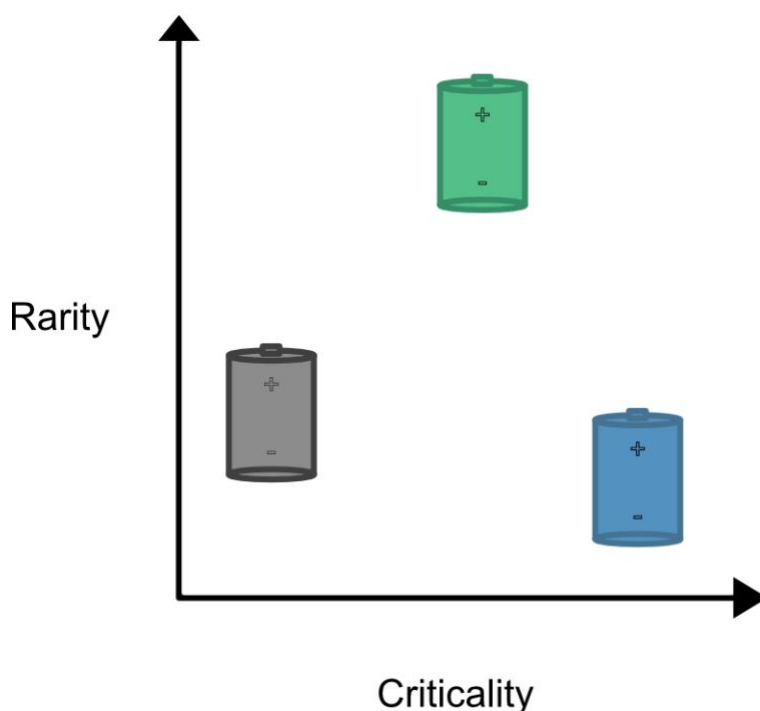




Screening resource assessment of next-generation battery chemistries

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CHALMERS UNIVERSITY OF TECHNOLOGY
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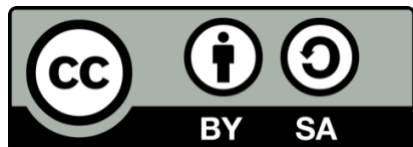
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SUMMARY

Rechargeable batteries are used in a number of applications of high societal importance, including various types of electronics and electric vehicles. Many of those batteries currently in use contain rare and/or critical chemical elements and materials. In this study, we identify next-generation battery chemistries based on a survey sent out to organizations within the Batteries Sweden (BASE) competence centre. The identified chemistries are then assessed regarding their resource requirements, applying a screening resource assessment method developed within the study. The method considers the crustal rarity and criticality of the materials contained within the battery cell, from the perspective of the European Union. The results from the screening assessment show that two types of multivalent batteries (one specific calcium-based battery cell and one specific aluminium-based cell) contain the lowest number of rare and critical materials of the batteries assessed, while a certain type of lithium-ion battery cell (nickel-manganese-cobalt, NMC) contains the highest number of rare and critical materials. The developed screening method can be used by BASE members and other relevant actors to identify battery chemistries with promising resource performance for further, more detailed resource assessments, such as life cycle assessment and material flow analysis.

SAMMANFATTNING

Laddbara batterier används i flera applikationer av stor samhällelig vikt, såsom olika typer av elektronik och elfordon. Många av dessa batterier som används för närvarande innehåller sällsynta och/eller kritiska kemiska grundämnen och material. I denna studie identifierar vi nästa generations batterikemier utifrån en enkät som skickades ut till organisationer inom kompetenscentrumet Batteries Sweden (BASE). De identifierade batterikemierna bedöms sedan gällande sin resursanvändning genom att applicera en förenklad resursbedömningsmetod som tagits fram inom ramen för studien. Metoden tar hänsyn till sällsyntheten i jordskorpan och kritikaliteten hos materialen i en battericell utifrån den Europeiska unionens perspektiv. Resultaten från den förenklade bedömningen visar att två typer av multivalenta batterier (en särskild kalciumbattericell och en särskild aluminium-baserad cell) innehåller det minsta antalet sällsynta och kritiska material av de batterier som bedöms, medan en särskild typ av litiumjonbatteri (nickel-mangan-kobolt, NMC) innehåller flest sällsynta och kritiska material. Den framtagna förenklade metoden kan användas av medlemmar inom BASE och andra relevanta aktörer för att identifiera batterikemier med lovande resursprestanda för ytterligare, mer detaljerade resursbedömningar, såsom med livscykelanalys och materialflödesanalys.

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1. Introduction

1.1 Background

Rechargeable batteries are nowadays used in many applications, including electric vehicles, various types of electronics and large-scale energy storage, and batteries are seen as key enablers for decarbonizing the transportation and energy sectors (Eurobat, 2020). According to Edström et al. (2020), the global battery demand will increase 14 times between 2018 and 2030, with almost 20% of that increase projected to be produced in the European Union. Lithium-ion batteries represent the dominant rechargeable battery technology today, and their success is linked to a high energy density, long cycle life and safety (Armand et al., 2020). However, many lithium-ion batteries contain geochemically rare metals, such as cobalt, nickel and lithium. In addition, all the mentioned metals plus the material graphite, which is used as anode material, are considered critical from a European perspective (European Commission, 2020a). Meanwhile, there is ongoing research that explores a wide range of new batteries based on at least two underlying rationales. One is the strive for increased technical performance, where, e.g., the lithium-sulfur battery is expected to reach a practical energy density 2-3 times higher than the current state-of-the-art lithium-ion batteries (Demir-Cakan et al., 2017). Another rationale is related to resource availability, where, e.g., sodium-ion batteries are being advocated because they show great promise from a resource point of view (Tapia-Ruiz et al., 2020).

Since some natural resources used for producing batteries, primarily metals and minerals, are non-renewable, it is important to understand how they can be used in a sustainable way. Furthermore, if Europe is to succeed in producing 20% of the global battery demand in 2030, the battery raw materials must be available. There are different perspectives on resource availability, such as physical availability from a long-term perspective as well as availability stemming from more short-term economic and societal constraints (Sandén et al., 2014). The latter perspective is captured in the term “criticality”, which refers to the risk of supply disruption of a given raw material of high economic importance for a certain actor, e.g., ranging from larger economies, such as the European Union (EU), to single companies within its economy (Graedel and Reck, 2015). Hence, materials that are critical for one economy might not be critical for another. Examples of criticality assessment approaches can be found in, e.g., Bach et al. (2017) and Erdmann and Graedel (2011). The physical availability, on the other hand, is captured in geochemical “rarity”, i.e., the concentration of the elements in Earth’s crust (Graedel et al., 2015b; Skinner, 1976). A third term relevant in this context is “scarcity”. A raw material is scarce when it is not available in sufficient quantities to meet societal demands (Sandén et al., 2014). As a summary, it can be noted that a rare raw material is at risk of becoming scarce when demand increases, and then also even critical for a particular industrial sector. However, in neither case does this only depend on the materials’ average rarity, but also on the societal capacity to make this material available to those who need it, in terms of extracting and refining, as well as in terms of distribution through global trade.

When assessing the resource implications of new batteries, it is challenging to select a representative assessment object considering that there are often a high number of variants of a certain new battery. This is a well-known phenomenon when it comes to new technologies. Gröbler (1998) describes the early stage of technology development as a chaotic phase, where many different designs are explored. Another issue when assessing emerging technologies, regardless if a study includes environmental impacts, resource impacts or other types of impacts, is the lack of data. At the same time, the early development stage constitutes an opportunity for making changes in the technology, since some design parameters have not yet been locked into a dominant solution. This is sometimes referred to as the “control dilemma” after being described by Collingridge (1980), which states that: when a technology can be controlled, there is too little information about its implications, whereas when there is sufficient information, the technology is entrenched in society and therefore very difficult to challenge or modify to any larger extent. Rarity is one aspect of resource use that could be important to consider when developing new batteries, when there is still a possibility to alter them, as it links to a risk for long-term raw material scarcity. Current EU statements on materials regarded as critical for its internal market as a whole can also be an interesting aspect to consider for current battery development within this geographical region, despite the shorter time horizon captured by this classification, as it points to raw material production and supply challenges that might persist also for the coming decades.

One way to identify, at an early stage of technology development, if the materials used in a battery are critical and/or rare, is to assess those battery materials using a screening method with low data demand. Most resource assessment methods, such as life cycle assessment (Finnveden et al., 2009) and material flow analysis (Graedel, 2019), have a relatively high data demand, which is generally difficult to fulfill at an early development stage. An available tool for simple screening of resource implications with a European perspective is the Resources Scanner. Using this tool, the developer can screen to what extent materials that the new technology depends on pose a risk to the developer’s business (Grundstoffenscanner, 2021). The developer can choose to screen different product groups, categories or raw materials of their interest, and obtain information regarding e.g. price fluctuations, reserve magnitudes and recycling rates. There is currently no data on batteries in Resources Scanners’ database, but there are several important battery materials included, such as natural graphite, lithium and cobalt. However, the Resources Scanner mainly considers short-term resource implications, rather than long-term impacts. In addition, it provides information about several (>10) different parameters. Such comprehensive information allows for a detailed analysis about possible supply disruptions, but it does not give a definite answer to, e.g., whether a material should be considered critical. Considering the absence of a simple screening tool that can be used to assess both the rarity and the current EU criticality of battery materials, such a method was developed within this study.

1.2 Aim

This study was conducted within the scope of Batteries Sweden (BASE). BASE, which this study aims to assist, is a platform for developing materials, components, and devices for future generation batteries (BASE, 2021). The aims of this study are:

- to identify batteries that members of BASE currently work with, but also those that can constitute the next generation of batteries,
- develop an easy-to-use resource screening method, and
- to conduct a screening assessment of the identified batteries in terms of resource rarity and criticality, using the developed method.

Based on the assessment results, BASE members and other relevant actors can obtain indications of which next-generation batteries are promising from a resource perspective. In addition, the screening method will be developed to enable relevant actors to assess their own batteries under development regarding criticality and rarity at early stages of battery development, far in advance of commercialization. Since this study aims to assess criticality as one of aspects of resource use, it follows that a specific geographical scope has to be defined. BASE has a Swedish focus, but we select the EU as the most relevant region for three reasons: (i) Sweden is a member of the EU, (ii) the future projected battery production within the union is relatively high and (iii) there is readily available EU data regarding criticality. However, while an EU perspective is used for the criticality assessment, the screening assessment can still be conducted for other regions given that data is available about which materials that are critical for that specific region.

2. Methods

2.1 Survey and literature study

The information on battery chemistries in this report is gathered through a survey, sent out to all 20 organizations within BASE. The survey is sent out via the respective contact person of the organization with the aim of mapping which battery chemistries members are working on today (Question 1 below), and which battery chemistries members consider promising for the future (Question 2 below). The survey consists of four questions:

***Q1:** Which battery chemistries do you work with right now?*

***Q2:** Which battery chemistries do you find promising for the future, regardless if you work with them or not? Please also motivate why you think so.*

***Q3:** Do you know of any review articles or roadmaps of post lithium-ion chemistries that you find interesting and/or important? Please provide references.*

***Q4:** Other companies or organizations that might be of interest for this study?*

Questions 3 and 4 are asked in order to facilitate the literature study and dissemination of results, respectively. It is also possible for the participants to leave any additional comments they find important.

The response rate of the survey is 50%. Based on the answers, a number of new and current battery chemistries that are considered promising by several respondents are identified. It should be noted that battery chemistries can be promising for many different reasons, such as high energy density, usage of low-cost materials and safety aspects.

The literature study is conducted in order to obtain information about the identified battery chemistries. The main roadmaps, review articles and other types of publications studied are:

- The roadmap “Inventing the sustainable batteries of the future. Research Needs and Future Actions” by Edström et al. (2020)
- The roadmap “2020 Roadmap on Sodium-Ion Batteries” by Tapia-Ruiz et al. (2020)
- The review paper “Lithium-ion batteries – Current state of the art and anticipated developments” by Armand et al. (2020)
- The book “Li-S Batteries. The challenges, chemistry, materials and future perspectives” by Demir-Cakan et al. (2017)
- The review paper “Lithium solid-state batteries: State-of-the-art and challenges for materials, interfaces and processing” by Boaretto et al. (2021)
- The book “Batteries for Electric Vehicles. Materials and Electrochemistry” by Berg (2015)
- The review paper “Current status and future perspectives of lithium metal batteries” by Varzi et al. (2020)
- The review paper “Multivalent rechargeable batteries” by Ponrouch et al. (2019)
- The review paper “Magnesium batteries: Current picture and missing pieces of the puzzle” by Dominko et al. (2020)

2.2 Screening resource assessment

A screening resource assessment method is developed and applied for a total of nine battery chemistries, which are selected based on which battery chemistries are reported as promising in the survey. The assessment is performed both to test the usefulness of the developed screening resource assessment method, but also to assess the battery chemistries and obtain results regarding their resource implications. The procedure of this screening assessment method is outlined in the following paragraphs.

First, different components of the battery chemistry are identified in more detail. The working unit of a battery is the electrochemical cell, i.e., the battery cell, which consists of the following components: an anode (the negative electrode), a cathode (the positive electrode), an electrolyte and one or two current collectors, as shown in Figure 1 (Berg, 2015). For the purpose of defining the material composition of different cell components, it can be useful to categorize batteries on different conceptual levels. We base this categorization on Berg (2015) and Edström et al. (2020). First, batteries can be divided into different general battery *concepts*,

such as solid-state batteries, liquid electrolyte batteries, flow batteries and similar broad categories. In addition to these concepts, there are other types of general battery concepts which relate to the constituting active materials of the battery, such as lithium-ion batteries and lithium-sulfur batteries. In order to differentiate the terminology for different types of concepts in the design, we refer to the latter material-related type of concept as a *group* in this report. Additionally, within each concept and group there are specific battery *chemistries*. An example of a chemistry is the nickel-manganese-cobalt (NMC) cathode combined with a graphite anode and an organic electrolyte, which constitutes a specific chemistry within the liquid electrolyte concept and the lithium-ion group. In Figure 2, a Venn diagram illustrating the relationship between the terms is presented. On an even more detailed level, there are variants on *component* level, e.g., the NMC 333 cathode and the NMC 811 cathode, where the difference is in the mass composition of the three constituent elements nickel, manganese and cobalt. For the assessment, we include the cell components anode, cathode and electrolyte. In addition, specific example component materials are selected from descriptions in relevant review articles.

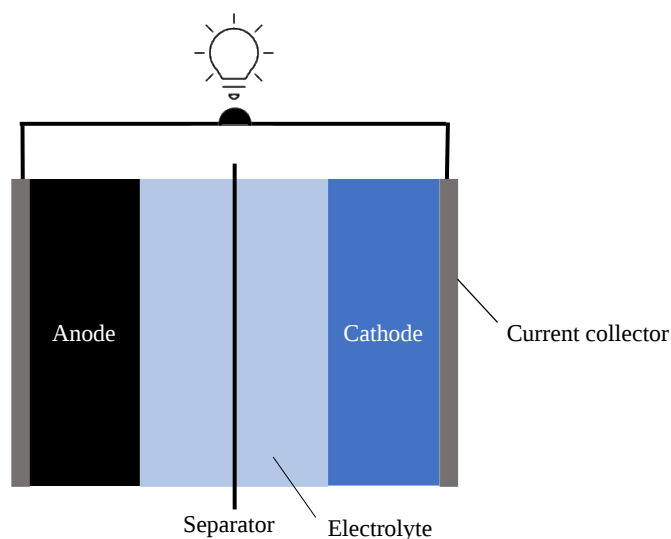


Figure 1. Components of an electrochemical cell based on Berg (2015).

Note that the illustration in Figure 1 specifically represents one of the most common battery concepts, namely a liquid electrolyte battery. For this battery concept, a separator is also required to avoid contact between the anode and cathode through the electrolyte (Berg, 2015). As can be seen in Figure 1, the anode and cathode are separated by an electrolyte. Most cathode and some anode materials are coated onto current collectors, which in turn connect to tabs. The tabs can then be connected to an external conductor. Separator materials are not included in the cell configurations presented in the Results section (Section 3), since one type of separator is dominating (microporous polymeric membranes), in particular for current lithium-ion batteries (Berg, 2015) but also as envisioned for some next-generation batteries (Arvidsson et al., 2018). These membranes often consist of polyolefin compounds and are therefore of limited interest in a resource screening of the kind performed here. Minor electrolyte additives are also excluded, since they vary notably and generally constitute minor shares of the electrolyte

material content. Finally, current collectors and tabs are also excluded since they are normally not considered parts of the cell chemistry.

When a cell configuration in terms of concept, group, chemistry and common components have been specified, both the criticality and rarity of the battery cell are assessed. Criticality assessments usually assess materials using two parameters, namely (i) the risk of supply disruption and (ii) economic importance, thus having a relatively short time horizon due to the focus on current supplies and the current economic situation. The higher the value of both parameters, the more critical is a material considered to be. Depending on the method, materials can be regarded as critical or non-critical on a binary scale, as in the EU method (European Commission, 2020b), or materials can be compared based on their relative criticality, as in the Yale method (Graedel et al., 2015a). The latter method also includes a third criticality parameter, which is environmental implications. For this study, the EU's method and its list of critical raw materials is applied (European Commission, 2020a).

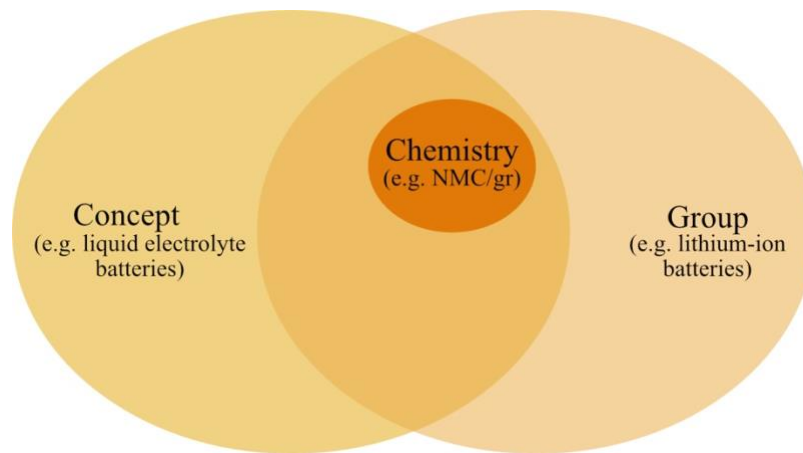


Figure 2. A Venn diagram showing the relationship between three different battery category terms: (1) Concept, (2) Group and (3) Chemistry. NMC/gr=nickel-manganese-cobalt/graphite. The area where concepts and groups overlap represent all chemistries for the given combination of concept and group.

Long-term resource impacts of resources in Earth's crust are connected to their geochemical rarity and therefore apply on a global level. For these impacts, we use a newly developed life-cycle impact assessment method called the crustal scarcity indicator (CSI) developed by Arvidsson et al., (2020a), which is based on crustal concentrations of chemical elements. For a given element, its crustal concentration is compared to the crustal concentration of silicon, since silicon is the most abundant element in the crust, and the resulting value is referred to as the element's crustal scarcity potential (CSP). The CSP of an element i extracted from Earth's crust is calculated as:

$$CSP_i = \frac{1/c_i}{1/c_{Si}} \quad (\text{Eq. 1})$$

where C is the crustal concentration (ppm). In addition to chemical elements, this method has been extended to include also minerals, rocks and ores based on their respective elemental composition (Arvidsson et al., 2020b). While this method is developed to be used within the life cycle assessment framework, the CSPs can also be used in general assessments of geochemical rarity since a CSP merely represents the inverse crustal concentration of an element relative to that of silicon.

Figure 3 shows a decision tree with the different steps used to assess resource rarity and criticality in this study. The idea is that the decision tree should also be possible to use for developers or other relevant actors themselves in order to screen their own specific battery chemistries under development regarding resource rarity and criticality. As can be seen in Figure 3, all chemical elements and materials that the specific battery cell contains should be considered. Then, starting with criticality, the actor must know which geographical or organizational setting that is applicable. In line with the aim of this study, the EU list of critical materials is used here in this assessment. Rarity can be assessed regardless of the geographical context, but it is important to know whether the raw material is likely to be extracted from the crust or not. Other options are if (purely or mainly) recycled materials are used or if extraction is made from, e.g., the sea or the atmosphere, as is the case for nitrogen (Sanderson, 2020). Table 1 is used for the last step of the rarity assessment, where different elements are grouped based on their relative rarity. To facilitate interpretation, an ordinal scale is used to categorize the elements into three categories based on their CSPs. Category 1 includes elements that are the least rare, whereas category 3 contains the rarest elements. EU's latest list of critical materials is presented in Table 2. Here, the categorization is on a yes-or-no scale, i.e., either the material is critical for the EU, or it is not.

Since the screening assessment is solely performed at cell level, any additional upstream or downstream resource requirements along the life cycle of the batteries are not accounted for. Furthermore, this study does not consider any specific amounts of battery materials used, since such amounts are not always known for next-generation batteries at an early stage of technological development. Consequently, the screening resource assessment method can only point to potential resource issues inherent in the cell chemistries due to the inclusion of rare and/or critical materials.

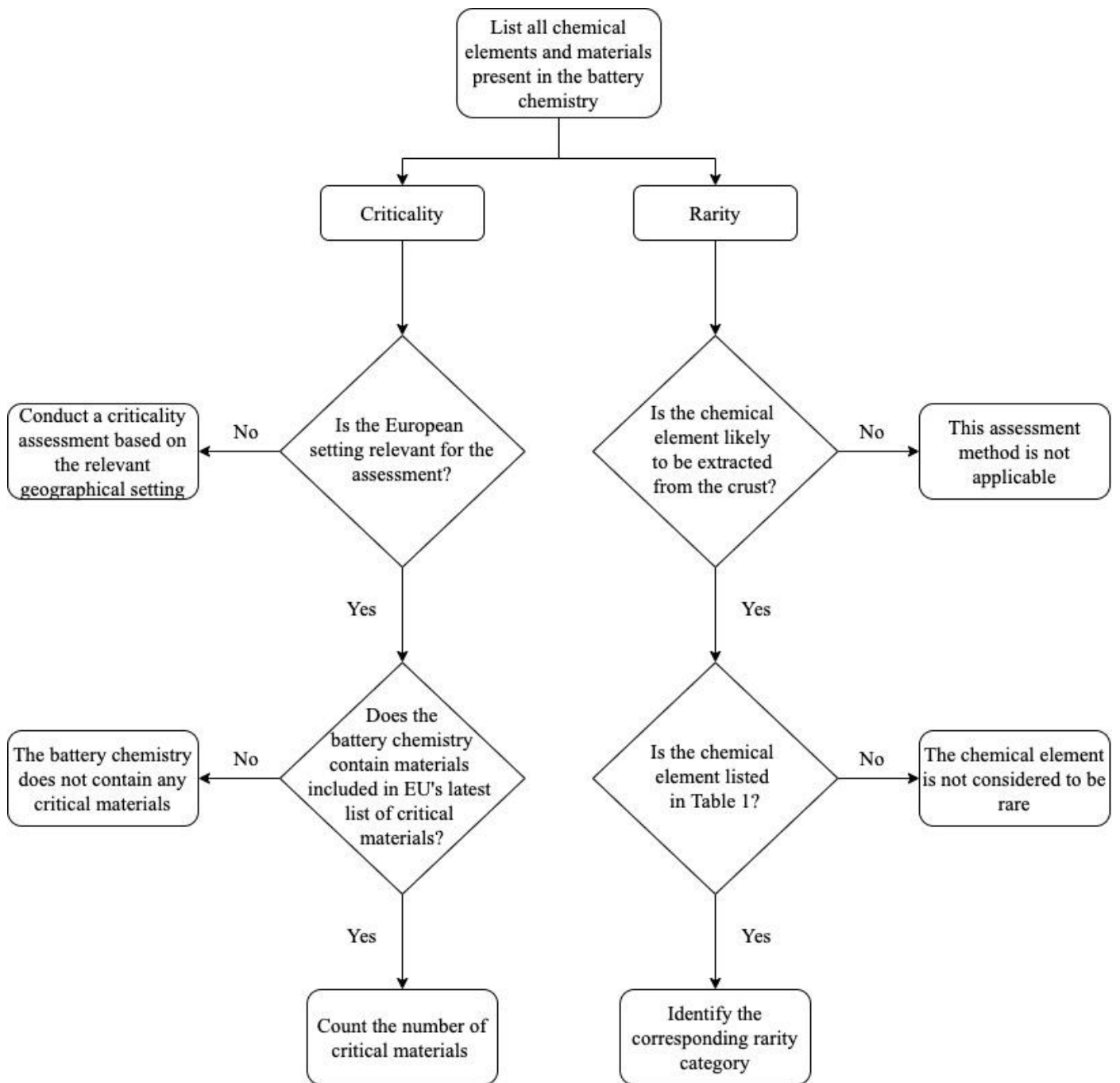


Figure 3. Decision tree for how to conduct the resource screening assessment.

Table 1. Categorization of rarity, which is based on CSPs from Arvidsson et al. (2020a).
Unit: kg silicon equivalents per kg element.

Category 1 (1000≤CSP≤10,000)	Category 2 (10,000<CSP≤100,000)	Category 3 (CSP>100,000)	
Chlorine	Cobalt	Arsenic	Antimony
Vanadium	Scandium	Erbium	Bismuth
Zirconium	Neodymium	Cesium	Selenium
Chromium	Lanthanum	Ytterbium	Cadmium
Zink	Yttrium	Beryllium	Silver
Nickel	Lithium	Tin	Indium
Nitrogen	Gallium	Uranium	Mercury
Rubidium	Germanium	Europium	Tellurium
Praseodymium	Lead	Wolfram	Platinum
Cesium	Boron	Bromine	Palladium
Copper	Niobium	Molybdenum	Gold
	Thorium	Holmium	Ruthenium
	Samarium	Tantalum	Rhenium
	Hafnium	Iodine	Rhodium
	Gadolinium	Terbium	Osmium
	Dysprosium	Thallium	Iridium
		Lutetium	Thulium

Table 2. EU's list of critical raw materials (European Commission, 2020a).

Antimony	Germanium	PGM***
Baryte	Hafnium	Phosphate rock
Bauxite	HREE*	Phosphorus
Beryllium	Indium	Scandium
Bismuth	Lithium	Silicon metal
Borate	LREE**	Strontium
Cobalt	Magnesium	Tantalum
Coking coal	Natural graphite	Titanium
Fluorspar	Natural rubber	Tungsten
Gallium	Niobium	Vanadium

*HREE=heavy rare earth elements, which include europium, gadolinium, terbium, dysprosium, holmium, erbium, thulium, ytterbium, lutetium and yttrium

**LREE=light rare earth elements, which include cerium, lanthanum, praseodymium, neodymium, samarium and scandium.

***PGM=platinum group metals, which include ruthenium, rhodium, palladium, osmium, iridium and platinum

3. Results and discussion

3.1 Survey results

Here, the survey results regarding the first two questions are presented.

Q1: Which battery chemistries do you work with right now?

The level of specificity in the survey answers vary, some refer to battery chemistries while others refer to groups or concepts. The answers to question 1 can however be divided into five main categories, whereof four refer to battery groups and one, the solid-state category, refers the concept of switching from a liquid to a solid electrolyte. The categories are listed according to the number of times each category was mentioned by the respondents.

1. Lithium-ion battery group
2. Lithium-metal battery group
3. Solid-state battery concept
4. Sodium-ion battery group
5. Multivalent battery group

In addition to the concepts and groups mentioned above, organic batteries utilizing carbonyl-coordinating organic compounds, lead-acid batteries, nickel-cadmium batteries, nickel metal hydride batteries, potassium batteries, potassium-ion batteries, anode-less batteries, dual ion batteries and redox flow batteries are also found among the answers. These responses are, however, only given once each and are therefore not addressed further in this report.

Q2: Which battery chemistries do you find promising for the future?

The survey answers for question 2 are divided into the same five main categories as for question 1, although in a slightly different order of preference based on the response frequency:

1. Lithium-ion battery group
2. Sodium-ion battery group
3. Lithium-metal battery group
4. Solid-state battery concept
5. Multivalent battery group

In addition to these groups, magnesium-sulphur batteries, nickel-cadmium batteries, potassium-ion batteries and organic batteries are listed among promising future chemistries. However, as these are only answered by one or a few respondents, they are not included in the resource assessment. Why the respondents consider these five groups of batteries to be promising for the future are described below for each group.

For the *lithium-ion battery group*, nickel-rich nickel-manganese-cobalt (NMC) cathodes with a lower cobalt content than the NMC 333 chemistry are generally found promising. Another respondent states that lithium-ion chemistries with a completely cobalt-free cathode, i.e., the lithium iron phosphate (LFP) cathode, are promising due to constraints in cobalt supply and

price levels for cobalt. In addition to this, lithium-ion batteries in general are seen as promising due to “good capacity” and “decent power characteristics”.

Sodium-ion batteries are seen as promising for the future due to their presumed lower environmental impacts, possibility to achieve circular flows, usage of low-cost materials and high voltage. In addition, their ability to maintain power density is mentioned as another reason for being promising.

Lithium-metal batteries are seen as promising because of their potential for achieving high energy densities. It is mentioned that they can be used for niche applications that do not require many charge-discharge cycles. In addition, provided that certain cathode materials are used, e.g., sulphur-based ones, a potentially lower raw material cost is also seen as promising.

The solid-state battery concept is seen as promising because the batteries are presumably safe, cheap and powerful, and because they could enable higher energy density and or cycle life. Various battery groups and chemistries can be utilized using solid-state electrolytes; however, the prevalent ones are based on lithium anodes (Edström et al., 2020; Kim et al., 2015; Lim et al., 2020). Most survey respondents have specified lithium-based solid-state batteries as the promising ones, although sodium-based batteries are also mentioned.

Different *multivalent batteries* are considered promising for different reasons. For example, aluminium-based batteries are seen as promising due to their potentially high energy density, while calcium-based batteries are claimed to combine sustainability with high voltage cells.

In general, the main arguments brought up by the respondents often relate to different technical performance characteristics of the battery cells, such as energy density and number of charge-discharge cycles. In some cases, the high performance might not yet have been achieved in practice but is based on theoretical values that are aimed for in the future. In addition, short-term resource aspects, such as supply risks and cost of certain battery materials, are also provided as reasons for why some battery chemistries are considered promising. Several respondents also mention sustainability-related aspects as reasons, such as low environmental impacts and the absence of cobalt. Though cobalt is not an abundant metal, it is not much rarer than copper. It is, however, considered a critical material. Additionally, cobalt mining is linked to sustainability issues, since the mining largely occurs in the Democratic Republic of the Congo (Watts, 2019), which includes harsh working conditions and child labor (Sovacool, 2019; Tsurukawa et al., 2011). Using cobalt is thus perceived as a problematic for a number of reasons and hence, battery developers try to minimize its use in batteries.

3.2 Defining battery cell configurations

In this subsection, chemistry specific cell configurations, for the battery groups and concepts considered most promising by the survey respondents are defined on a component level; see Table 3 for an overview. The purpose of this specification is to enable a screening resource assessment of example configurations. It can be noted in the survey results that most

respondents referred to groups or specific battery chemistries (Section 3.1). Only one concept is mentioned specifically by the respondents – the solid-state electrolyte. Thus, as can be noted, this concept is reported as a category of its own alongside the other batteries which belongs to more specific groups. This also implies that for all other groups and chemistries, the more common liquid electrolyte concept can be assumed.

Many lithium-ion batteries, which are commercially available, currently consist of cells that have a graphite anode, a cathode based on layered oxides, an electrolyte containing a lithium salt and a current collector for each electrode (Armand et al., 2020). According to the survey results, the commercially available LFP cathode is a promising alternative to the NMC cathode, because it does not contain the element cobalt. Thus, two example chemistries within the lithium-ion group are assessed: NMC/graphite and LFP/graphite.

Regarding sodium-ion batteries, there are several cathode and anode materials mentioned in the roadmap by Tapia-Ruiz et al. (2020). Also, several electrolytes are being considered since no standard composition exists yet. For this assessment, a cathode based on a layered transition metal oxide is selected, which is mentioned in both the review by Liu et al. (2020) and in the roadmap by Tapia-Ruiz et al. (2020). The layered oxide has a general formula of NaMO_2 , where M is one or several transition metals – typically metals in the d-block of the periodic table. When different layered oxides are screened in Liu et al. (2020), nickel and iron seem to be two of the more frequently used transition metals for this purpose. Thus, these are selected to represent M in this case. Regarding anode materials, there are five categories of materials mentioned in the road map, where examples include hard carbon, titanium-based oxides and alloy and conversion materials. However, hard carbon is reported to be the most popular choice for sodium-ion batteries and is therefore selected as the example anode material in the assessment.

The lithium-sulfur battery is an example of a lithium-metal battery, applying a lithium metal anode. Composites of sulfur and different carbonaceous materials are often reported as the cathode material of choice and one such example composite is selected in this case (Cairns and Hwa, 2017; Manthiram et al., 2013). The electrolyte generally consists of lithium salts in an organic solvent, which is therefore chosen as example for this assessment.

Another option in the lithium-metal group, i.e., when lithium metal is assumed for the anode, assessed in this study is the lithium-oxygen battery. Porous carbon is an often-reported cathode material (Berg, 2015; Varzi et al., 2020). According to Berg (2015), a metal catalyst is combined with the carbon material, where for example manganese, cobalt and silver are studied examples. For the assessment, a porous carbon cathode with a manganese-based catalyst is selected as example. Based on Guo et al. (2018), an ether-based electrolyte with a lithium salt is considered in the assessment.

Table 3. Example configurations of the battery concepts, groups, chemistries and components assessed in this study.

Battery	Anode material	Cathode material	Electrolyte	Chemical elements present*
Lithium-ion, NMC	Graphite	Layered oxide: NMC	Lithium hexafluorophosphate, LiPF_6 , in an organic solvent	Lithium, nickel, manganese, cobalt, phosphorus, fluorine, carbon
Lithium-ion, LFP	Graphite	Lithium transition metal phosphate: LFP	Lithium hexafluorophosphate, LiPF_6 , in an organic solvent	Lithium, iron, phosphorus, fluorine, carbon
Sodium-ion	Hard carbon	Layered oxide: NaMO_2 where M=nickel and iron	Sodium hexafluorophosphate, NaPF_6 , in an organic solvent	Sodium, nickel, iron, phosphorus, fluorine, carbon
Lithium-sulfur	Lithium	Sulfur-carbon composite	Lithium bis(trifluoromethanesulfonyl)imide, $\text{LiC}_2\text{F}_6\text{NO}_4\text{S}_2$, (LiTFSI) in organic solvents	Lithium, carbon, sulfur, fluorine
Lithium-oxygen	Lithium	Porous carbon with manganese catalyst	LiTFSI	Lithium, carbon, fluorine, sulfur, manganese
Solid-state battery	Lithium	NMC	LLZO, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	Lithium, lanthanum, nickel, manganese, cobalt, zirconium
Magnesium-metal	Magnesium	Chevrel Phase consisting of magnesium, molybdenum, selenium and sulfur	Magnesium tetrakis(hexafluoroisopropoxy)borate, $\text{Mg}[\text{B}(\text{hfip})_4]_2$, in an organic solvent	Magnesium, molybdenum, selenium, sulfur, boron, fluorine,
Calcium-metal	Calcium	Vanadium pentoxide	Calcium perchlorate, $\text{Ca}(\text{ClO}_4)_2$, in an organic solvent	Calcium, vanadium
Aluminium-metal	Aluminium	Vanadium pentoxide	Ionic liquid-based electrolyte, 3-ethyl-1-methylimidazolium chloride with excess aluminium chloride (AlCl_3 -EMICl)	Aluminium, vanadium, carbon

*Elements that are considered inexhaustible, such as oxygen and hydrogen are not listed. Also, elements not likely extracted from the crust, such as nitrogen and chlorine, are not listed either.

Solid-state batteries represent a different type of concept than the liquid electrolyte battery, as mentioned already in Section 2.2. As mentioned earlier, various battery groups and chemistries can be utilized using solid-state electrolytes, however the prevalent ones are based on lithium anodes. Therefore, a lithium metal anode is assumed as example in the assessment. Since the cathode materials used for commercial lithium-ion batteries are also the ones often studied for solid-state batteries, the NMC cathode is selected (Boaretto et al., 2021). The solid electrolytes applied in solid-state batteries are categorized as inorganic, polymer-based or hybrid solid electrolytes (Boaretto et al., 2021; Varzi et al., 2020). The inorganic electrolytes are considered to be more preferable for these batteries, and thus an inorganic electrolyte is assumed, specifically the lithium lanthanum zirconium oxide (LLZO) electrolyte (Varzi et al., 2020).

Multivalent batteries is the last group of batteries that are considered promising according to the survey respondents. These batteries all use multivalent ions as charge carriers, often magnesium ions, calcium ions and aluminium ions (Ponrouch et al., 2019). Starting with the magnesium battery, a magnesium metal anode is selected (making the battery a magnesium-metal battery), together with one of the cathode materials currently investigated, which is called Chevrel Phase (Berg, 2015; Dominko et al., 2020). Chevrel Phases have the general formula $Mg_xMo_6T_8$, where T represents either sulfur, selenium or both. In this assessment, we assume a mixture of sulfur and selenium. Berg (2015) exemplifies promising electrolytes for magnesium batteries, where one of them is based on magnesium organoborates, such as magnesium tetrakis(hexafluoroisopropoxy)borate. In a life cycle assessment study assessing magnesium batteries, this electrolyte type is also used to represent current state of the art (Bautista et al., 2021), and is thus selected for this assessment.

The calcium battery is another multivalent battery mentioned in the survey. For this battery, a calcium metal anode and a vanadium pentoxide cathode are selected (Ponrouch et al., 2019; Stievano et al., 2021). The electrolyte considered is calcium perchlorate in an organic solvent.

The last multivalent battery chemistry that is included is the aluminium battery. As for the other multivalent batteries, a pure metal anode is considered plausible, in this case aluminium (Ponrouch et al., 2019). Vanadium pentoxide is assumed to be a relevant example of a cathode material, based on Ponrouch et al. (2019). In the same review article, ionic liquid-based electrolytes are mentioned as being studied for aluminium-based batteries and one such example is therefore chosen.

3.3 Resource assessment

A screening resource assessment is conducted as described in Section 2.2. The results in Figure 4 show that the lithium-ion NMC/Gr chemistry contains the highest number of critical elements (five), whereas the example solid-state battery contains the highest number of rare elements (five). The example calcium-metal cell and the example aluminium-metal cell both contain the lowest number of both rare and critical elements and materials – only one element that is both rare and critical. A notable element is the selenium potentially used in the example magnesium battery cell. While magnesium batteries are considered promising from a sustainability point

of view by some survey respondents, it is important to note that selenium is a geochemically very rare material, with a crustal concentration of only 0.13 ppm (Rudnick and Gao, 2014). Configurations of magnesium battery cells using only sulfur in the cathode are thus preferable from a rarity point of view. Boron, another possible constituent of magnesium batteries, is also counted among the geochemically rare elements, with a crustal concentration of about 11 ppm. It can also be noted that criticality and rarity assessments partly highlight different materials. For example, fluorine (550 ppm) and phosphorus (440 ppm) are relatively abundant in the Earth's crust, but are nevertheless considered critical for the European Union. The sodium-ion battery is also mentioned as beneficial from a sustainability perspective in the survey, specifically for having low environmental impacts. The results in Figure 4 indicate that given this specific example cell, sodium-ion batteries indeed have few rare and critical constituents. If iron is used instead of nickel in the cathode, there are no rare materials and only two critical ones (fluorine and phosphorus).

One way to use Figure 4 and the proposed screening assessment method is to consider the lithium-ion LFP example as a benchmark, since it is a lithium-ion battery regaining attention. Other battery groups and chemistries can therefore be compared to the LFP chemistry in terms of rarity and criticality. This can be done by comparing the number of critical and rare elements/materials included in the assessed chemistry to that of the lithium-ion LFP example (four critical materials and one rare elements) to get an early indication of whether the other cell configuration is promising from a resource perspective given a European setting. Based on such an approach, it can be seen in Figure 4 that four out of nine example battery chemistries have the same number of rare elements, while most of the example battery chemistries have fewer critical materials.

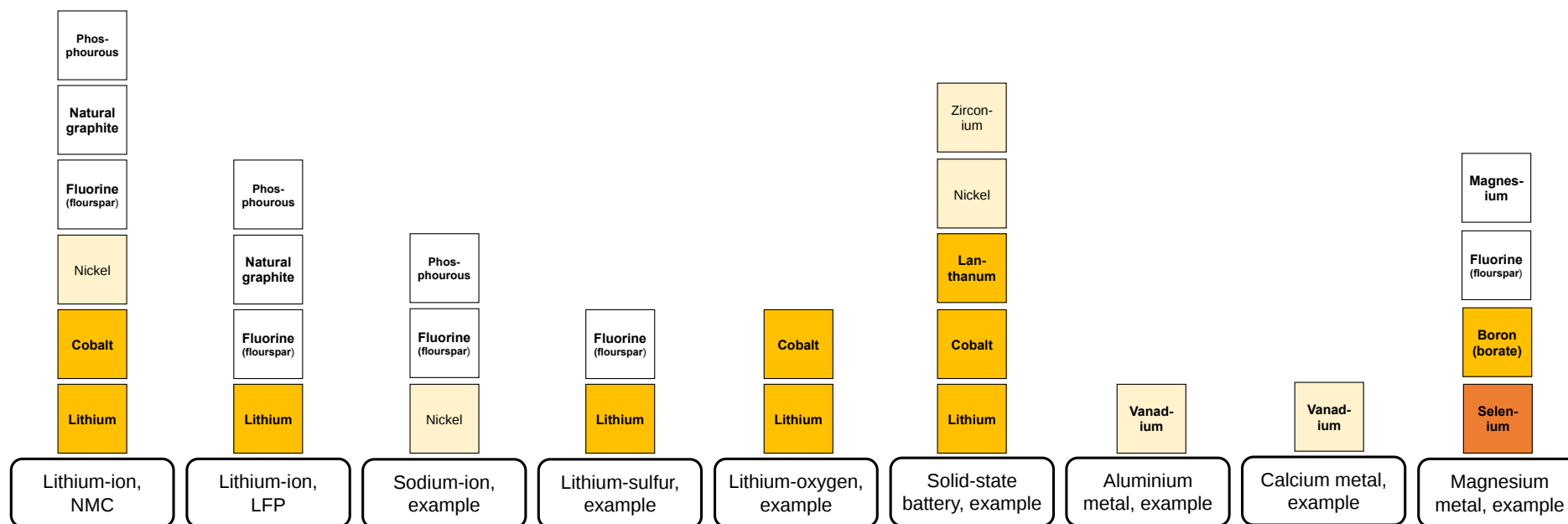


Figure 4. Battery materials used in the example battery chemistries that are either geochemically rare, critical or both. A colored background indicates that the element is rare, with orange being rarer than dark yellow, which in turn is rarer than light yellow (see Table 1). Elements and materials in bold font are critical according to the EU's list of critical materials.

4. Conclusions

It is difficult to draw general conclusions regarding the resource performance of a battery concept or a group, since each may include a wide range of possible cell design solutions in terms of the detailed chemical composition and the components. The resource performance of a battery is not decided by its categorization in terms of concepts or groups: a specific lithium-based battery might be as promising as some type of multivalent battery from a resource point of view. Rather, the “devil is in the details”, i.e., in the specific material selection within battery concepts, groups and even chemistries. The option to use either the rare selenium or the much more abundant sulfur in the magnesium-metal battery cathode materials constitutes an example of this. It is also important to remember the European perspective and how it influences the results in terms of criticality. If another perspective would have been used, other battery solutions might have come out as more (or less) promising. Nevertheless, by applying the screening resource assessment method developed in this study, some situations where rare and/or critical materials are included in battery cells can potentially be avoided at an early stage of technological development.

When performing more detailed assessments of resource implications of batteries, the amounts of different chemical elements and materials in battery cells will influence the resource performance. For example, if a rare element is used in only small amounts, it might not influence the results notably. Furthermore, with material recycling, the need for primary resource extraction could in some situations still be kept low. With more data available, more accurate assessments can be performed. The screening resource assessment has highlighted a number of battery chemistries with seemingly promising resource performances. More detailed assessments of such battery chemistries are recommended in order to verify or falsify these preliminary screening results.

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