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Virtual Material Design

BASE
Digital Battery Passport – common ontology concept for various systems

BASE

Digital Battery Passport – common ontology concept for various systems

- **Why digital passports? What is BASE?**
- **What is a Lithium Ion Battery?**
- **What is a DBP?**
  - Which questions to answer?
  - organizing the data

Motivation: EU-Regulation 2023/1542

From February 2027, each … battery … ≥ 2kWh… on the market … shall have a … **BATTERY PASSPORT**

- improve **sustainability, safety, labelling, marking and information** for batteries within the European Union.
- minimum requirements for **producer responsibility, the collection and treatment of waste batteries** and for reporting.
- battery **due diligence obligations** on economic operators
- requirements for **green public procurement**

Regulation applies to Lithium Ion Batteries

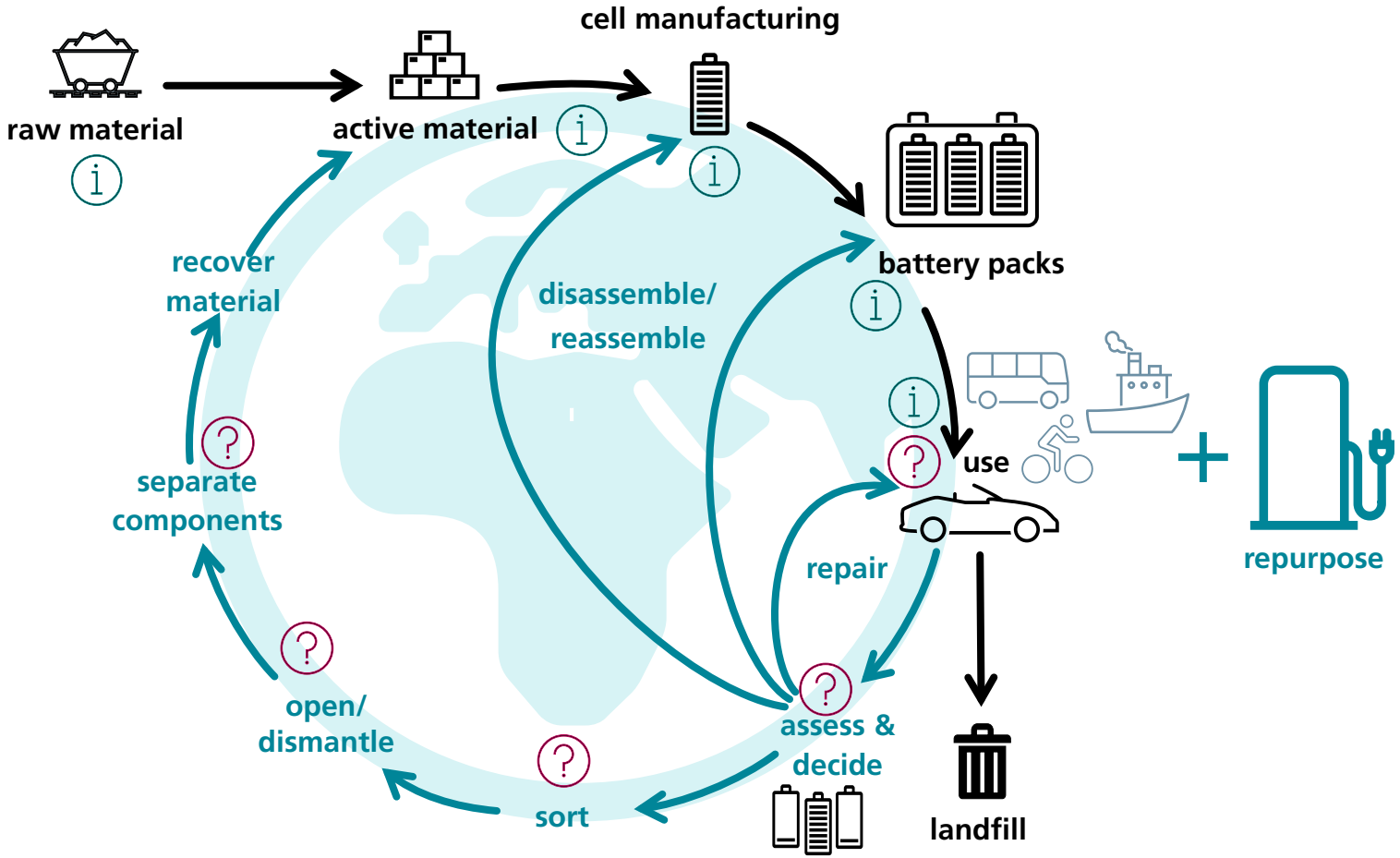
icons from Dall-E + stock.adobe.com

DBP = ELECTRONIC RECORD
with information accessible to

- the general public
- notified bodies
- persons with legitimate interest

Motivation: Lithium ion battery lifecycle

Transition from linear to circular economy



Aim: Make best use of resources

- maintain & prolong 1st service life
- repurpose packs/cell for 2nd life
- recycle
- faciliate informed decisions

Challenges

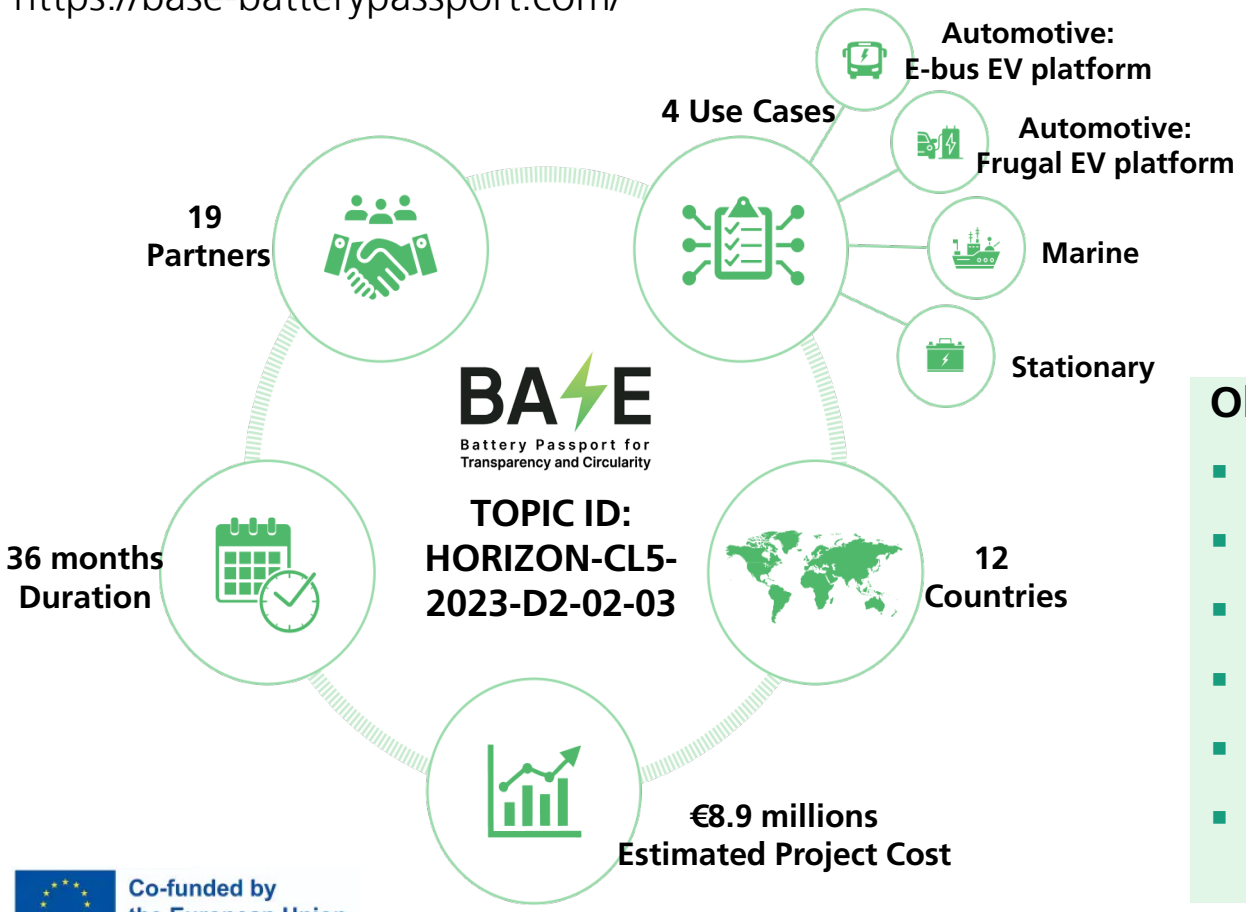
- batteries age
- business secrets → data protection
- leap in time → data available/reliable
- applications = zoo of curiosities

→ Several initiatives developing DBPs

BASE

Battery Passport for Resilient Supply Chain and Implementation of Circular Economy

https://base-batterypassport.com/



Co-funded by the European Union

Objectives

- service satisfying legal obligations
- secure data
- state of health & safety diagnosis
- remaining useful life prediction
- life cycle analysis assessment
- environmental, socio-economic & governmental indicators

Consortium Partners

Fraunhofer
TECHNOVATIVE SOLUTIONS
cleantron
Seraph.
ARTECH
FORD OTOSAN
Corvus Energy
Mercedes-Benz
adscensus
NAVTEK
EXITCOM recycling for future
BePlanet factory
SQM
GENEVA GRADUATE INSTITUTE
ROK METALS
aspilsan
UNIVERSITY OF SURREY
eLi Lithium Institute
Parakeet BV

Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or CINEA. Neither the European Union nor the granting authority can be held responsible for them.
This project has received funding from the Horizon Europe Framework Programme (HORIZON) Research and Innovation Actions under grant agreement No 101157200.

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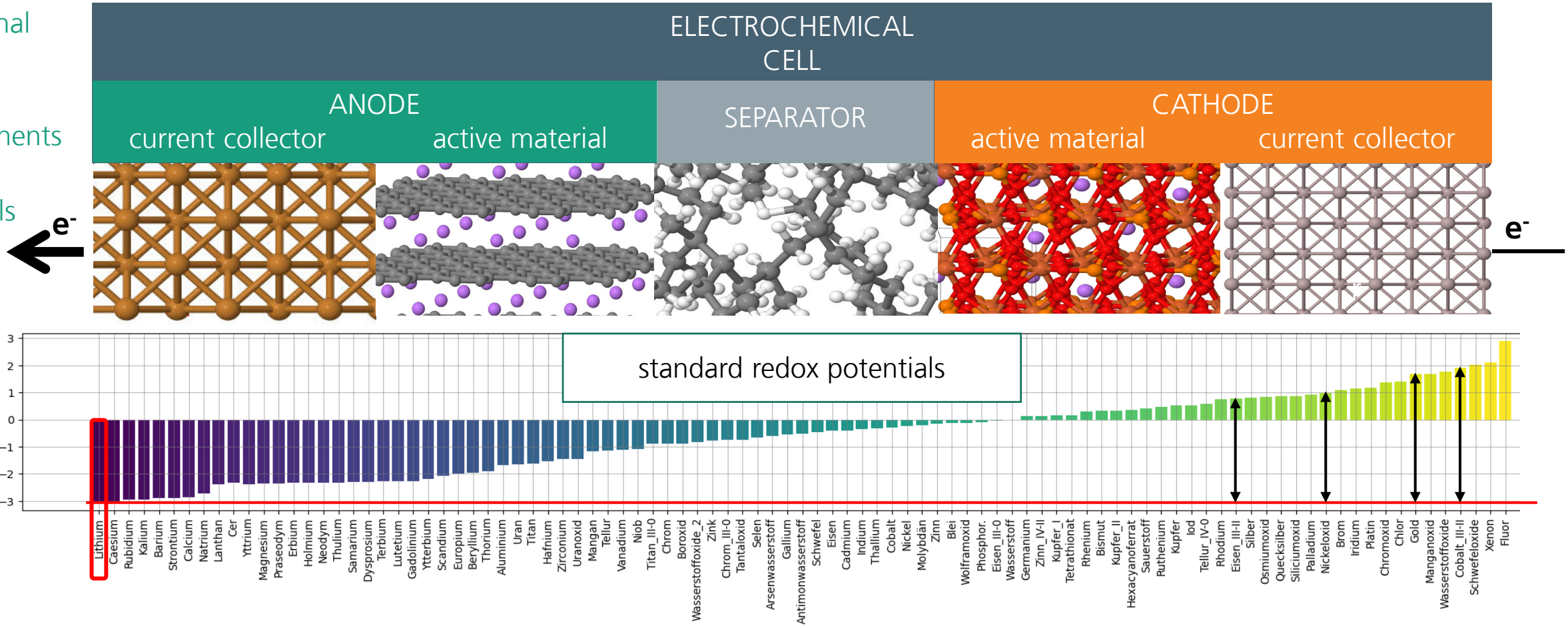
“Batteries”

Functional Unit

Components

Materials



chemistry → specific voltage

ionic mobility → amperage

amount of material → capacity

Diverse applications require varying levels of assembly

Application dictates number of cells: parallel → current↑ – series → voltage↑

Practicality recommends grouping (identical) cells into (robust) subunits (cells, modules, packs)

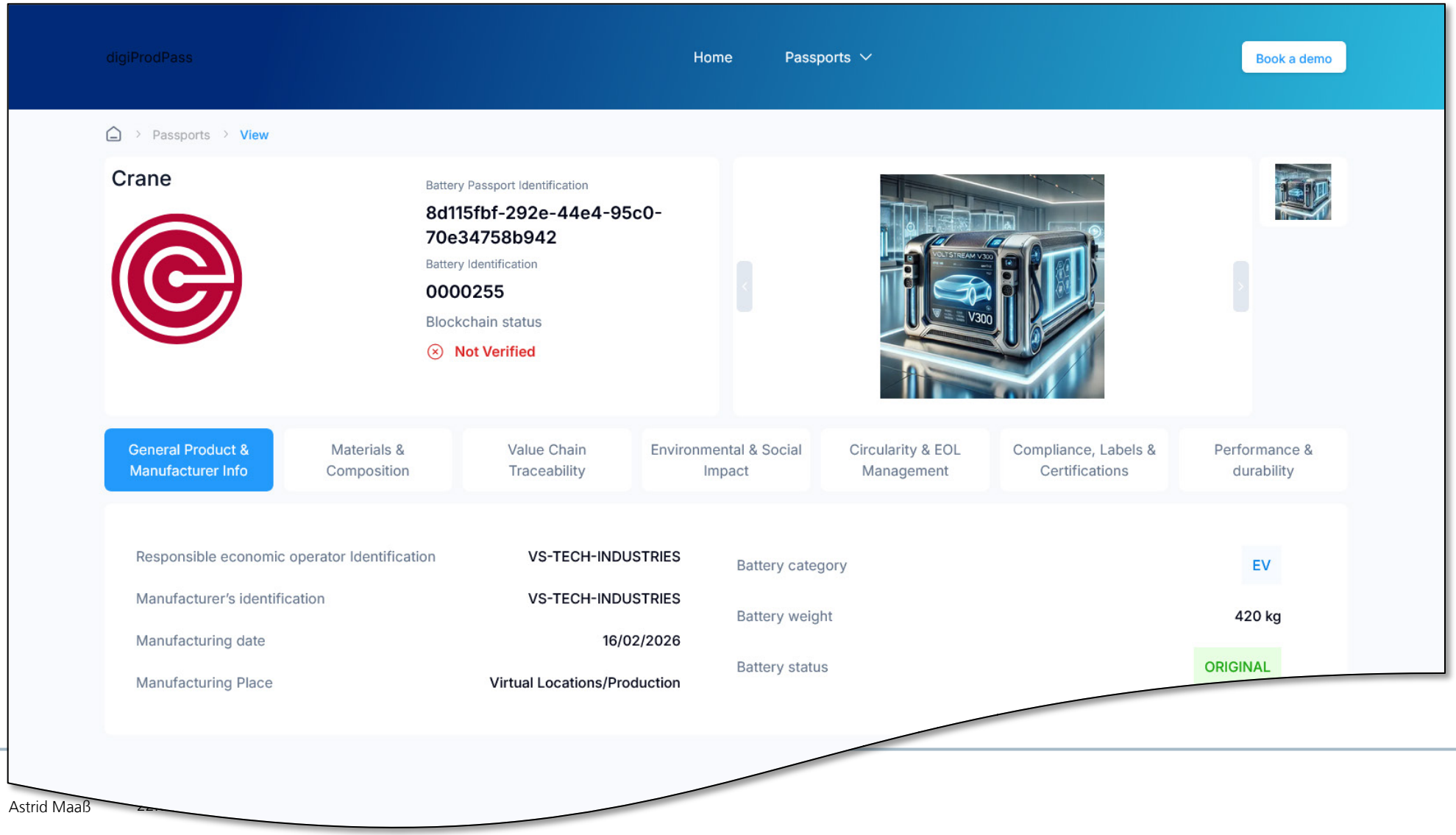
→ improve production, handling, maintenance & replacability

→ varying degrees of voltage/current, safety & data at each level of assembly

- → the higher the level, the more accessory components: control, thermal management, safetey
- → no consistent naming convention

Life Cycle Assessment of a Lithium-Ion Battery Pack Unit Made of Cylindrical Cells, https://www.mdpi.com/2313-0105/8/8/76#app1-batteries-08-00076

DBP-Draft



- **static data**: all except:
- **dynamic data**: performance & durability

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Some questions to answer

- supply chain → responsibility, reliability
- material → critical raw materials, hazardous, virgin materials/recycled shares
- usage/handling/transport → state of health & safety, remaining useful life, safety precautions
- reusing, repurposing, recycling → history, state of health, assessment of options, dismantling instructions, material content
- data → currentness, protection/role-based access

→ capture batteries & components in full detail
→ track history & prospective future of individuals/parts
→ consider context (situation of battery/updates of databases)

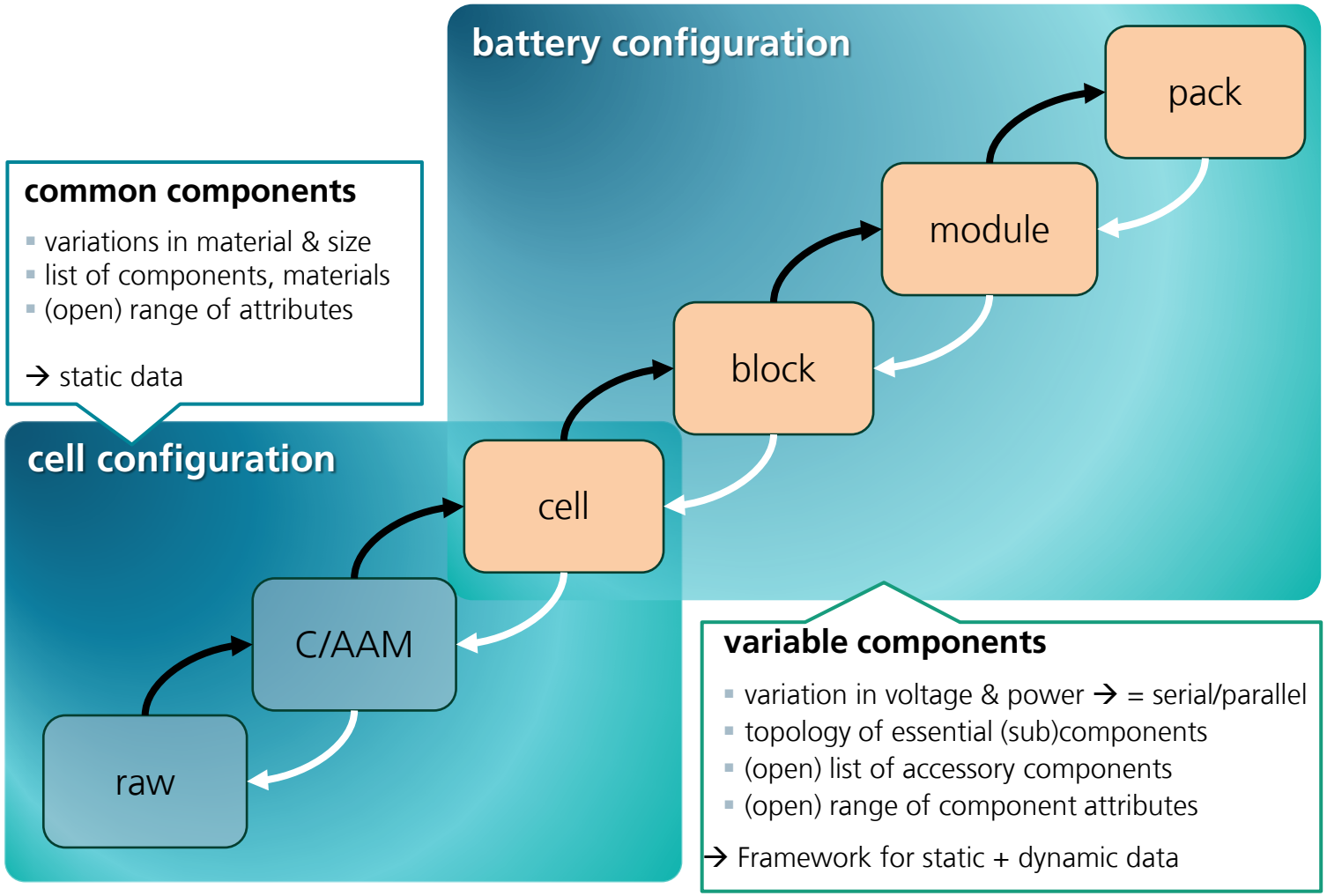
Common description for all types of batteries

Aim

- chemistry/technology agnostic solution
  - full detail & resolution
  - easy to update

Approach

- slim ontology, elaborate knowledge graphs
  - ontology build on existing ones/based on project results
  - KG structure according to application
  - based on **object-centered view**
  - complemented by **process-centered view**



Common description for all types of batteries

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- chemistry/technology agnostic solution
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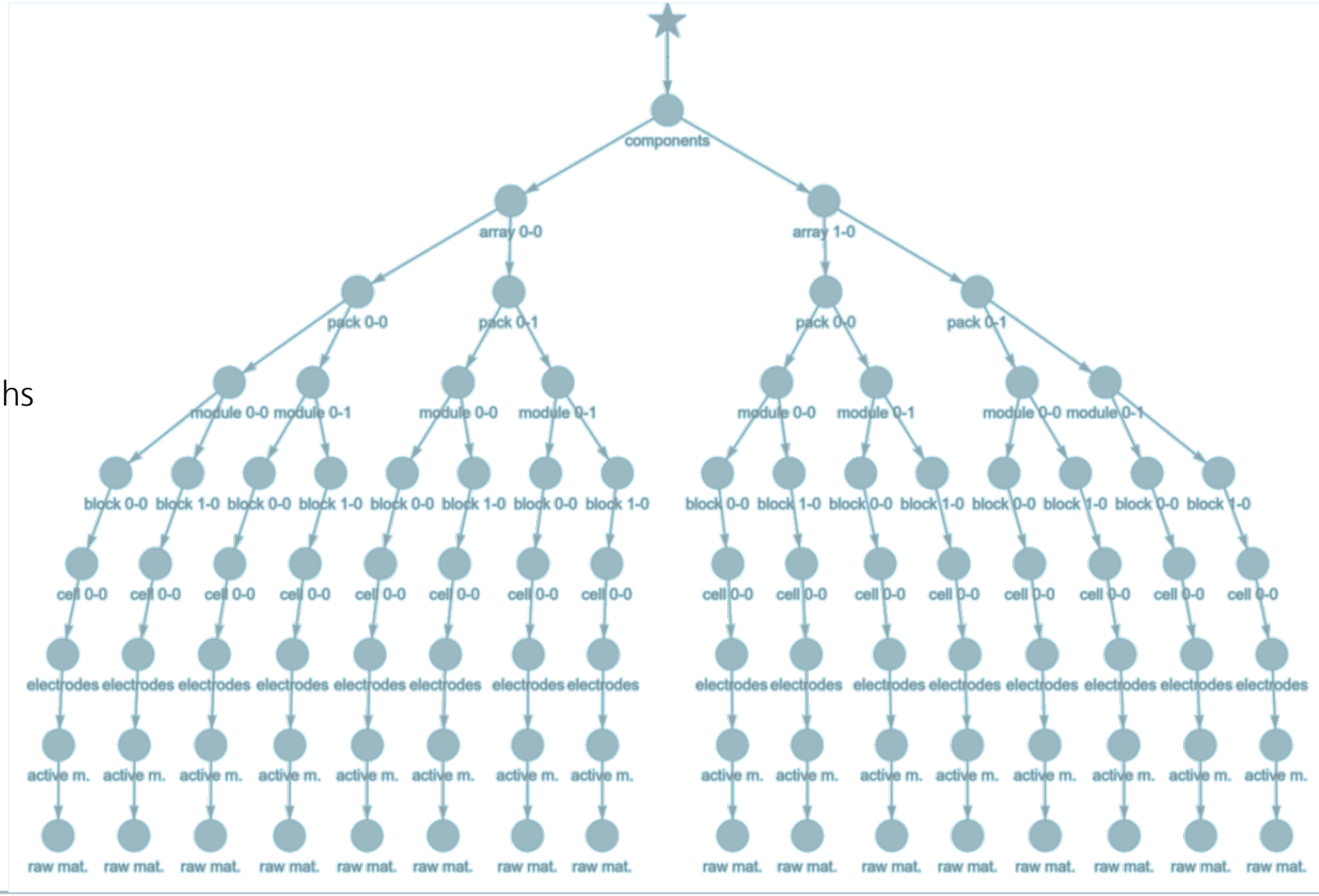

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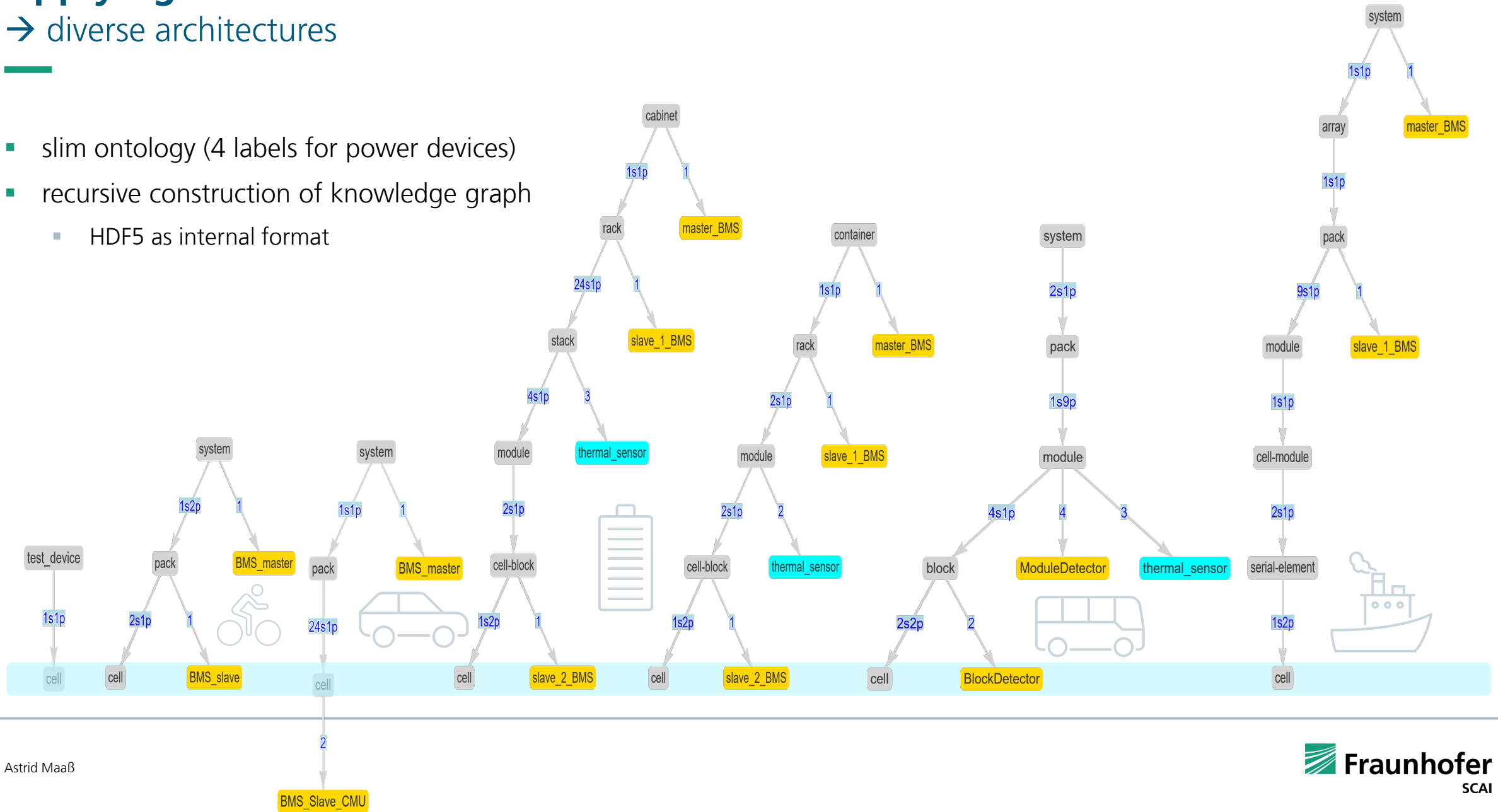
Applying to use case data

→ diverse architectures

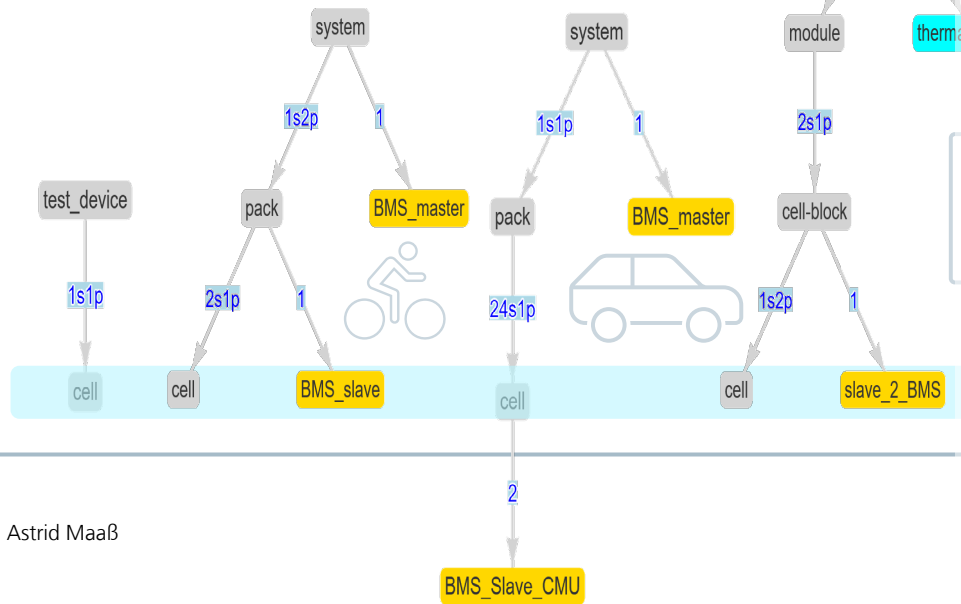
- slim ontology (4 labels for power devices)
- recursive construction of knowledge graph
  - HDF5 as internal format

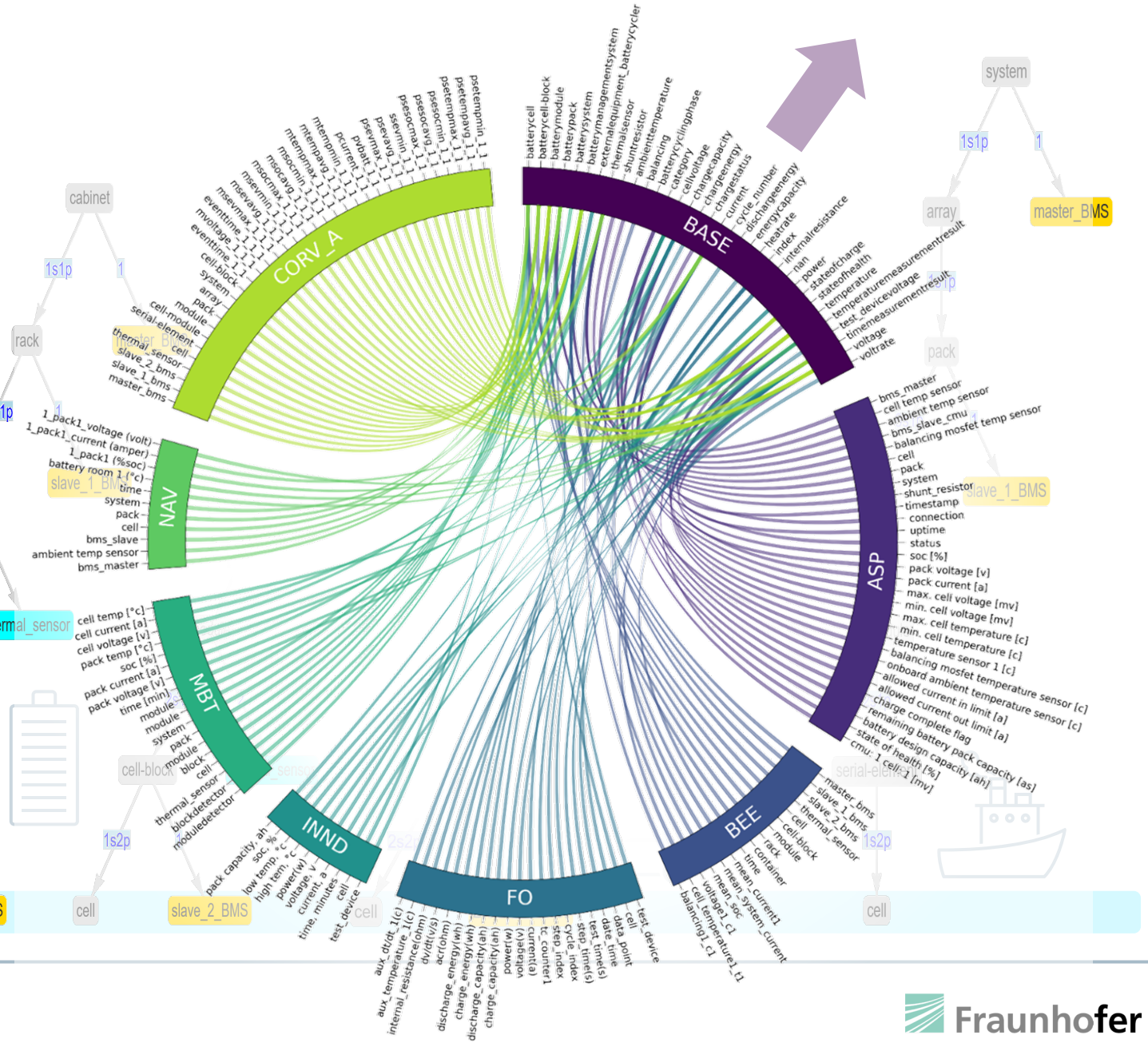


Applying to use case data

Mapping

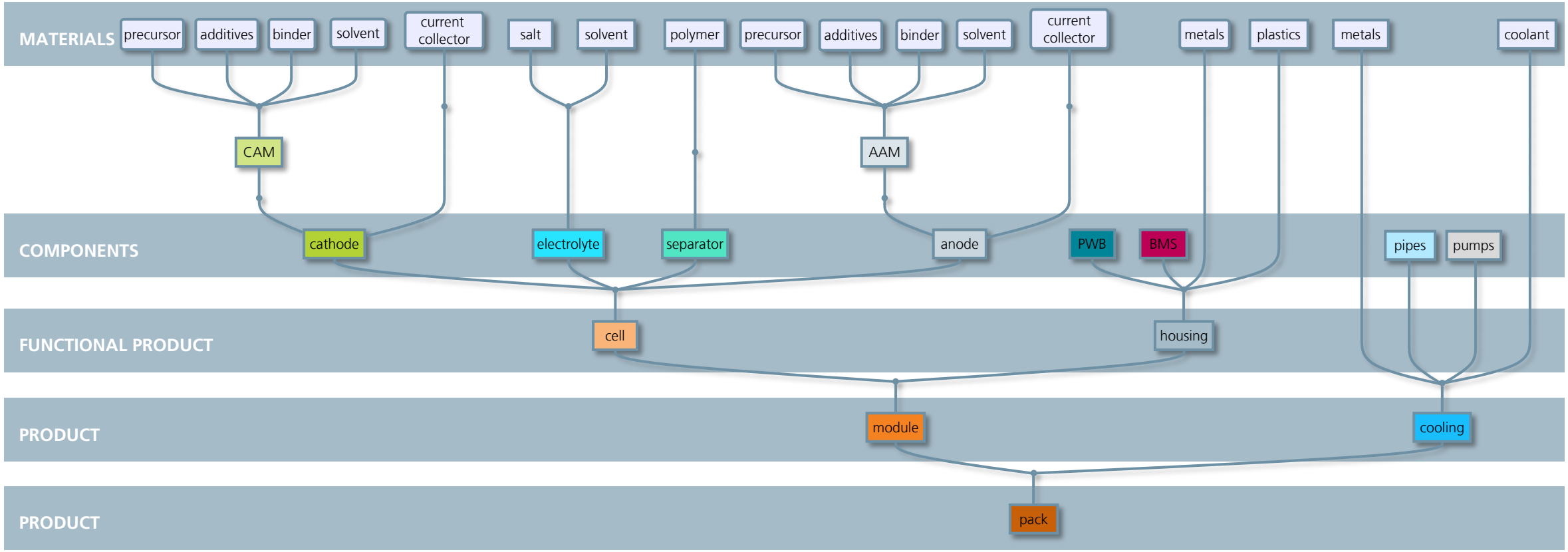
- slim ontology (4 levels only)
- recursive construction of knowledge graph
  - HDF5 as internal format
- plenty of synonyms; contradicting usage





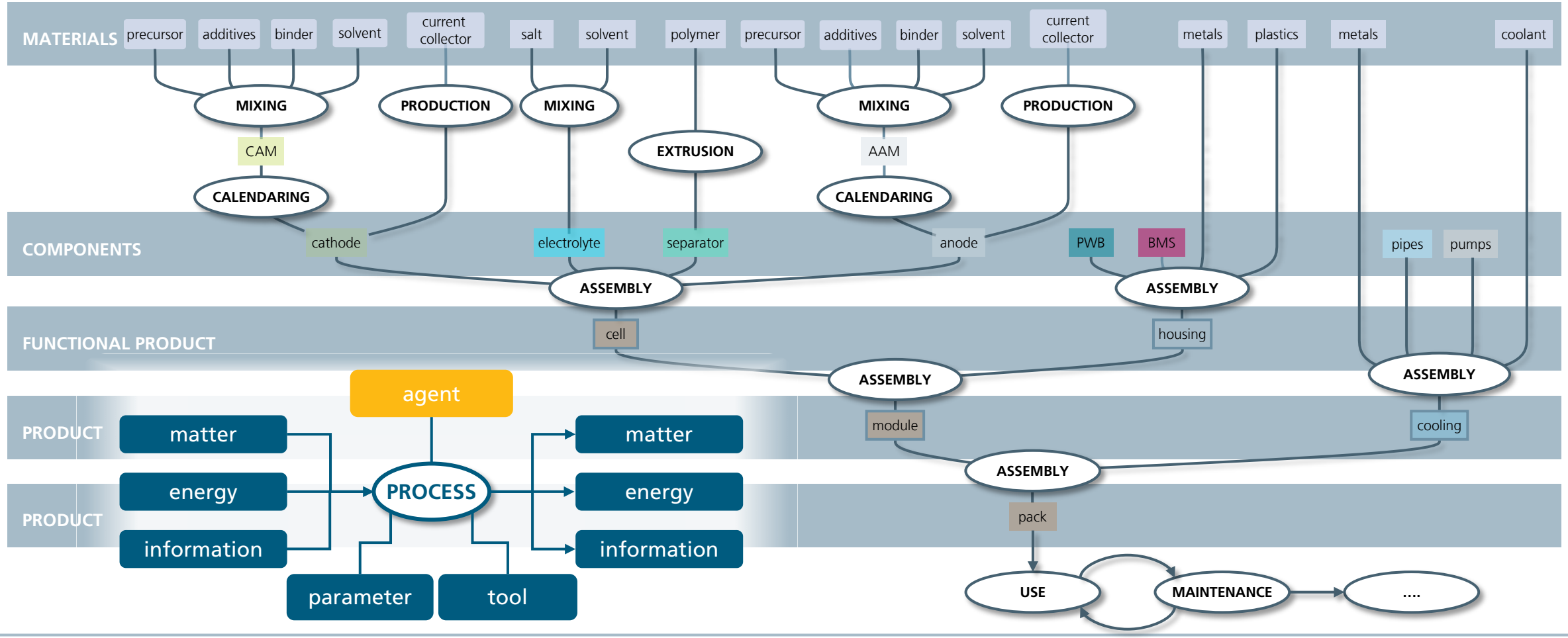
Object centered view

Parthood concept

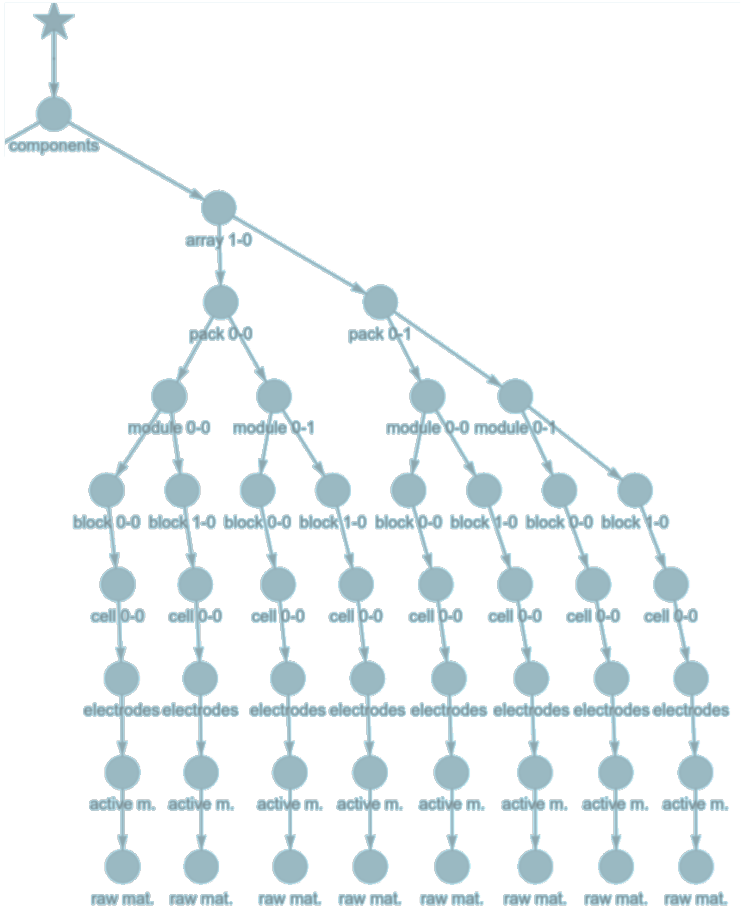


Process centered view

Changes in time via General Process Ontology



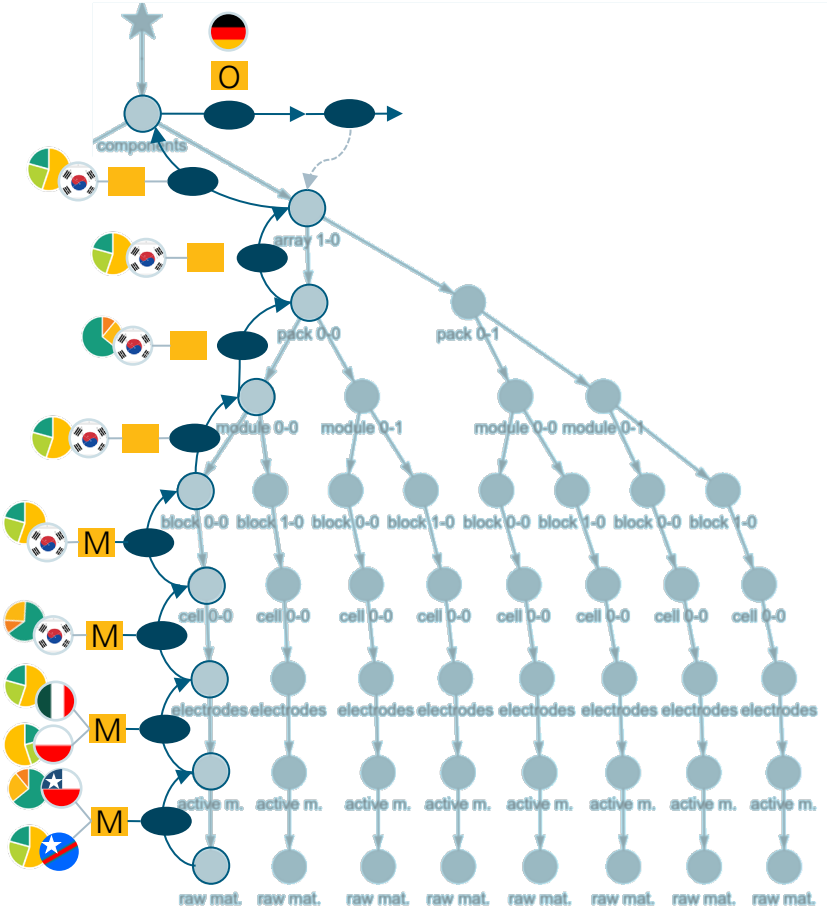
Summary



Ongoing work

- representation of battery guided by physical principles
  - → information on individual battery encoded in substructure of KG
  - slim ontology → flexibility & generic applicability; reduced interaction complexity
  - link data bases to KG → updates

Summary



Ongoing work

- representation of battery guided by physical principles
  - → information on individual battery encoded in substructure of KG
  - slim ontology → flexibility & generic applicability; reduced interaction complexity
  - link data bases to KG → updates
- model history as sequence of processes
- complex KG → run complex queries
  - basis for deriving data, e.g. aggregated product scores (ESG, LCA)
  - upload detailed inspection reports → transparency
  - tracking replacement of components
  - transfer history upon repurposing

challenges & risks

- data availability
- data ingestion

No DBP, no business!

Thank you

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Use existing ontologies

Elementary Multiperspective Material Ontology

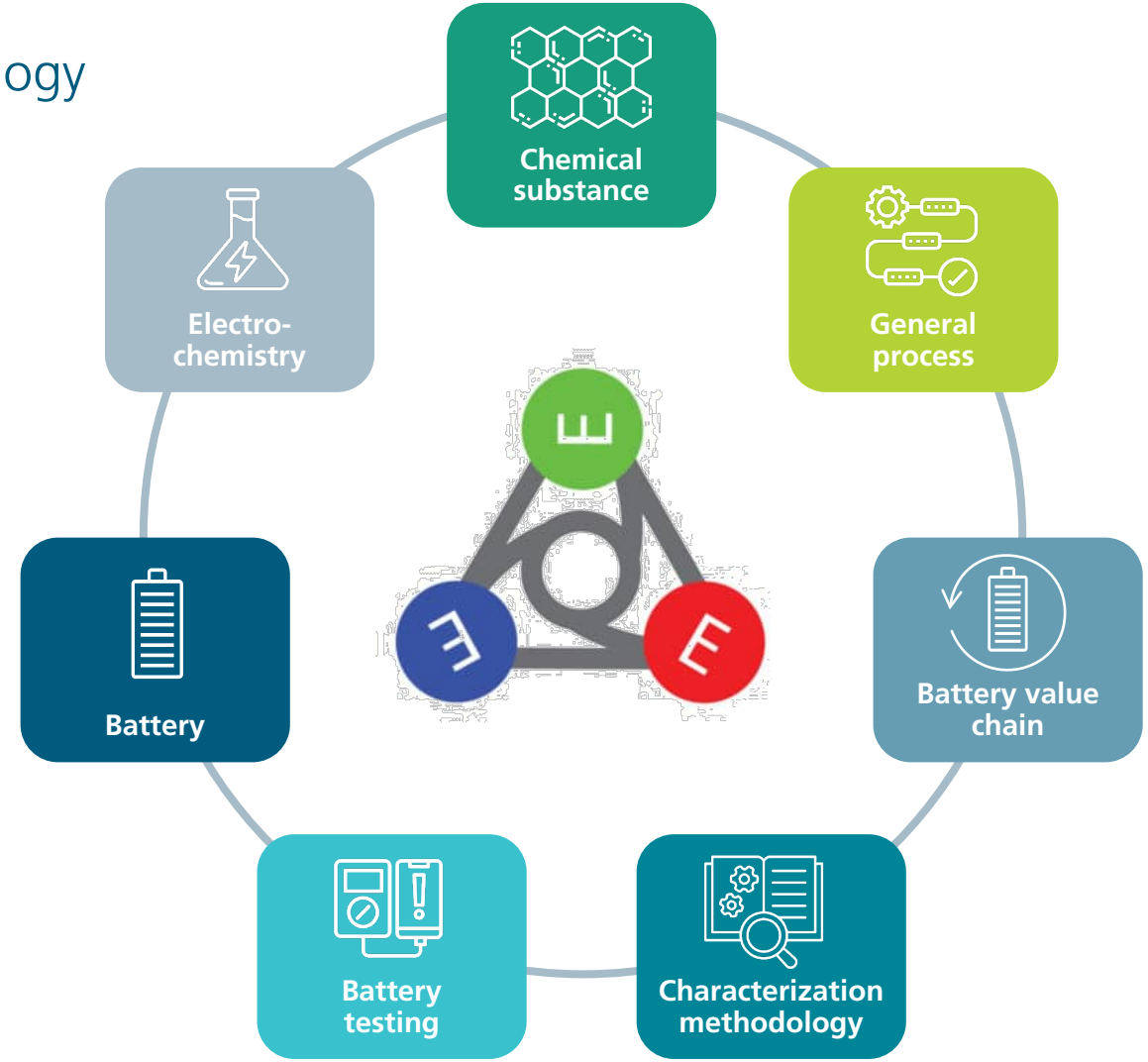
https://github.com/emmo-repo/EMMO

Representational ontology framework based on current materials modeling and characterization knowledge, relying on recognized authorities.

- standardized nomenclature (IUPAC/IEC)
- persistent identifiers
- CC BY 4.0

Extensions

- integrated with the EMMO universe
- focus on representing physical world
- + project specific definitions



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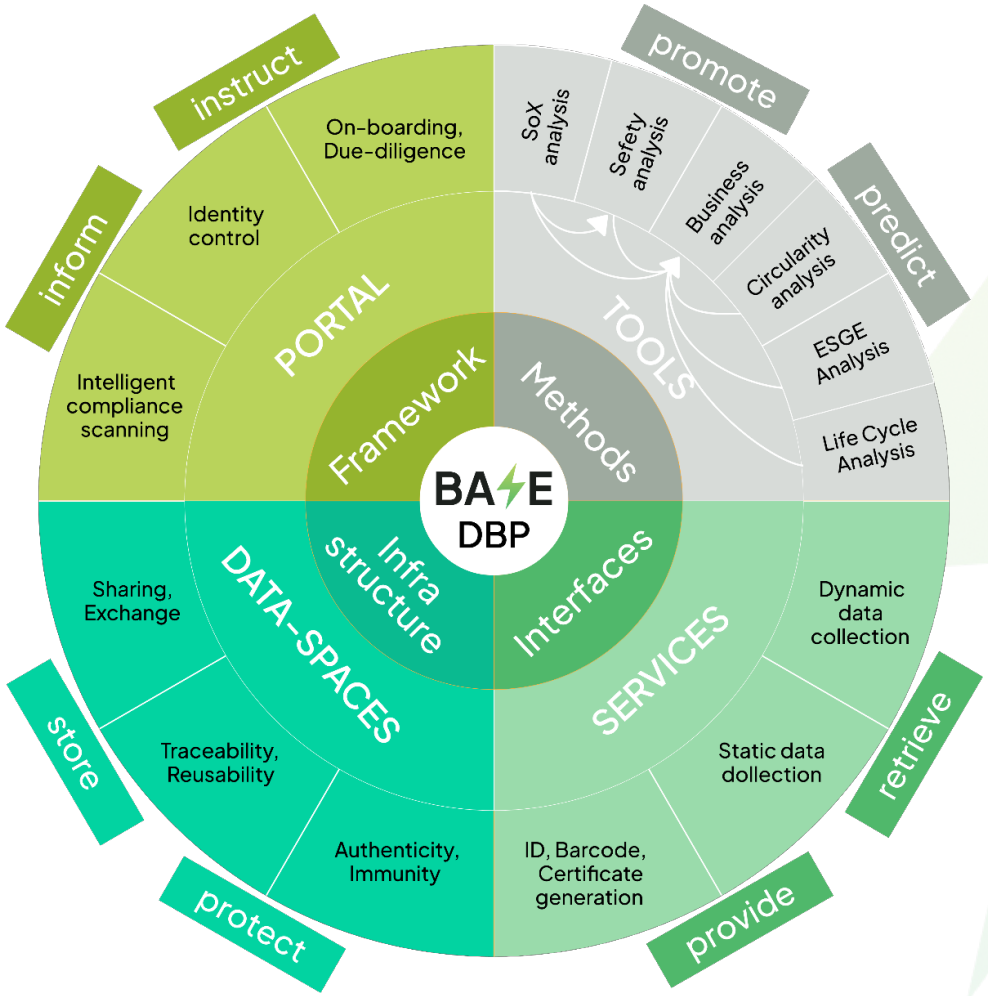
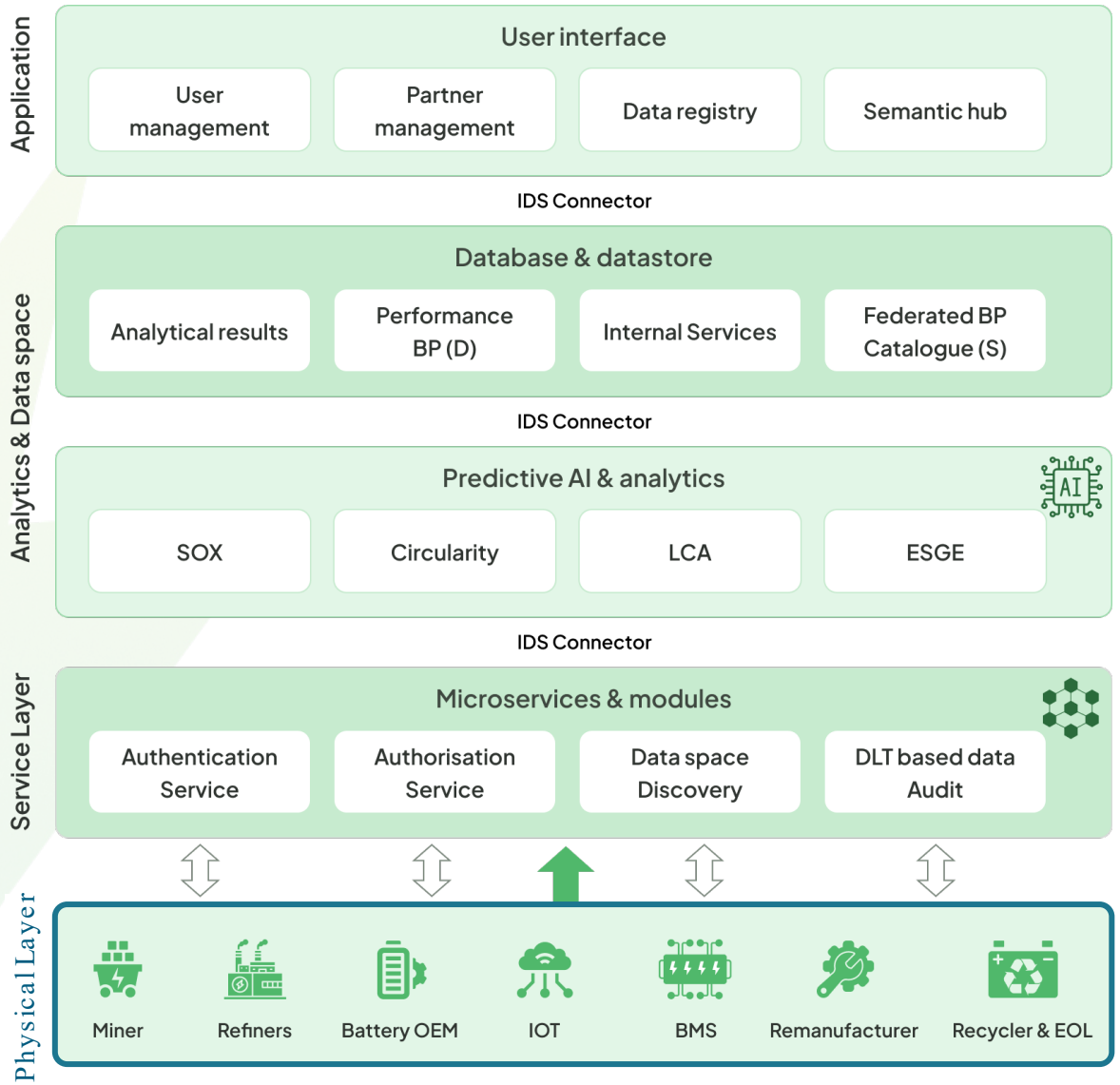
Concept & Architecture

Project BASE





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Use Cases and Demonstration Methodology

Project BASE

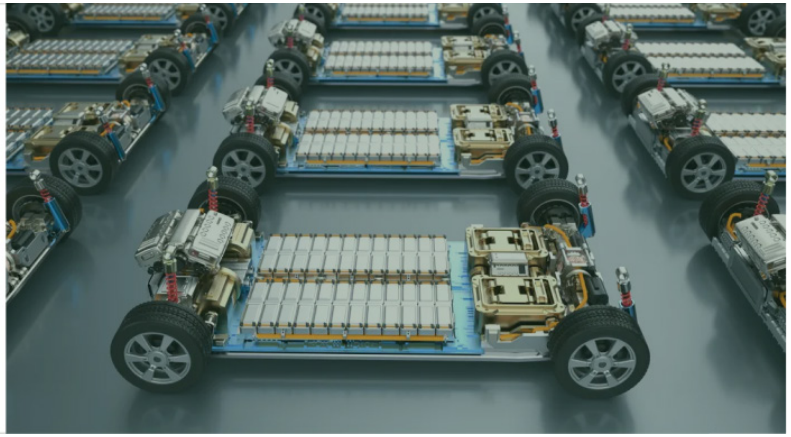
General Objectives for each Pilot

- Secure and reliable access to federated DBP infrastructure
- Systematic immutable data inputs to DBP
- Transparency, accuracy, and reliability of battery indicators
- DBP data provisions with a realistic product development lifecycle
- Interoperable data sharing among value network members
- Real physical data for circularity index tuning, ESGE analysis and business impact analysis

Use-Case-1

Automotive: E-bus EV platform production pilot for MERCEDES-BENZ

Use-Case-2



Automotive: frugal EV platform production pilot for FORD Motors

Use-Case-3

Marine: electric tugboat production pilot

Use-Case-4

Stationary: 2nd-life electric energy storage production pilot

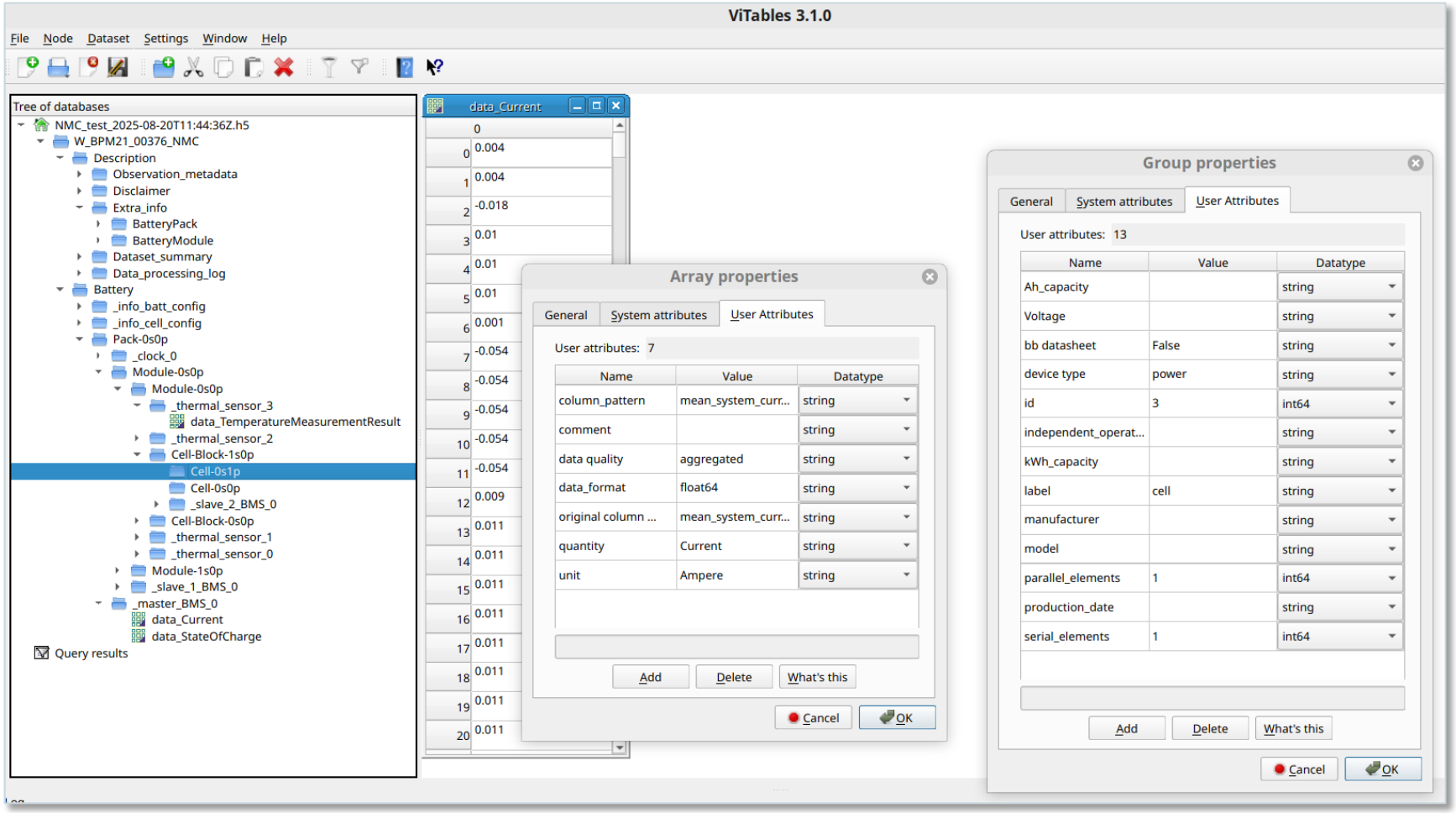
Current Definitions – Regulation vs. Ontology

Component	EU Battery Regulation (2023/1542) Annex I – Definitions, specifically in Article 3 of the Regulation	BASE Definition (Proposed Ontology)	Technical Characteristics
Battery Cell	This term is not explicitly defined on its own in the EU Battery Regulation (2023/1542), but referred to indirectly in other definitions as: "the basic functional unit in a battery, composed of electrodes, electrolyte, container, terminals and, if applicable, separators, and containing the active materials the reaction of which generates electrical energy"	**The smallest electrochemical unit** in a battery system, consisting of electrodes, electrolyte, terminals, and a container (with separators if needed). It contains the active materials that generate electrical energy through chemical reactions and comes in various formats (e.g., pouch, coin, cylindrical, prismatic) depending on the application.	• **Generates and carries its own electrical current** • Delivers voltage typical for its chemistry • Operates as an independent electrochemical unit • Can be connected in series or parallel to form blocks or modules
Battery Cell-Block	Attn: This term is not explicitly defined in the EU Battery Regulation (2023/1542)	A group of battery cells connected in parallel and monitored as a unit by the Battery Management System (BMS). If no parallel connection exists, it corresponds to a single battery cell. In a module or pack, it is the smallest unit with a voltage typical for its chemistry.	• **Shares current across parallel-connected cells** • Delivers a fixed voltage level depending on cell chemistry • Monitored as a single unit by the BMS • Acts as the basic electrical building block within a module or pack
Battery Module	Article 3(17): "'battery module' means a unit comprising multiple battery cells that are connected together and used as a building block of a battery pack."	**A mid-level unit** made of battery cells (or cell blocks), protected by an outer casing. It is the smallest unit that can be easily exchanged. In non-modular systems (e.g., Cell-to-Pack), the module equals the pack.	• May contain multiple cell blocks or sub-modules • **Shares electrical current across its internal units** • Replaceable as a serviceable unit • Provides electrical and structural interface to the pack
Battery Pack	Article 3(16): "'battery pack' means a unit that comprises battery modules or cells and is fitted with a battery management system;"	**The largest unit** in a battery system, made of connected modules or cell blocks. It includes thermal, electrical, and safety systems and operates as a standalone power source, while internal units cannot operate independently.	• **Shares total system current across modules or blocks** • Delivers power to external systems or vehicles • Contains structural housing, cooling, and control systems • Not designed for disaggregated operation of internal components

Source: European Union (2023). *EUR-Lex - 32023R1542 - EN - EUR-Lex*. [online] Europa.eu. Available at: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=celex%3A32023R1542.

Use case data

Converted to HDF5



- annotated sample data
- harmonized format

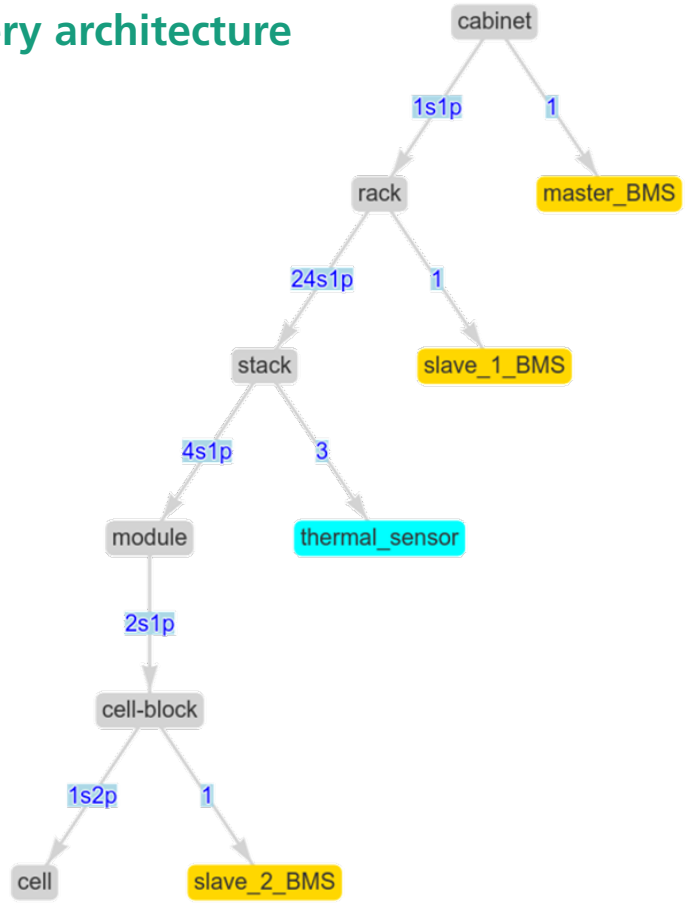
use for

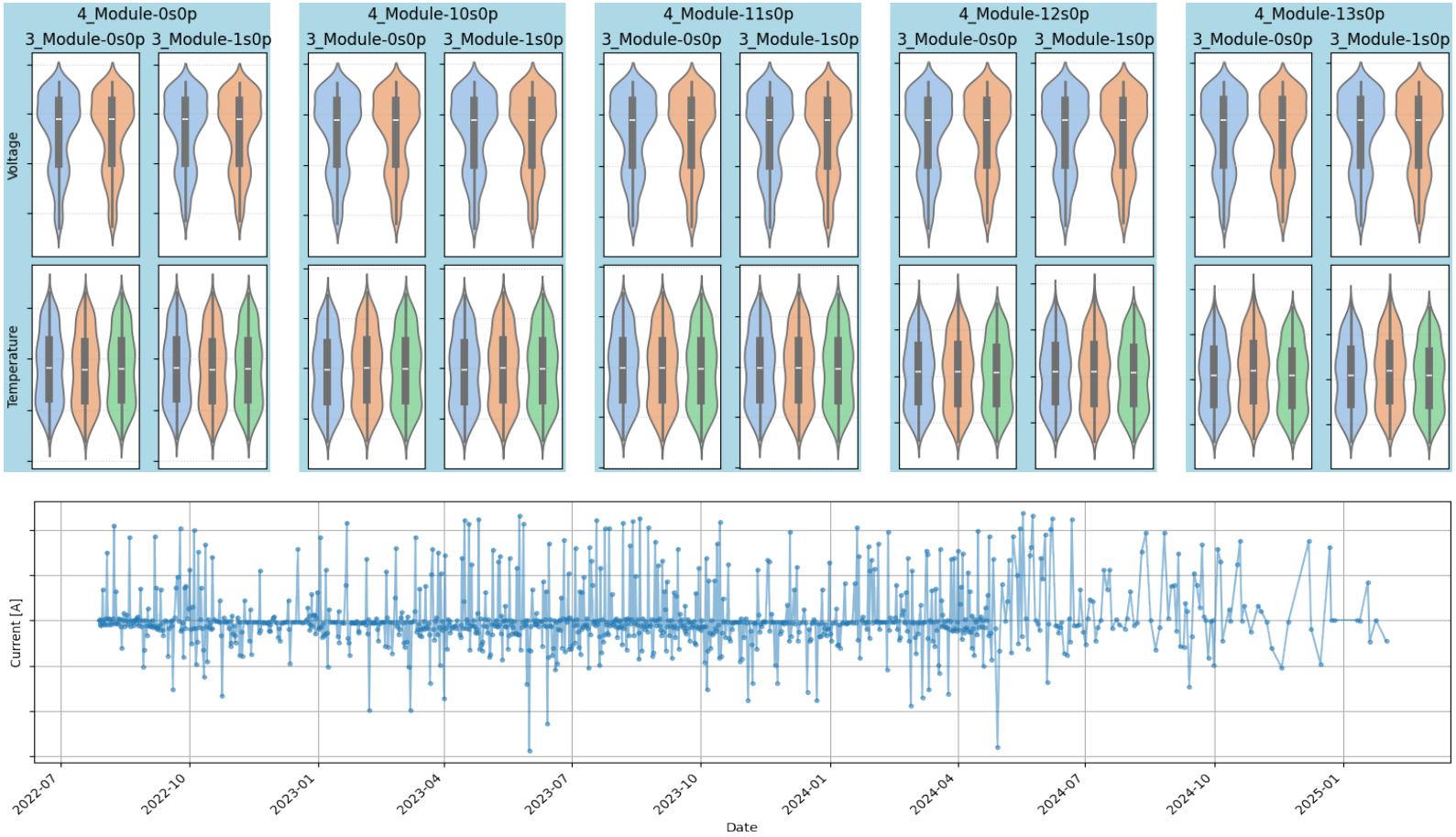
- data analysis
- semantic modelling

Sample data

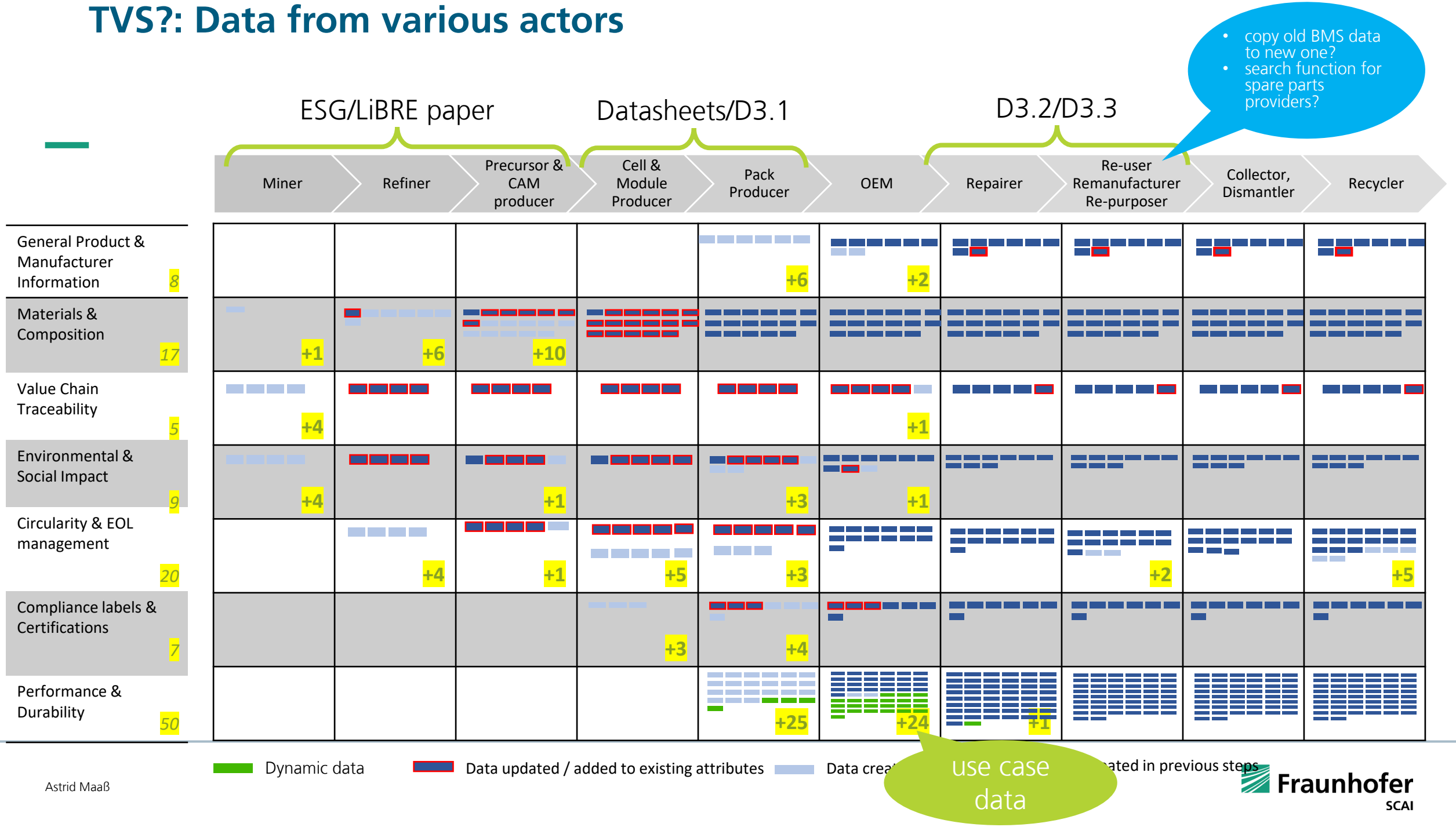
Storage application

Battery architecture





TVS?: Data from various actors



ESG: company-based to product-based score?

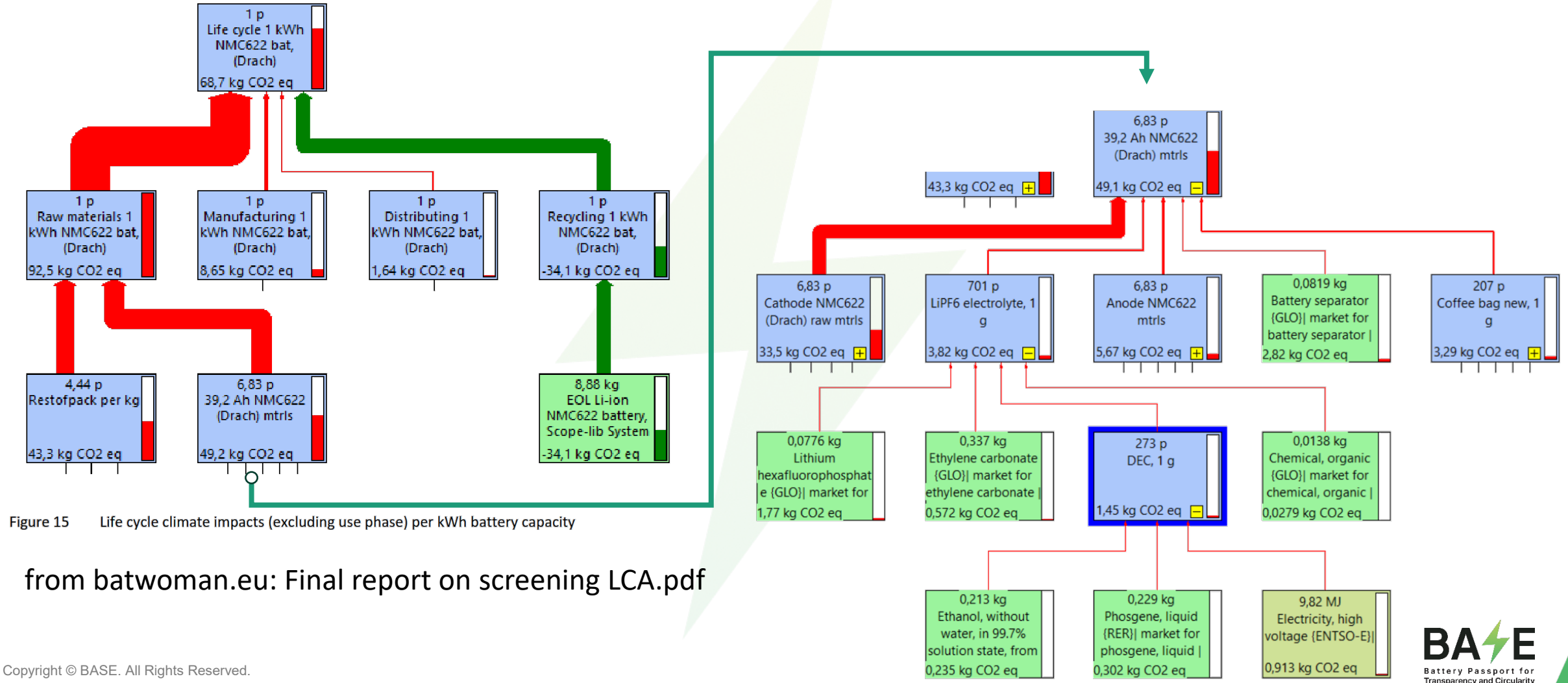


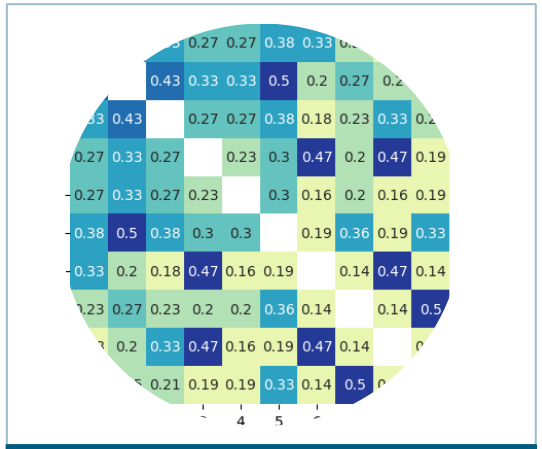
Figure 15 Life cycle climate impacts (excluding use phase) per kWh battery capacity

from batwoman.eu: Final report on screening LCA.pdf

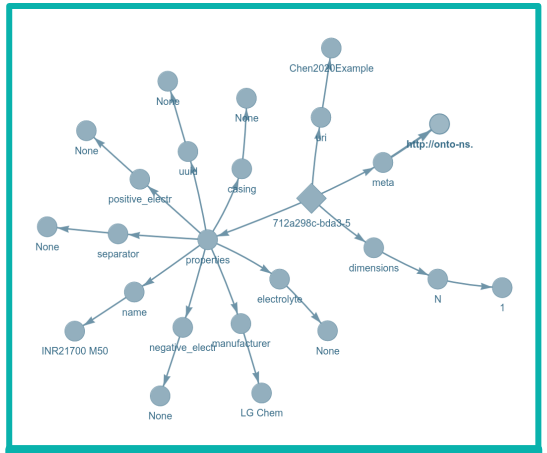
BASE
Battery Passport for Transparency and Circularity

BASE Semantic model

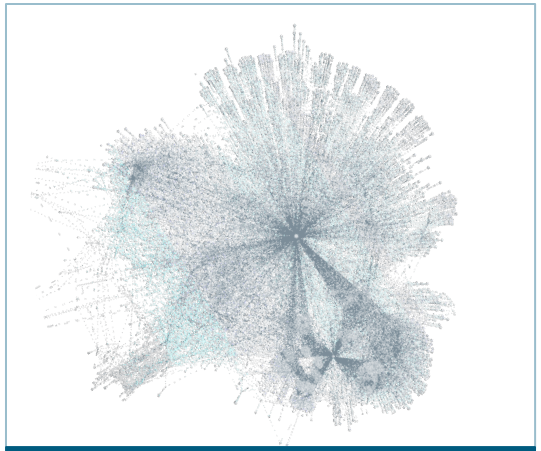
A generic approach applicable to various scenarios



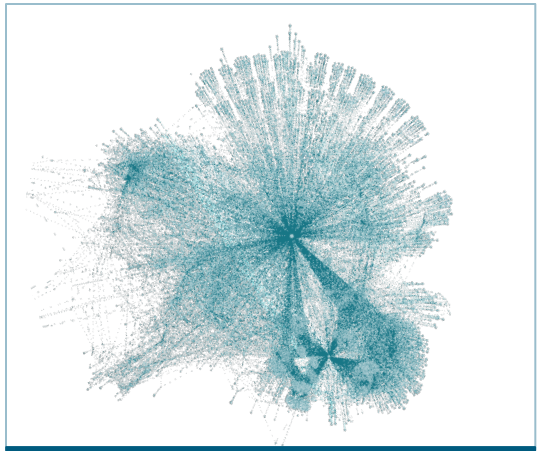
USE CASE DATA
Application-specific data originating from local environments and measurements. While familiar, non-standardized naming conventions can limit interoperability.



METADATA
Contextual annotation transforms raw data into interoperable assets.
It provides essential information for accurate interpretation and processing, relying on standardized formats.

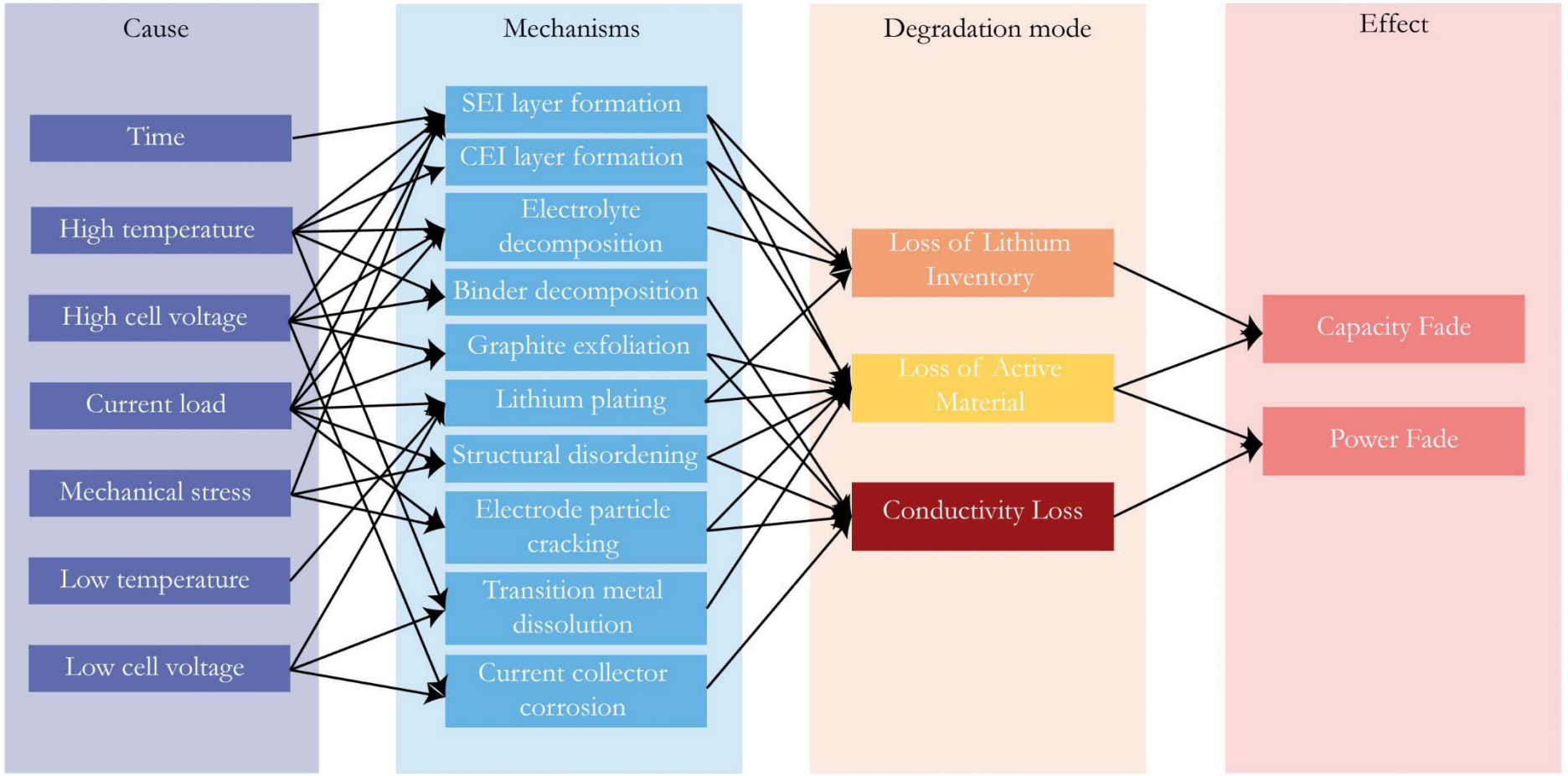


ONTOLOGY
Defined by expert communities, ontologies establish the general principles and concepts of their domains in both human- and machine-readable formats.



KNOWLEDGE GRAPH
A synthesis of principles and data, forming a well-structured, queryable system. This unified dataset enables insights, enhanced AI applications, and optimized data retrieval.

LIB-Ageing phenomena



Wikipedia, Vermeer 2022

Annotation tables

dynamic

cell: static data
global info section:
key = value

csv table
essential components + data

optional attributes section

list of components

static #1
universal

battery
global info section:
key = value

csv table

- unit → sub unit
- unit → sensor/other
- sensor/other

optional attributes section

list of components + **config section,** mandatory

static #2
app specific

observations
global info section:
key = value

csv table

list of column names + metadata

battery config file & Circularity & EOL

2. INFORMATION RELATING TO THE BATTERY MODEL ACCESSIBLE ONLY TO PERSONS WITH A LEGITIMATE INTEREST AND THE COMMISSION

A battery passport shall include the following information relating to the battery model, which shall be accessible only to persons with a legitimate interest and the Commission:

(a) detailed composition, including materials used in the cathode, anode and electrolyte; → cell config file

(b) part numbers for components and contact details of sources for replacement spares;

(c) dismantling information, including at least:

— exploded diagrams of the battery system/pack showing the location of battery cells,

— disassembly sequences,

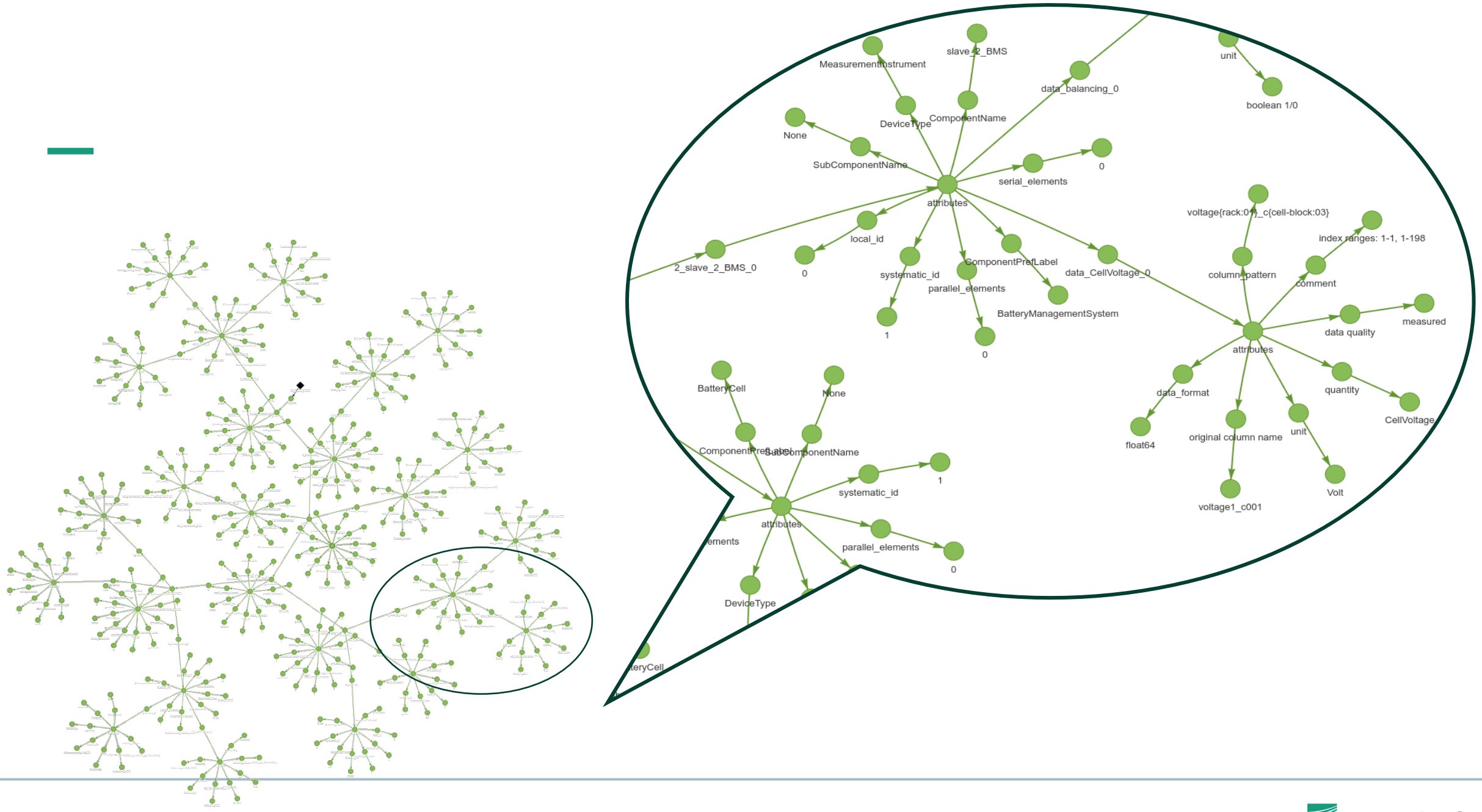
— type and number of fastening techniques to be unlocked,

— tools required for disassembly,

— warnings if risk of damaging parts exist,

— amount of cells used and layout; → battery config file

(d) safety measures.


MeasurementInstrument
slave_2_BMS
DeviceType
ComponentName
None
SubComponentName
data_balancing_0
unit
boolean 1/0
serial_elements
0
attributes
2_slave_2_BMS_0
local_id
0
systematic_id
parallel_elements
ComponentPrefLabel
BatteryManagementSystem
1
0
data_CellVoltage_0
voltage{rack:01}_c{cell-block:03}
index ranges: 1-1, 1-198
column_pattern
comment
data quality
measured
attributes
data_format
quantity
CellVoltage
float64
original column name
unit
Volt
voltage1_c001
BatteryCell
None
ComponentPrefLabel
SubComponentName
systematic_id
1
attributes
parallel_elements
0
DeviceType

principles of organisation

application defines requirements in terms of power & voltage

form follows function

start with cell, build up from there

follow physics

connect cells to meet power/voltage requirements (serial→ voltage; parallel → power)

fix cells/contacts to satisfy robust & safe usage → encapsulate

add whatever else is needed

control

safety

Circularity & EOL

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(d) safety measures.

needed in future!! automated search for suppliers?

BASE Battery Passport for Transparency and Circularity

Project Consortium

Co-funded by the European Union

This project has received funding from the Horizon Europe Framework Programme (HORIZON) Research and Innovation Actions under grant agreement No 101157200