This project has recived funding from the European Union's Horizon Europe research and innovation programme under grant number No. 101104022.

An interactive semantic battery knowledge base

Philipp Veit, Christian Punckt, Simon Stier, Lukas Gold, Simon Clark, Eibar Flores

Karlsruhe Institute of Technology

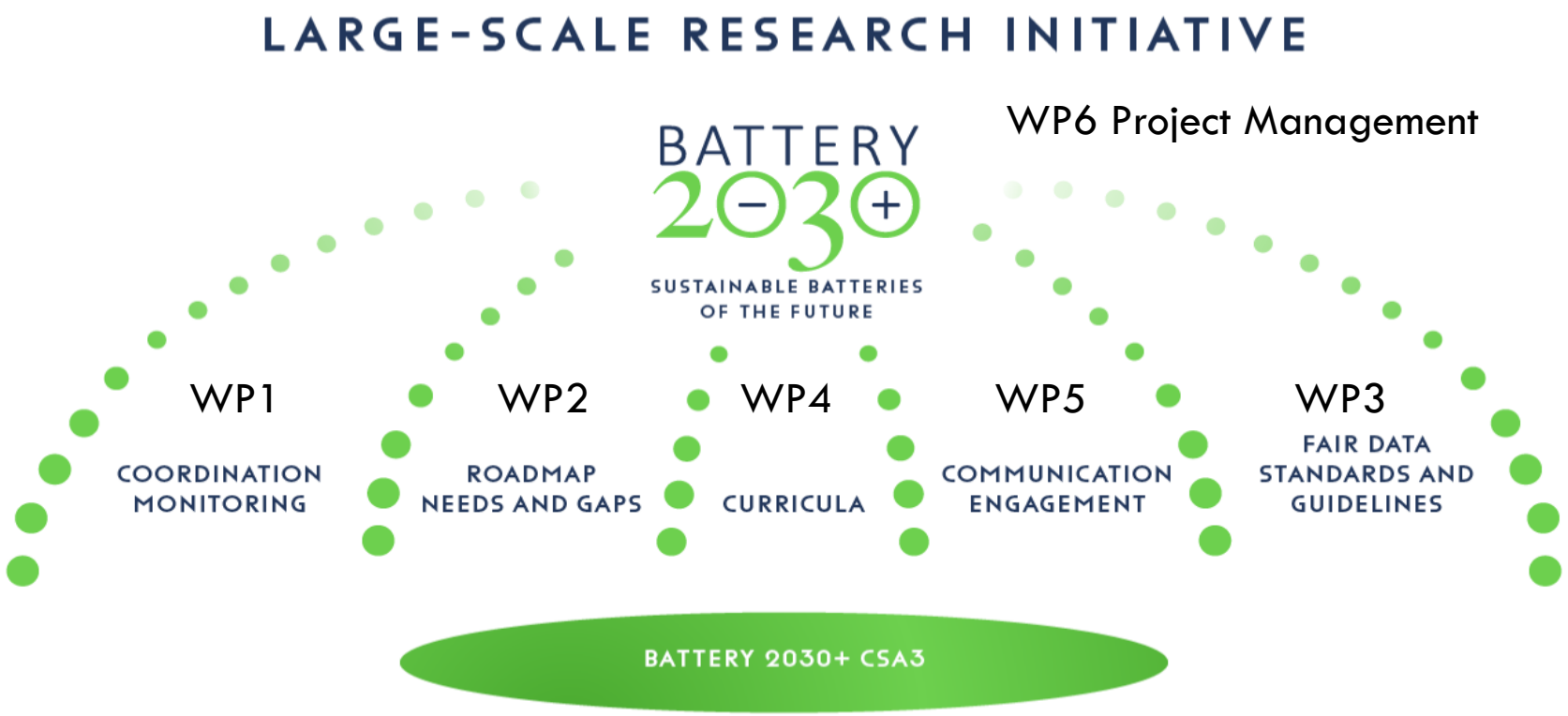
Standards and Best Practice Workshop Oslo

June 26th 2024

BATTERY 2030+

Structure of the initiative

This project has recived funding from the European Union's Horizon Europe research and innovation programme under grant number No. 101104022.



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LARGE-SCALE RESEARCH INITIATIVE

BATTERY 2030+
SUSTAINABLE BATTERIES OF THE FUTURE

WP6 Project Management

WP1 COORDINATION MONITORING

WP2 ROADMAP NEEDS AND GAPS

WP4 CURRICULA

WP5 COMMUNICATION ENGAGEMENT

WP3 FAIR DATA STANDARDS AND GUIDELINES

BATTERY 2030+ CSA3

SALAMANDER

RENOVATE

phoenix

OPINCHARGE

STREAMS

Revitalise

REUSE

BATTwin

HEALING BAT

OPERA

UltraBat

CICERO

BatCAT Battery Cell Assembly Twin

Why do we need standard protocols?

Comment | Published: 12 February 2024

My cell is better than yours

Nella M. Vargas-Barbosa

Nature Nanotechnology **19**, 419–420 (2024) | Cite this article

4735 Accesses | **10** Altmetric | Metrics

Editorial | Free Access

Ten Ways to Fool the Masses When Presenting Battery Research**

Prof. Patrik Johansson, Dr. Sajid Alvi, Pedram Ghorbanzade, Martin Karlsmo, Dr. Laura Loaiza, Dr. Vigneshwaran Thangavel, Kasper Westman, Fabian Årén

First published: 01 October 2021 | https://doi.org/10.1002/batt.202100154 | Citations: 9

** Heavily inspired by and a homage to Ref. [1]. Editorial note: This Editorial article is written in a humorous tone and has been peer reviewed. It should not be taken as literal advice by the scientific community.

Research Article | Open Access

Round-robin test of all-solid-state battery with sulfide electrolyte assembly in coin-type cell configuration

Alexander Beutl, Ander Orue, Pedro López-Aranguren, Andrea Itziar Pitillas Martinez, Maria Helena Braga, Ville Kekkonen, Artur Tron

First published: 29 March 2024 | https://doi.org/10.1002/elsa.202400004

Research Article | Open Access

Potential and Limitations of Research Battery Cell Types for Electrochemical Data Acquisition

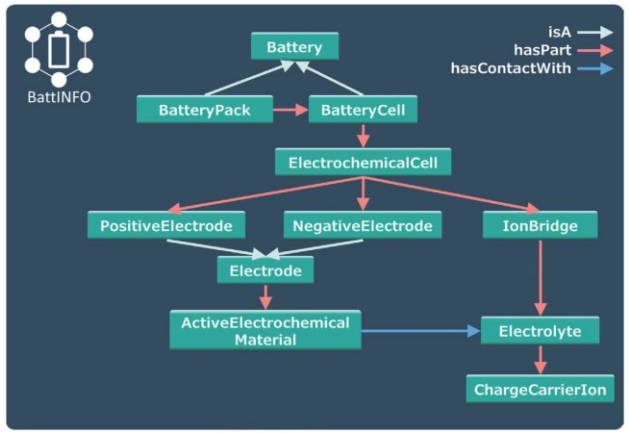
Dr. Anna Smith, Dr. Pirmin Stüble, Dr. Lea Leuthner, Dr. Andreas Hofmann, Dr. Fabian Jeschull, Liuda Mereacre

First published: 20 March 2023 | https://doi.org/10.1002/batt.202300080 | Citations: 4

- → Compare results from different “competing” labs
- → Compare results from different collaborating labs
- → **Boost collaboration & innovation**

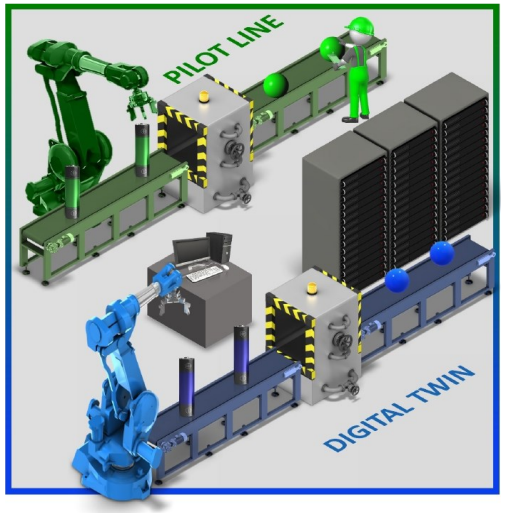
Best Practices for standard protocols for theory and experiment

Ontologies & Dynamic DMPs



Clark et al., *Adv. Energy Mater.* (2021) 2102702

Modelling & Digital Twins



DEFACTO / LiPlanet

Underlying data must be not only FAIR but FAI**R**^{4}

Best Practices – Battery2030PLUS

FAI**R**^{4} **Data:**

F	-	Findable
A	-	Accessible
I	-	Interoperable
R^4	-	Reusable
	-	Reproducible
	-	Reliable
	-	Relevant

Data „Quality“

BATTERY 2030+ Memorandum on Research Standards and Guidelines

114 Signatures from 57 Affiliations

Read and Sign the Memorandum today:

Combined, RDM tools and standardisation will not only improve the general quality of research within BATTERY 2030+ and enable the FAIR* data principles. More importantly, the collaboration will be possible on entirely new levels, allowing for a novel, autonomous research approaches, accelerated materials discovery, and data-based research in a field that has thus far mostly adhered to classical trial and error research.

Read **BATTERY 2030+ Memorandum on Research Standards and Guidelines**.

Endorse BATTERY 2030+ Memorandum by sending an email to **battery2030@uu.se** including your full name and affiliation or fill out this form below.

Your name

Your email

Affiliation

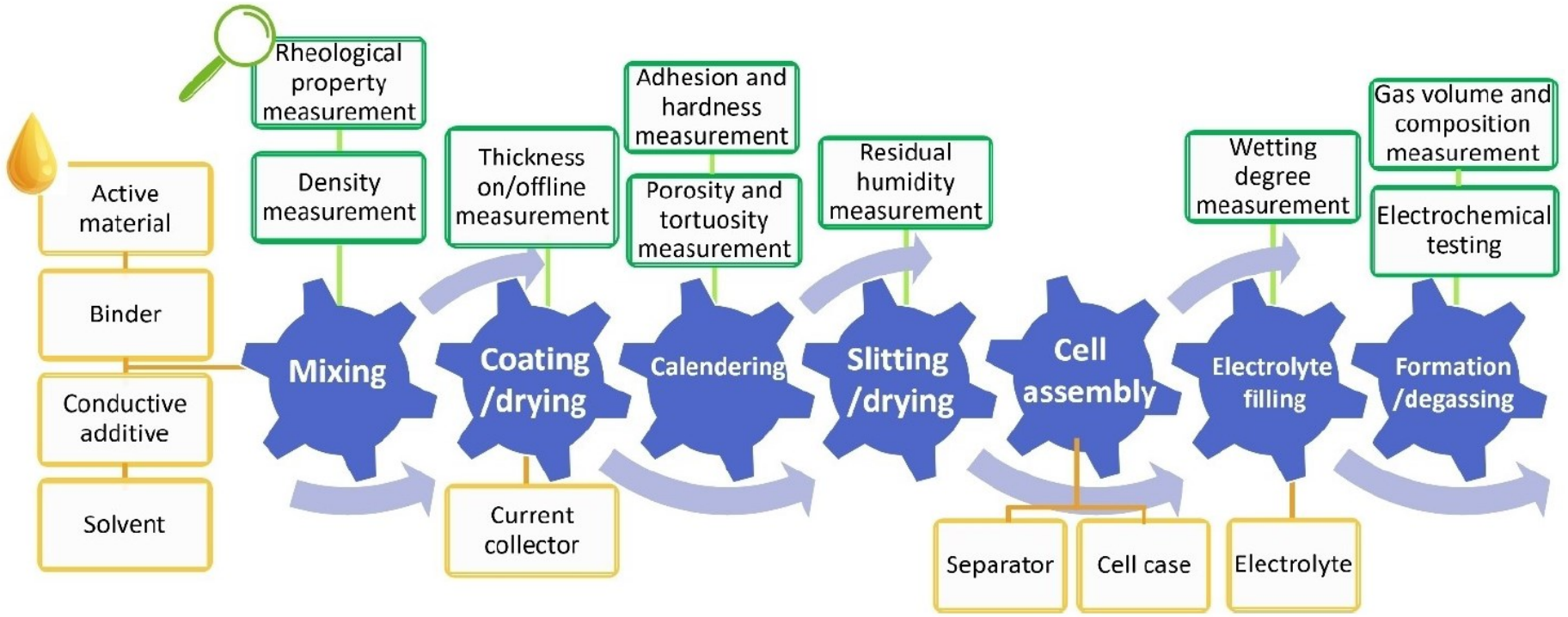
Submit

*FAIR data stands for **F**indability, **A**ccessibility, **I**nteroperability, and **R**euse of digital assets.

https://battery2030.eu/research/research-data-management-rdm-standards/

Protocols & Standards

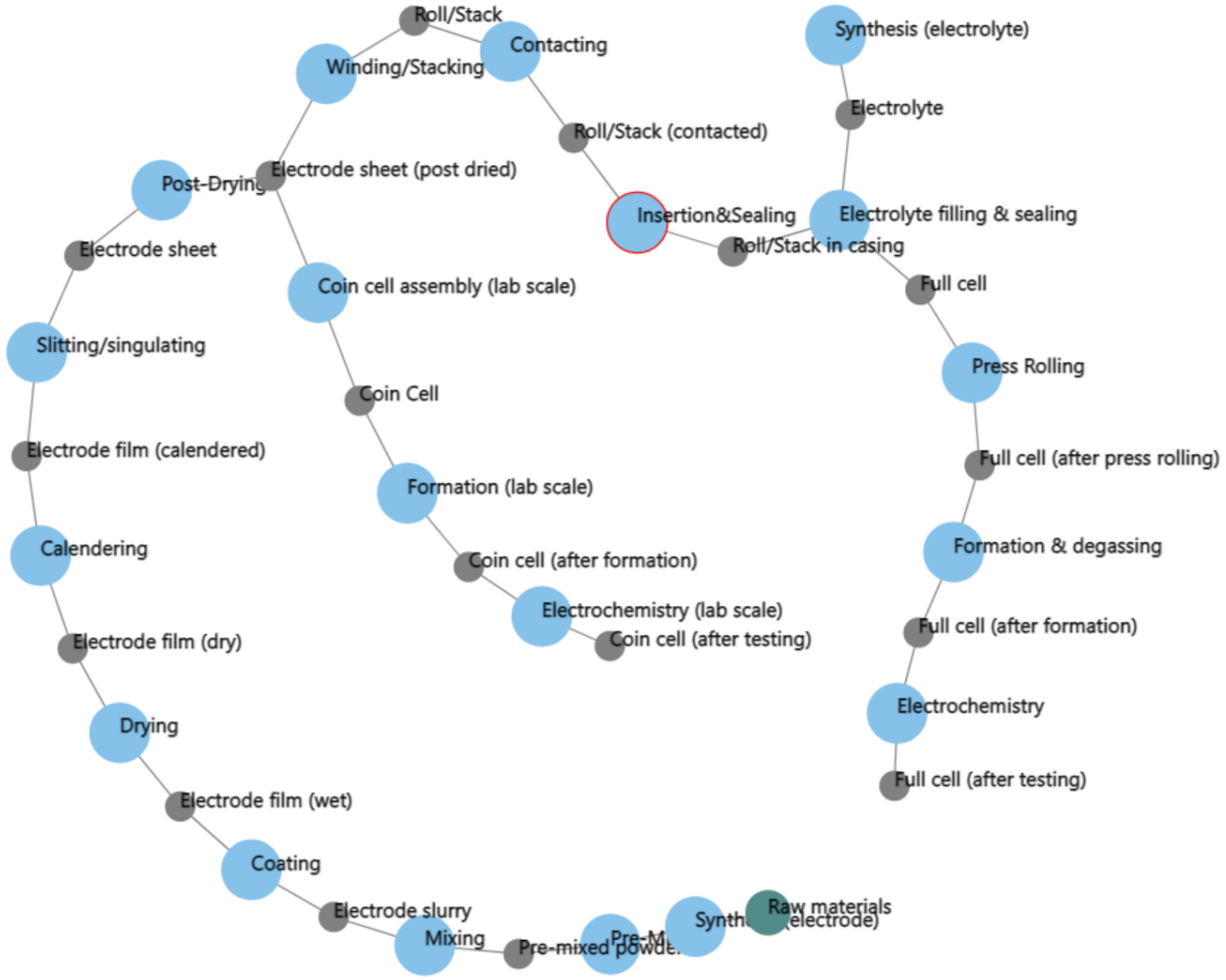
- **Key Performance Indicators (KPIs) & Process Parameters (PPs) along the R&D process chain for batteries – FOCUS ON CELL FABRICATION**



From: F.M. Zanotto et al. "Data Specifications for Battery Manufacturing Digitalization", Batteries & Supercaps (2022) e202200224

Protocols & Standards

- **Key Performance Indicators (KPIs) & Process Parameters (PPs) along the R&D process chain for batteries – FOCUS ON CELL FABRICATION**

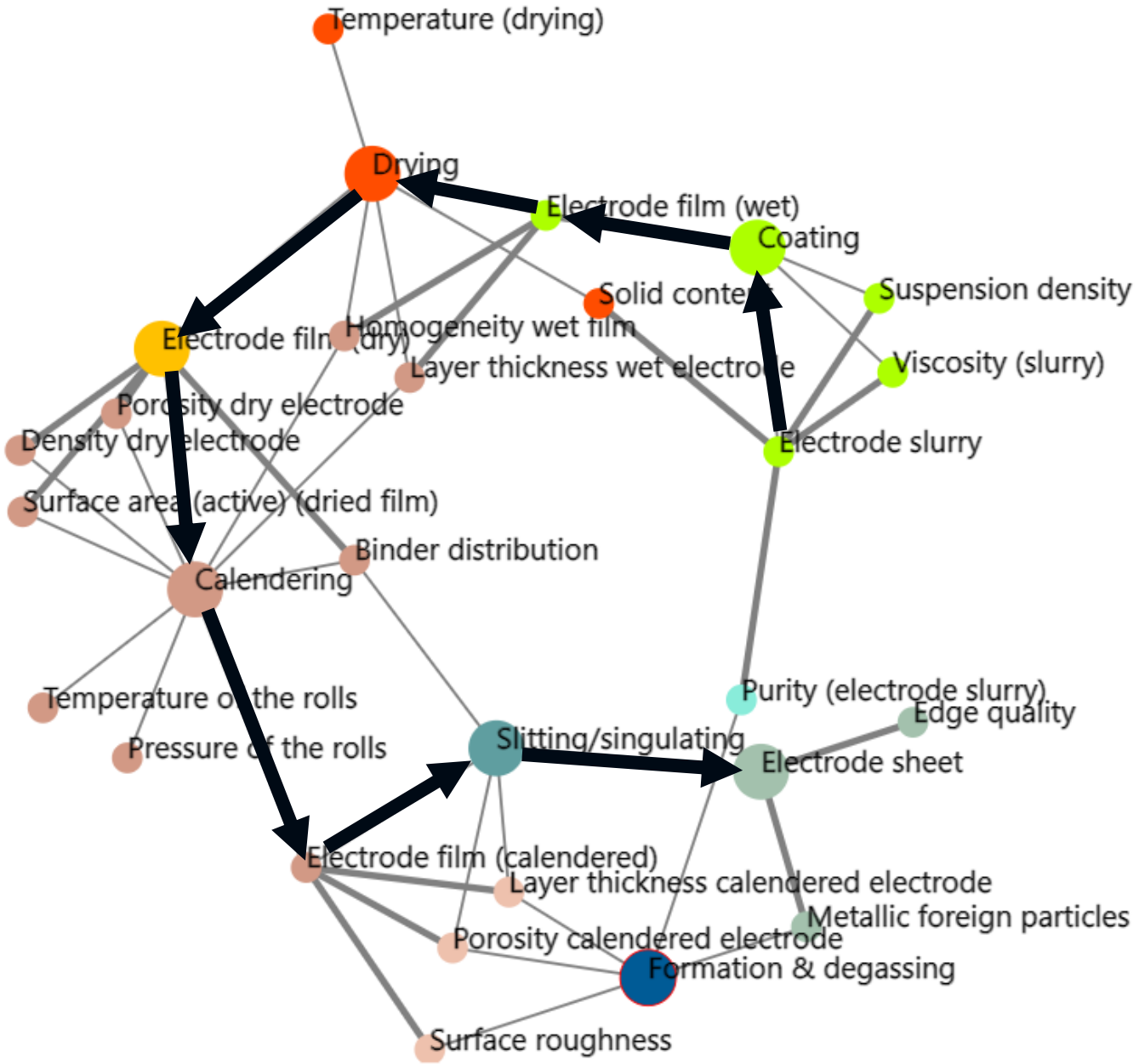


- **PPs and KPIs for each step and intermediary "product" identified**

Network is being created, as KPIs of one step become PPs for subsequent steps

- **First measurement methods and protocols for PPs & KPIs identified**

Protocols & Standards



OVERALL NETWORK:

- **150+ KPIs and PPs**
- **Each associated with method of measurement**
- **Data & Metadata**
- **Protocols and procedures**
- **Blank Detail Specifications**

HUGE TASK!

- **Focus on pilot activities and best practice examples**

Protocols & Standards

Extract from full data base:
Calendering process, KPIs of calendered electrode

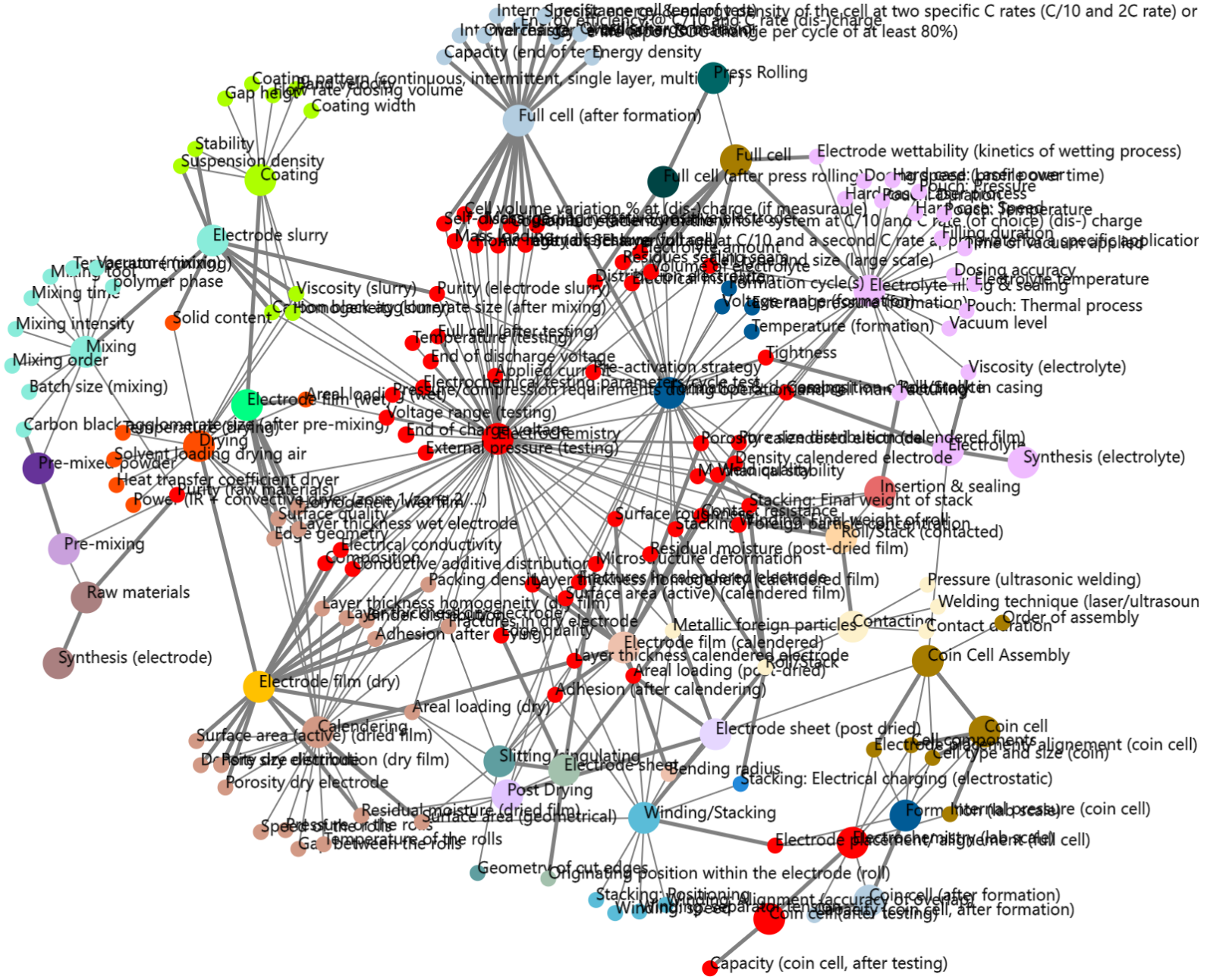
Selection of 3 KPIs w/ connection to several subsequent steps

KPI	PP 1 for	PP 2 for	PP 3 for	Measurement technique
Layer thickness calendered electrode	Slitting/singulating	Post Drying	Electrochemistry	Thickness gauge, SEM, Laser triangulation
Porosity calendered electrode	Electrolyte filling & sealing	Formation & degassing	Electrochemistry	Laser triangulation, mercury porosimetry
Surface roughness	Formation & degassing	Electrochemistry		SEM, Reflectometer

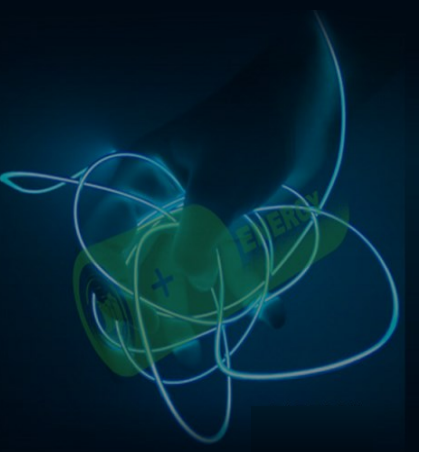
Let‘s take a look at the complete network of process steps, KPIs and PPs…

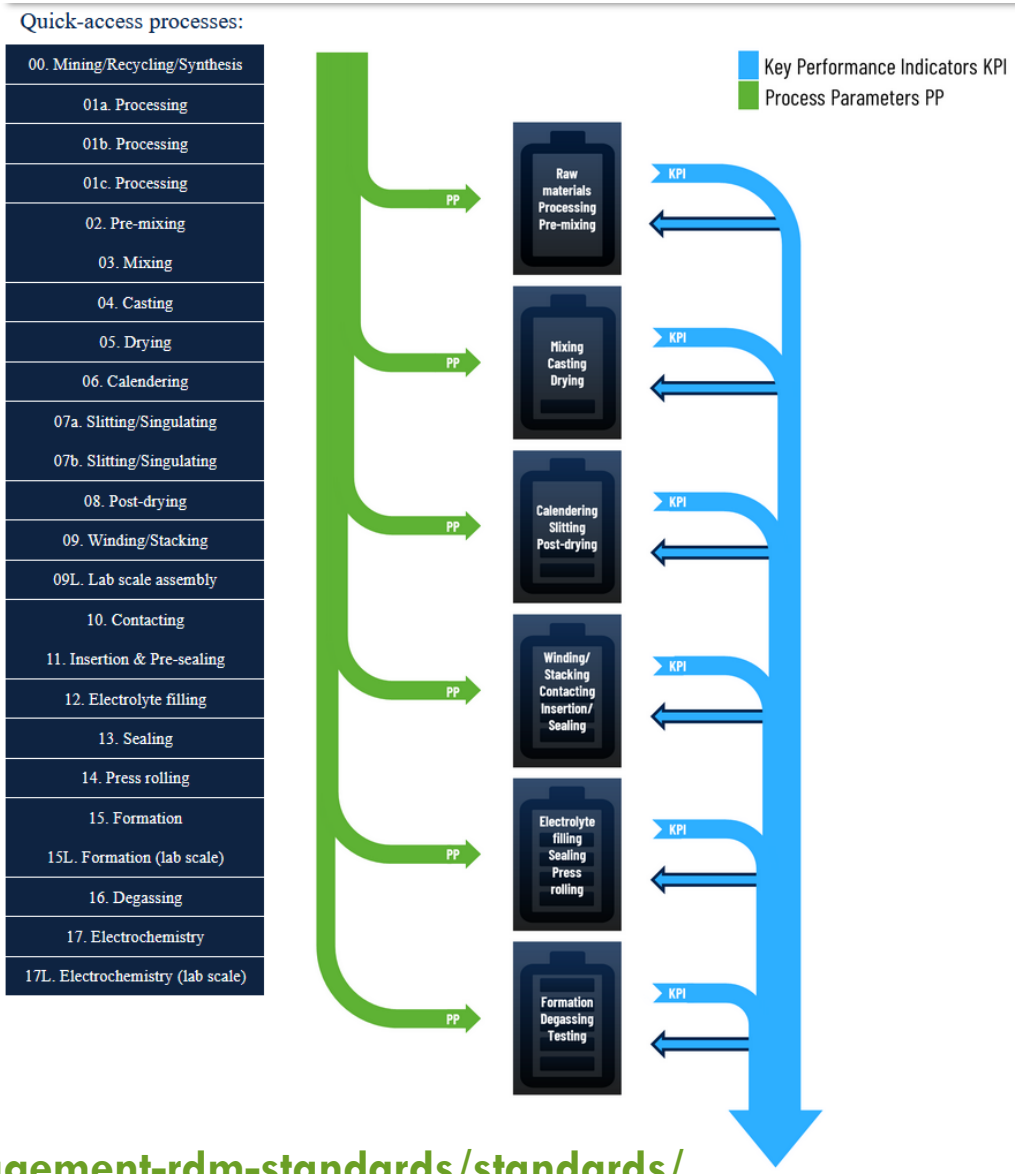
BATTERY 2030+

Visualisation in Power BI



BATTERY 2030+ Knowledge base (1.0) for standards and protocols in battery research & development





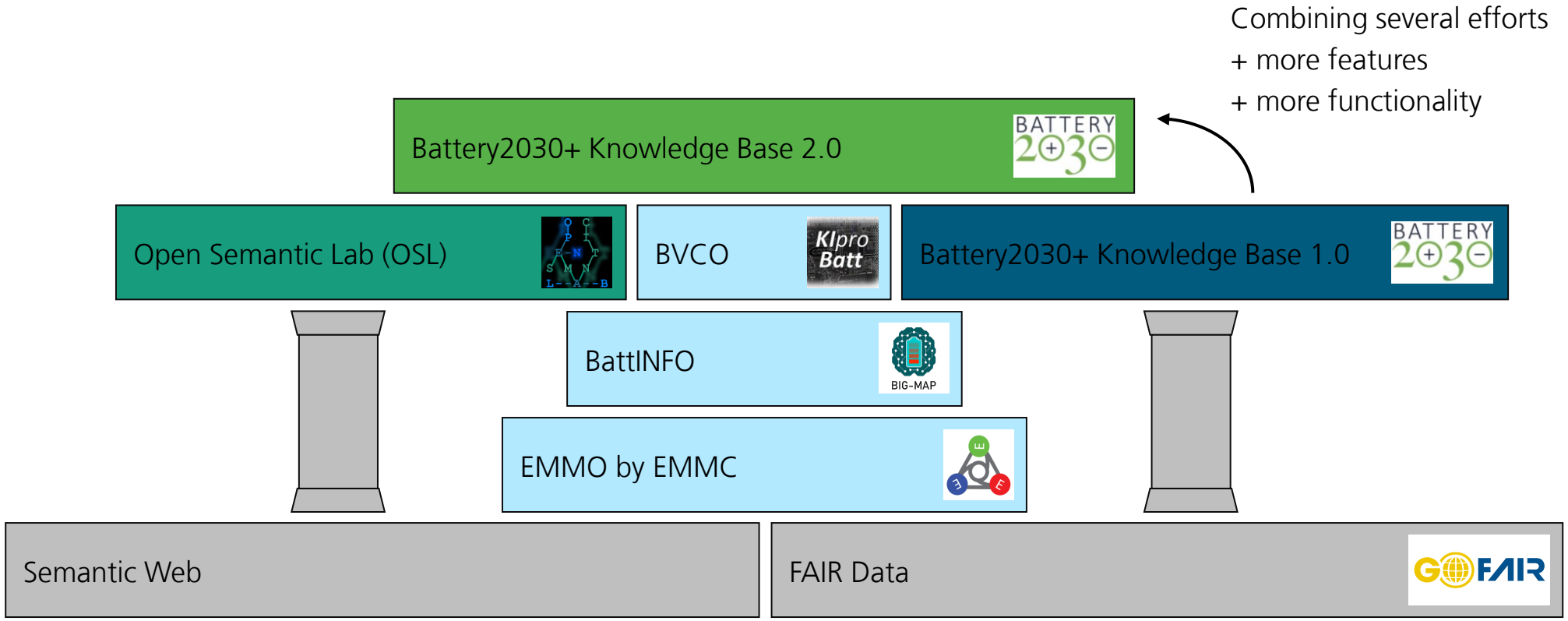
- Only desktop version running at the moment

https://www.celest.de/en/or/layer1

https://battery2030.eu/research/research-data-management-rdm-standards/standards/

Implementing Semantic Web Technology

To the battery domain - A brief retrospective



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Motivation

Linking Research Data to Ontology (Terms)?

QUDT
Quantity, Unit, Dimenson and Types Ontology

EMMO
Elementary Multiperspective Material Ontology

Ok, Great! BUT…

How to do this mapping?
(in everyday research work)

Do I have to do it again?

Where to put this mapping?

How should I describe my Sample?

- Production parameters?
- Usage & storage history?

Example:
Bio-Logic EIS spectrum

unit:HZ
emmo:Frequency

unit:OHM
emmo:ElectricImpedance

unit:SEC
emmo:Time

unit:V
emmo:ElectricPotential

unit:MilliA
emmo:ElectricCurrent

*Cell025_PEIS.mpt - Editor

Datei Bearbeiten Format Ansicht Hilfe

freq/Hz	Re(Z)/Ohm	-Im(Z)/Ohm	|Z|/Ohm	Phase(Z)/deg	time/s	<Ewe>/V	<I>/mA
1,9999814E+005	-5,0842005E-004	-2,8044581E-002	2,8049190E-002	9,1038605E+001	4,131745615463762E+003	3,8452442E+000	1,2709299E+002
1,6482334E+005	7,4216514E-004	-2,3246864E-002	2,3258708E-002	8,8171432E+001	4,132296617783315E+003	3,8452420E+000	1,1706958E+002
1,3582802E+005	1,6357927E-003	-1,9288411E-002	1,9357650E-002	8,5152512E+001	4,132845593249367E+003	3,8452537E+000	1,1183223E+002
1,1194515E+005	2,2274035E-003	-1,6020076E-002	1,6174182E-002	8,2084442E+001	4,133396612315555E+003	3,8452654E+000	1,0645662E+002
9,2256156E+004	2,4567349E-003	-1,3307923E-002	1,3532788E-002	7,9540558E+001	4,133946614741639E+003	3,8452506E+000	1,0256559E+002
7,6028055E+004	2,6373817E-003	-1,1062559E-002	1,1372598E-002	7,6590645E+001	4,134497596261150E+003	3,8452423E+000	9,8932236E+001
6,2657734E+004	2,7039335E-003	-9,2100762E-003	9,5987897E-003	7,3638588E+001	4,135047597007302E+003	3,8452401E+000	9,6577942E+001
5,1634871E+004	2,7133890E-003	-7,6447935E-003	8,1120497E-003	7,0458549E+001	4,135596592740039E+003	3,8452516E+000	9,3989075E+001
4,2551219E+004	2,7010620E-003	-6,3426504E-003	6,8938341E-003	6,6932930E+001	4,136146616446145E+003	3,8452468E+000	9,1498405E+001
3,5063469E+004	2,6747584E-003	-5,2436721E-003	5,8864616E-003	6,2974209E+001	4,136697601938969E+003	3,8452506E+000	9,0785957E+001
2,8902539E+004	2,6378180E-003	-4,3150596E-003	5,0574522E-003	5,8562344E+001	4,137248594151810E+003	3,8452463E+000	9,0007919E+001
2,3817920E+004	2,6050475E-003	-3,5300588E-003	4,3872073E-003	5,3574100E+001	4,137798613991297E+003	3,8452439E+000	8,8230858E+001

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github.com/emmo-repo/EMMO
qudt.org

Motivation

Linking Research Data to Ontology (Terms)?

➡ **Open Semantic Lab**

➡ **Object Oriented Linked Data**

- Object orientation
- Linked Data

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Theoretical Background

Object Orientation (OO)

Abstract concepts

Real-world (physical) Items

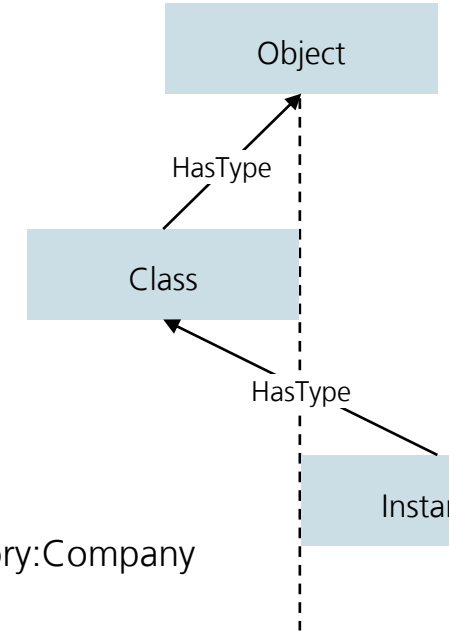
Object Orientation – a (subconsciously) often used concept

Everything

- Is an Object

Extension: Everything

- Has a Type
- Has an unique identifier



Item:MyElectricCar

Serial No.:	Y02-4256
Manufacturer:	Green Motion
Type No.:	Y02

Defines

- Set of properties
- Valid range thereof

Category:Car

Serial No.:	string
Manufacturer:	Category:Company
Type No.:	string

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BATTERY 2030+

Fraunhofer ISC

Theoretical Background

Object Oriented Linked Data (OO-LD)

Abstract concepts

- EMMO
- BattINFO
- BVCO
- Schema.org
- FOAF
- …

How to map to ontology terms?

schema:Corporation
https://schema.org/Corporation

owl:sameAs

schema:Car
https://schema.org/Car

owl:sameAs

schema:serialNumber
https://schema.org/serialNumber

owl:sameAs

schema:manufacturer
https://schema.org/manufacturer

owl:sameAs

emmo:Manufacturer
https://w3id.org/emmo#EMMO_c0afb341_7d31_4883_a307_ae4606df2a1b

Category:Car

Serial No.:	string
Manufacturer:	Category:Company
Type No.:	string

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Application Example

OO-LD in Action

Abstract concepts

Category:Vehicle (JSON Schema)

```
{
  "@context": [
    {
      "manufacturer": "schema:manufacturer",
      "manufacturer*": "emmo:EMMO_c0afb341_7d31_4883_a307_ae4606df2a1b",
      "serial_or_batch_number": "schema:serialNumber",
      "serial_or_batch_number*": {
        "@id": "Property:HasSerialNumber",
        "@type": "xsd:string"
      },
      "serial_or_batch_number**": {
        "@id": "Property:HasBatchNumber",
        "@type": "xsd:string"
      },
      "manufacturer**": {
        "@id": "Property:HasManufacturer",
        "@type": "@id"
      },
```

Ln: 14 Col: 9

defines

Category:Car (JSON Data)

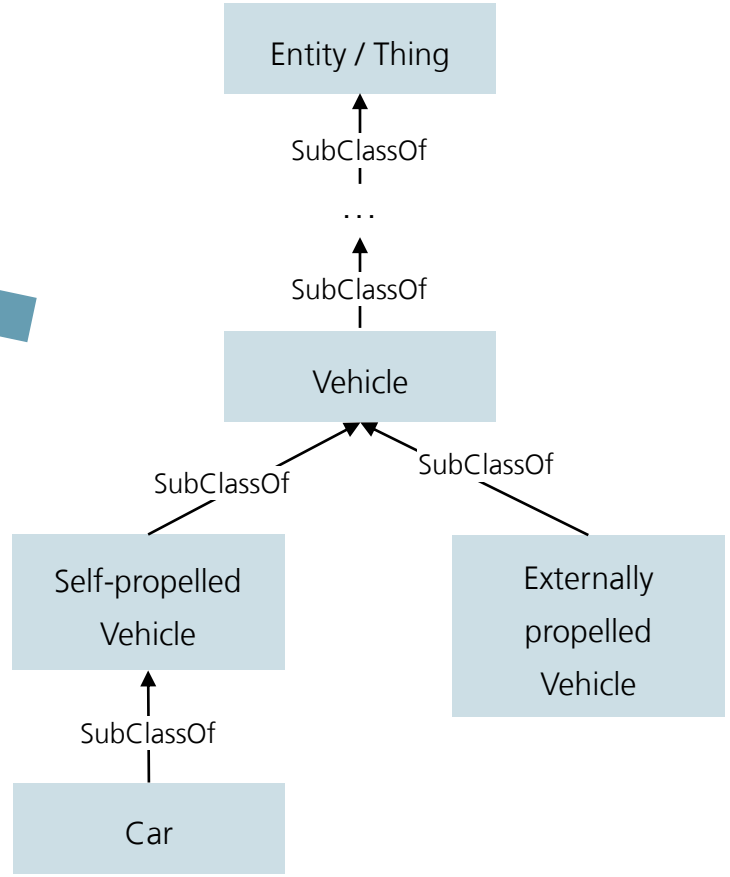
```
{
  "name": "Car",
  "subclass_of": [
    "Category:OSWaf7b11dea04e4ad189e32124956af9b6"
  ],
  "rdf_type": [
    "schema:Car"
  ],
  "label": [
    {
      "text": "Car",
      "lang": "en"
    },
```

Ln: 10 Col: 6

Self-propelled Vehicle

defines

Categories:



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Application Example

OO-LD in Action

Real-world (physical) Items

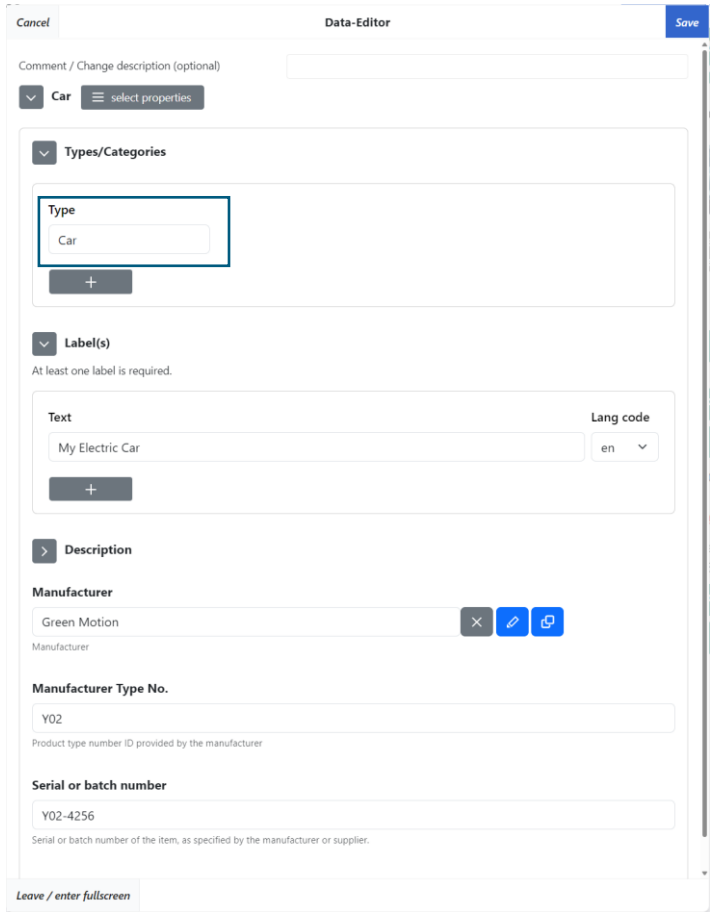
Abstract concepts

Item:MyElectricCar (JSON Data)

```
{
  "type": [
    "Category:OSWea8e435f766b484e9fbb53344c90a942"
  ],
  "manufacturer": "Item:OSWbd9d3e4203c94d488d10c1cdda84d985",
  "manufacturer_type_no": "Y02",
  "serial_or_batch_number": "Y02-4256",
  "uuid": "5538bdc6-bd0d-413a-9337-73136dade46b",
  "label": [
    {
      "text": "My Electric Car",
      "lang": "en"
    }
  ],
  "description": [
    {
      "text": "This is a made up car for demonstration purpose",
      "lang": "en"
    }
  ],
  "name": "MyElectricCar",
  "image": "File:OSW736e9efde3224d7e8c185f352cf53b0f.png"
}
```

Car

Creates



Define Editor layout & Input fields

HasType

Categories

- Entity / Thing
- SubClassOf
- ...
- SubClassOf
- Vehicle
- SubClassOf
- Self-propelled Vehicle
- SubClassOf
- Car

Data structured and annotated – Ready for export

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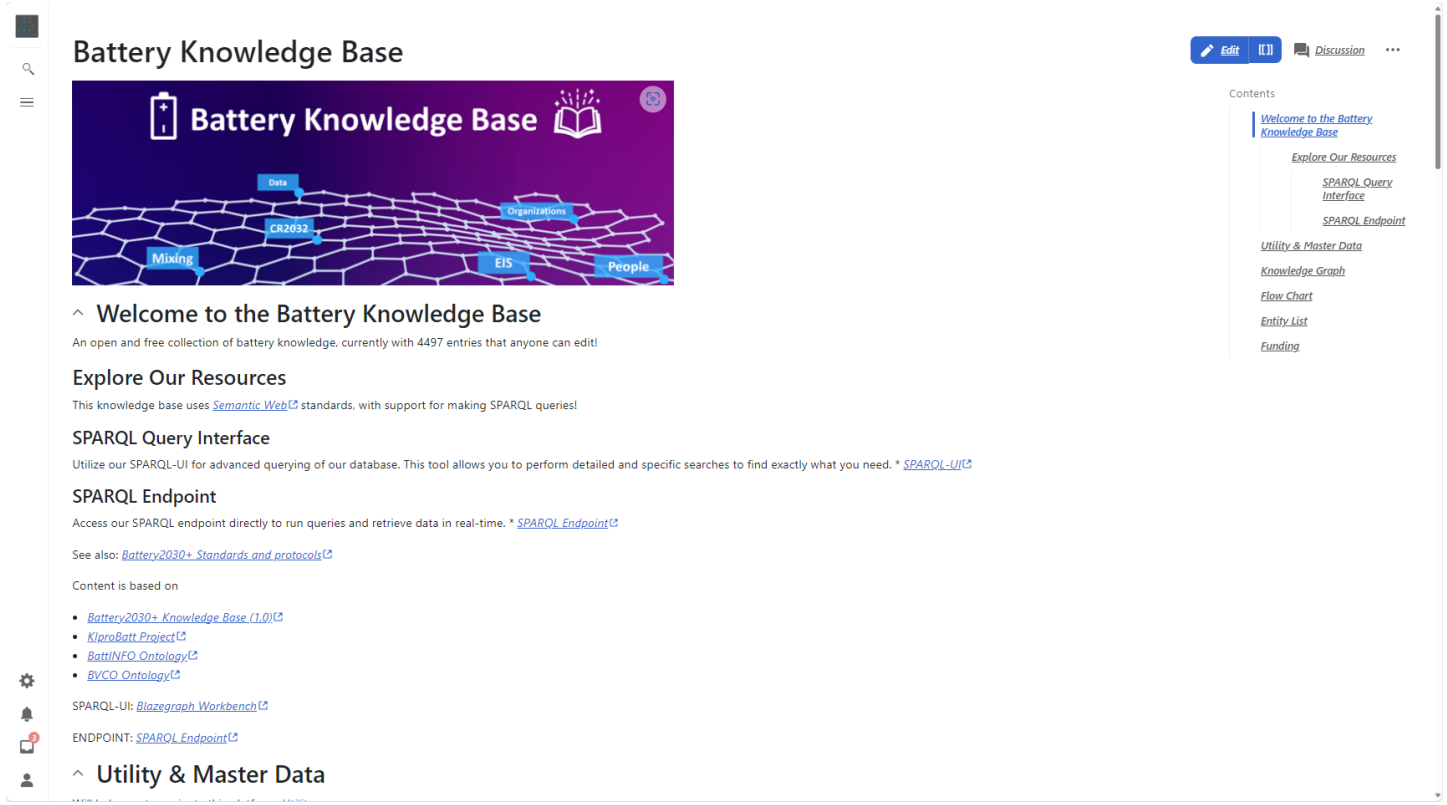
Battery2030+ Knowledge Base

Hands-on Tutorial



https://battery.knowledge-graph.eu

(Works best in desktop version)

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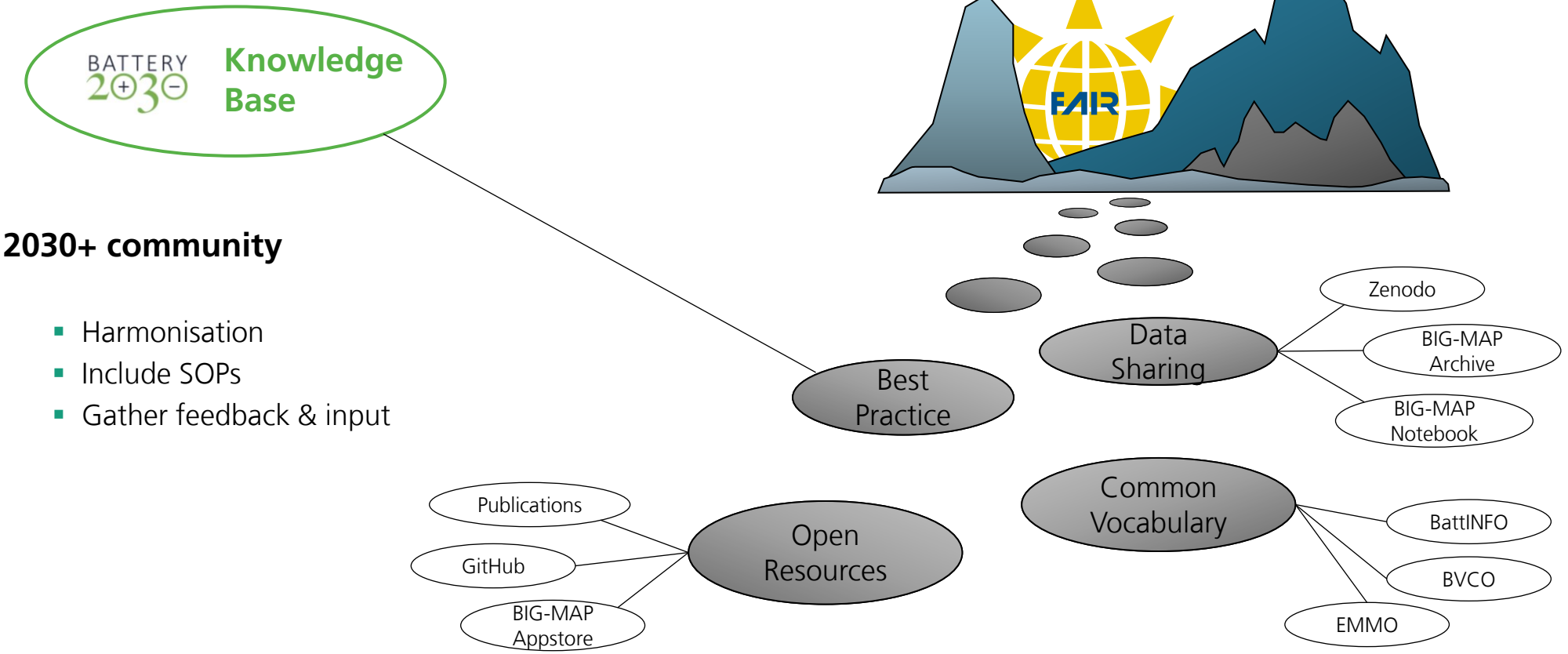
Outlook – What's next?

FAIR Data – Not very far ahead

Connect with ontologies
(complete the process)

Add more content on measuring techniques



Include the BATTERY 2030+ community

- Link standards
- Link research papers
- Fill Wiki articles
- Connect to BIG-MAP ELN
- Harmonisation
- Include SOPs
- Gather feedback & input

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github.com/OpenSemanticLab

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