal of Power Sources"^[1]. The editorial team at Joule (Cell Press) also recently published Standardized Battery Reporting Guidelines accompanied by a battery checklist. Authors submitting battery focused manuscripts should provide the checklist at the time of submission^[27]. Additionally, within the activities of WG1 in Batteries Europe, a series of critical reports have been compiled by leading scientists dealing with the most promising new and emerging cell chemistries^[6-13,28,29].

All the above-mentioned documents represent a good foundation for the proper reporting aiming at reducing the occurrence of "overly optimistic" predictions and claims and promoting a more realistic and effective assessment of new and emerging cell chemistries.

In the following, the most common parameters resulting from electrochemical tests, *i.e.*, reported in scientific literature, are defined and some critical observations are highlighted.

It is worth mentioning that some of these parameters can refer to a single electrode, *i.e.*, specific capacity, coulombic efficiency, while others, *i.e.*, energy and power density and energy efficiency, are always referring to cells.



Specific Capacity (Q in mAh g⁻¹): This quantity can be referred to a specific electrode material as well as to the entire cell. It represents the amount of electric charge delivered (discharge) or stored (charge) per unit mass. The specific capacity is the integral of the specific current (I in mA g⁻¹), m is the mass of the materials or the cell, flowing in an electrode or a cell in a discharge or charge time period (t in h), according to the equation:

$$Q = \int I(t) dt$$

It is worth noting that in most of the scientific literature, when calculating the specific capacity, only the mass of the active material is considered, excluding the weight of inactive components (binder, conductive agents, current collector, ...). In order to compare different electrodes, chemistries or morphologies, it is important that the exact electrode composition, including the current collector, and density are also given, as well as the testing parameters (temperature, specific current, pressure when gaseous reactants are used...). When reporting results or extrapolations to a complete cell, the specific capacity values can be given with respect to one or both of the active materials, but details about all inactive components should also be given.

Specific Cell Energy: (E in Wh kg⁻¹) is a quantity that can be defined only for complete (full) CEP cells. It is obtained by integrating the product of the specific current (I in A kg⁻¹) flowing through the cell and the voltage (U in V) upon the time (t in h) of discharge until the cut-off voltage is reached.

$$E = \int I(t) * U(t) dt \approx Q * (U)_{average}$$

Often the values reported in the literature are extrapolations based on results for one (versus a reference electrode, e.g., Li metal) or both electrodes, but taking into consideration only the weight of the active material(s). For Li-ion cells, it is assumed that the weight of inactive components accounts for roughly 50% of the total cell weight, enabling an easy evaluation of the cell's specific energy. However, this "rule of thumb" applies only for specific cell designs and cannot be easily transferred between different chemistries. This is especially true for chemistries in which the electrolyte is also an active component, or which require large amounts of conductive additives and/or binder, or non-flat current collectors. Once more, the detailed information mentioned above should always be included.



Specific Cell Power: (P in W kg^{-1}) of a complete CEP cell is obtained by multiplying the cell output voltage (U in V) by the specific current (I in A.kg^{-1}). The output voltage is a function of state-of-charge (Q) which is a measure of the specific capacity stored in the materials. It also depends on the current ($V=IR$)

$$P = U(Q) * I$$

The specific (gravimetric) values of, e.g., capacity, energy and power, can be converted into the volumetric equivalents (and vice versa) by considering the density (in g cm^{-3}) of the active material or the electrode or the entire cell. In the scientific literature, the volumetric performance values are rarely reported and difficult to calculate due to a lack of the cell component density values and the overall cell design. Among these, the geometrical electrode density is the easiest to evaluate and should always be supplied. In fact, it can be calculated by dividing the electrode's weight by its volume, which is the product of the electrode's thickness and (geometric) area. The minimum requirements should also include the crystallographic and tap density values, especially for those technologies claiming potentially high volumetric energy density.

Other important parameters for the evaluation of a specific cell chemistry are the Coulombic, Voltaic and energy efficiencies.

Coulombic efficiency: (C_{Eff} in %) defines the efficiency of a charge-discharge process as the ratio between the discharge and charge capacity.

$$C_{\text{Eff}} = (Q_{\text{discharge}} / Q_{\text{charge}}) \cdot 100\%$$

This parameter applies to both electrodes as well as complete cells.

The Coulombic efficiency is a fundamental parameter giving hints on the reversibility of the process. It is important in closed systems, e.g., Li-ion cells, where a low Coulombic efficiency value (besides the first cycle) indicates the occurrence of parasitic reactions to consuming one or more cell components. It is particularly important at low discharge rates where parasitic processes would affect the C_{Eff} the most. It can also provide hints on the occurrence of self-discharge processes.



Energy efficiency: (η in %) indicates how efficiently energy can be stored in the cell. It is obtained by dividing the specific energy (as described above) obtained on discharge divided by that obtained on charge.

$$\eta = (E_{\text{discharge}} / E_{\text{charge}}) \cdot 100\%$$

It is suggested that this important parameter has to be defined specifically at a complete cell level and between 0 and 100% SoC..

Voltaic efficiency: (V_{Eff} in %) is an index of the sum of all the different overvoltages present in the cell resulting by the presence of internal resistances. It is obtained by dividing the discharge average voltage ($U_{\text{discharge}}$) by that obtained on charge (U_{charge}).

$$V_{\text{Eff}} = (U_{\text{discharge}} / U_{\text{charge}}) \cdot 100\%$$

C rate: generally referring to CEP cells, the C-rate is a measure of the rate at which a cell is discharged relative to its nominal capacity. For instance, a 1C rate means that the discharge current will discharge the entire cell in 1 hour. For a cell with a capacity of 100 Ah, this equates to a discharge current of 100 A. A 5C rate for this cell would result in a 12 minute discharge at 500 A, and a C/2 rate would correspond to 2 hour discharge at 50 A. The C rate is used in order to normalize the cell performance against its capacity.

Cycle life: It is expressed in terms of the number of cycles that the cell can achieve before its capacity falls below a given threshold (usually 80% for EV). This parameter is very dependent on the depth of discharge (DOD) and the charge/discharge rate. Thus, it is important to report with the total number of cycles these testing parameters. In addition, the current density and the voltage range employed for the cycling test are also necessary parameters.

Self-discharge (%): Self-discharge occurs in every type of cell and depends on their chemistry. This characteristic is rarely reported and analysed for new cell technologies (at least in scientific publications) although it is of fundamental importance for determining the energy efficiency of the cell as well as it indicates the occurrence of unwanted side reactions.

Alignment of these reporting parameters to already available values is recommended to facilitate their wide implementation along the whole battery value chain.

5 Guidelines for the comparison of new cell technologies



With the introduction of new cell chemistries and technologies, new reporting guidelines need to be established.

Electrochemical cell tests should provide reproducible and useful data enabling the accurate comparison within a given cell chemistry and between different cell chemistries. The information and data provided need to be at least sufficient to characterize and define the initial cell performance but also to quantify degradation over the cell lifetime. Finally, preliminary safety testing and chemical hazard evaluations would be a valuable addition.

The new guidelines aiming at establishing comparable performance metrics and a transparent reporting methodology should include:

- Cell components characteristics
- Details on the electrochemical measurements (electrochemical set up, testing conditions and obtained KPIs)

Among all useful information, KPIs are a set of performance metrics enabling the initial comparison of cell chemistries and technologies. However, at the materials level, the characteristic of the active materials and the final electrode's composition and properties should be given with sufficient detail for a fair analysis of the material performance to be possible. In fact, cell components (and their constituents) are defined by characteristics and not by KPIs.

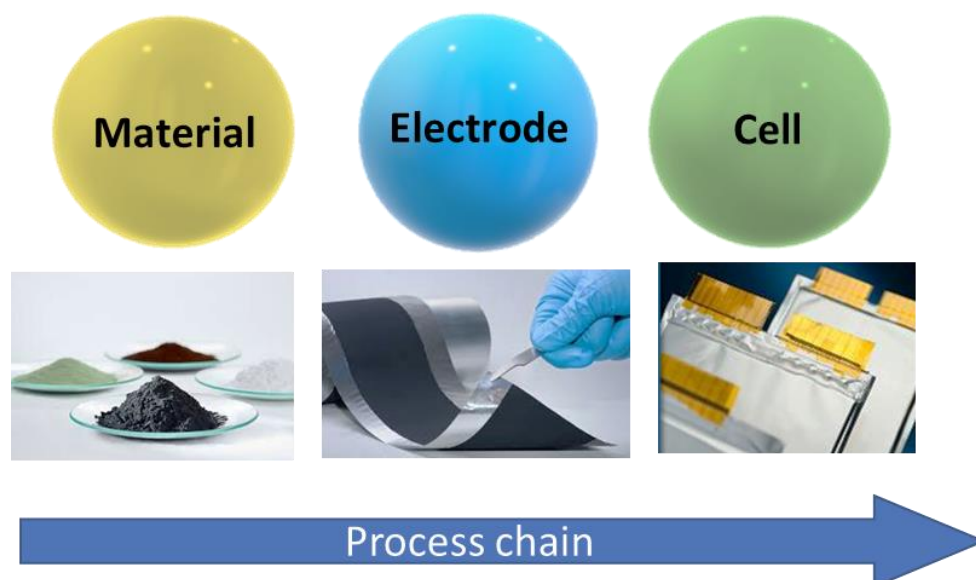


Figure 4. From materials to cell level.



5.1 Cell components characteristics

Comparing new cell chemistries and technologies with existing ones requires the evaluation of all the cell components that can influence the performance of the final cell. The following cell components are certainly the most important:

- Electrodes (for CEPc and DEPC)
- Electrolytes for CEPc
- Separators (for CEPc and DEPC)
- Current Collectors (for CEPc and DEPC)

5.1.1 Active electrode materials and electrodes

In the development of new and emerging cell chemistries, a large part of the ongoing research effort is devoted to new materials discovery and the assessment of their performance in electrochemical cells. In such endeavours, accurate reporting and precise description of the synthesis procedure is important to facilitate comparison of results among different reports.

In scientific publications, all synthesis steps should hence be described in detail, allowing for the assessment of reproducibility in other laboratories. Information associated to the scale of the synthesis (size of batch) should be provided. All the chemical precursors/solvents should be described in terms of supplier, purity, and other possible pre- and post-treatment processes (such as purification or drying) after purchasing. Synthesis conditions such as temperature, pressure, environment, concentration, amount of starting material, pH etc., should be given.

The obtained material should be described in terms of stability, and methods of further handling/storage (such as under either inert or ambient conditions) should be given.

Each new material should be characterized in terms of chemical composition, physical and mechanical structure and morphology. This should be accompanied by the detailed experimental conditions used for the analysis, including sample procedure preparation and experimental protocol for analysis and accuracy of determined values. This will ultimately enable a better comparison of data to be made, offering a clear overview of the materials properties.



Regarding the electrode assembly process, details should be provided about the binder and other non-active components, the solvent (if any) used for the slurry preparation, the drying procedure, calendaring and other relevant process parameters and compounds.

Overall, going from materials to electrodes (for tests in electrochemical cells) it is important that the following characteristics are given:

Table 1. Characteristics for active materials and electrodes used in CEPc and DEPC cells.

Coupled Energy and Power Cells (CEPc)
Active Material
Chemical composition and properties (stability, corrosiveness)
Thermal stability
Structural information (crystallographic properties, phase purity)
Morphology (imaging and particle size)
Bulk and tap densities, crystallographic density, porosity, surface area
Cost (at least a preliminary estimation, ore actual market price)
Toxicity (at least a preliminary estimation based on MSDS)
Sustainability of sourcing of raw materials (at least a preliminary estimation on availability of resources and ease of recycling)
Electrode
Formulation (including binder, conductive additives, slurry processing conditions, pH (if aqueous processing is applied), ...)
Type of electrode (compressed powder/pellet, (3D)-printed, coated on a metallic foil/mesh, ...)
Areal loading
Thickness (active material layer and substrate)
Porosity (pore volume) or geometrical density
Active and geometrical surface area
Packing density
Mechanical properties (adhesion and bending radius, if critical)
Current density (for standard charge and discharge)
Specific capacity (for standard charge and discharge)



Working potential (vs. counter or reference electrode) in V; (info on reference electrode should be given)
Test Temperature
Test pressure in the case of gaseous reactants
Operating Voltage window (upper and lower cut off voltage)
Decoupled Energy and Power Cells (DEPC)
Active Material
Chemical composition and properties (pH included, corrosiveness, ...)
Thermal stability
Physical-chemical properties (viscosity, density,..)
Volumetric and specific capacity (charge and discharge)
Voltage stability window
Long term stability (aging) (chemical, electrochemical, i.e., degradation potential)
Operating temperature limits
Cost (at least a preliminary estimation (ores actual market price)
Toxicity (at least a preliminary estimation based on MSDS)
Sustainability of sourcing of raw materials (at least a preliminary estimation of availability of resources and ease of recycling)
Inert Electrode
Chemical composition (formulation if composite material)
Porosity (pore volume) or at least the geometrical density of the electrode
Active surface area
Test cell structure (flow factor, static-flow mode, define kind of cell)
Current density in mA cm ⁻² (charge and discharge)
Working potential, degradation potential (vs. counter or reference electrode);
Thickness
Electronic conductivity (changes upon compression)
Wettability



5.1.2 Electrolytes

Table 2. Characteristics for electrolytes used in CEPc and DEPC cells.

Coupled and Decoupled Energy and Power Cells (CEPC and DEPC)
Chemical composition (at least for the main components, additives included (wt.% or vol.%))
Overall weight and volume employed in the cell (includes filling of electrode porosity and stoichiometric if participating in the electrochemical reactions)
Thickness (if critical)
Chemical properties
Thermal properties (including melting temperature and flash point)
Density
Rheology (liquid and hybrid gel-electrolytes)
Ionic Conductivity (total and effective, if feasible)
Electronic conductivity (Solid state technologies)
Electrochemical stability window on standard electrodes (Pt, carbon black, current collector, ...);
pH (for aqueous electrolytes)
Relevant impurities (H ₂ O for non-aqueous electrolytes)
Cost (at least a preliminary estimation on ore actual market price)
Toxicity (at least a preliminary estimation based on MSDS)
Sustainability of sourcing of raw materials (at least a preliminary estimation of availability of resources and ease of recycling)



5.1.3 Separators

Table 3. Characteristics for separators used in CEPc and DEPC cells.

Coupled and Decoupled Energy and Power Cells (CEPc and DEPC)
Chemical composition
Thickness
Areal weight
Density
Porosity & Tortuosity
Wettability toward electrolyte or surfactants
Cross over (selectivity)
Mechanical properties (swelling, shear force, fatigue)
Operative temperature range (less than 10% change of properties)

5.1.4 Current collectors

Table 4. Characteristics for current collectors used in CEPc and DEPC cells.

Coupled and Decoupled Energy and Power Cells (CEPc and DEPC)
Composition (including purity requirements)
Morphology (flat foil or three-dimensional structured)
Density (bulk material and current collector morphology)
Thickness
Surface treatments

5.2 Electrochemical set-up, measurements and KPIs

Transparency in reporting the selected electrochemical cell set-up and all testing conditions during electrochemical measurements is the first step for a realistic comparison between new cell technologies.



As several laboratory-scale cell setups (beaker, Swagelok-type, coin (button), and pouch cells) may be employed to test novel chemistries, the electrochemical performance of a material could be affected differently by the various cell configurations. Even when a new component such as an electrode is used in conjunction with standard commercially available components, particular cell characteristics such as a large electrolyte volume (e.g., in beaker cell) or a large counter electrode could artificially increase the performance of poor electrochemical systems.

A typical example is the common performance evaluation of electrode materials for application in lithium-ion cells employing oversized metallic lithium or well-known insertion materials as counter electrodes in the so-called “half-cell configuration”. This half-cell set-up is used to determine specific thermodynamic characteristics of the investigated materials, but requires the use of a counter electrode (e.g., lithium or sodium metal) which could contribute to the overall electrochemical activity. Additionally, these counter electrodes are usually oversized with respect to the investigated one, frequently hiding poor Coulombic efficiency in full cell configuration. On the other hand, these metal counter electrodes contribute, via side reactions with the electrolyte, to the formation of reactive compounds which in their turn affect the electrode under investigation. Therefore, additional limitations may apply when half-cells are used for characterization of a new material.

The assessment of the performance of cells requires the measurement and quantification of a series of performance metrics. Although performance metrics for individual electrodes are important (evaluated in half-cells), the evaluation of electrodes in practical cell configuration is critical for the identification of the true cell performance.

The following KPIs, referring to complete cells without casing (if casing is included it should be specified), are required for the appropriate performance comparison of different cell technologies including the commercial ones:

Table 5. List of KPIs for complete CEPc and DEPC cells.

Necessary KPI's
Cell type (pouch/cylindrical/prismatic, coin cells, two/three electrode T-cells) and size
Anode/Cathode balance (mass or capacity ratio)
Specific energy and energy density of the cell at two specific C rates (C/10 and 2C rate) or current densities upon (dis-)charge



Energy efficiency of the cell at C/10 and C rate (dis-)charge
Coulombic efficiency of the whole system at C/10 and C rate (of choice) (dis-)charge
Cycle life (upon SOC change per cycle of at least 80%)
Test temperature
Pressure/compression requirements during operation and cell manufacturing.
Cell volume variation % at (dis-)charge (if measurable)
Optional KPI's (according to availability of results)
End of charge voltage
End of discharge voltage
Average (dis-)charge voltage at C/10 and a second C rate appropriate for a specific application
Overcharge behavior
Overdischarge behavior
Preliminary safety assessment

It is also important to specifically identify the testing conditions including environmental conditions such as temperature, flow rate in flow systems, pH and the experimental set up (cell geometry, potential window for testing, etc...) which inevitable affect the above listed KPIs.

5.3 Safety testing & chemical hazards evaluation

Even if they are not paramount for a first level evaluation, preliminary safety testing and chemical hazards evaluations should be encouraged (especially for high TRL technologies) in order to ascertain the feasibility of developing a new cell chemistry. The following list identifies the simplest parameters that could be assessed and given along with the development of a new cell chemistry or, even more, the development of new materials for existing cell chemistry.



Table 6. List of *preliminary* safety, toxicity hazards characteristics for complete CEPc and DEPC cells.

Coupled and Decoupled Energy and Power Cells (CEPc and DEPC)
Cell component level;
Toxicity from MSDS (mandatory for commercial materials, if available for in lab made materials);
Thermal stability of electrolyte in combination with charged electrodes
Emissions related tests (mainly gas detection)
Flammability tests (determination of the flammability of each cell component and its emissions and decomposition products)
Cell level
Safety testing towards thermal runaway evaluation (e.g., short circuit, overcharge, overdischarge);
Self-heating properties (thermal behavior in adiabatic conditions);
Emissions related tests (mainly gas detection);

6 Summary and outlook

In order to homogenize cell information including new and emerging technologies, this document principally refers to characteristic and performance metrics at the cell level, including its constituent components.

Alignment to these reporting guidelines is highly recommended to facilitate the comparison of cell characteristics especially when considering new cell chemistries.

This document aims at defining reporting guidelines whose implementation should be as wide as possible.

For a successful implementation, the suggested reporting methodology needs to be adopted by a majority of scientists and implemented in all EU funded battery-related projects for monitoring the progress beyond the state-of-the-art. In addition, the reporting guidelines could, for example, be recommended as a requirement for publications originating from the EU funding in scientific journals.

Whilst this development will not have an immediate impact, it will set a best practice for results' reporting and will reduce the occurrence of "overly optimistic" claims often occurring in the field of battery research.



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