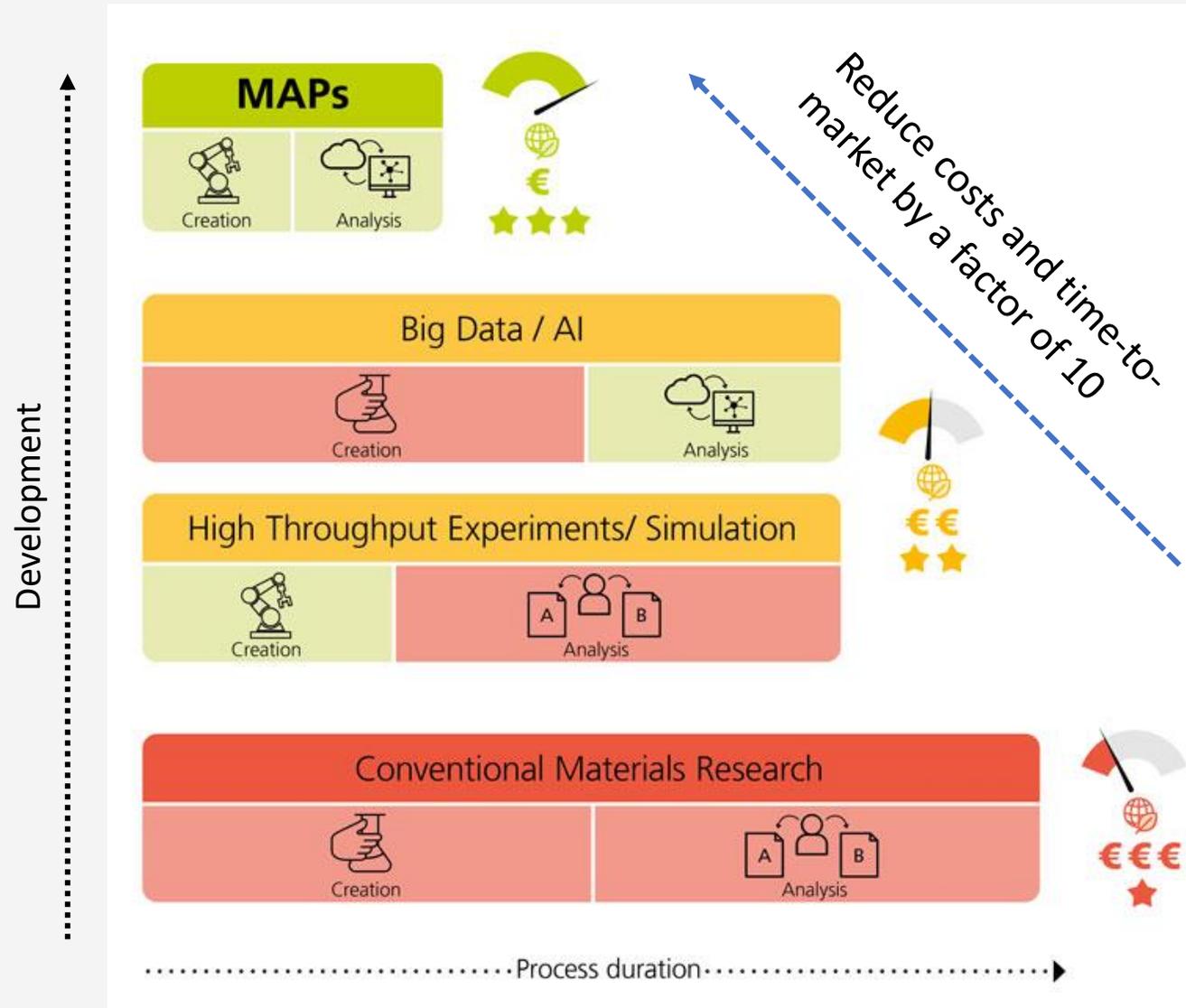


# **BIG-MAP, BattINFO & OpenSemanticLab**

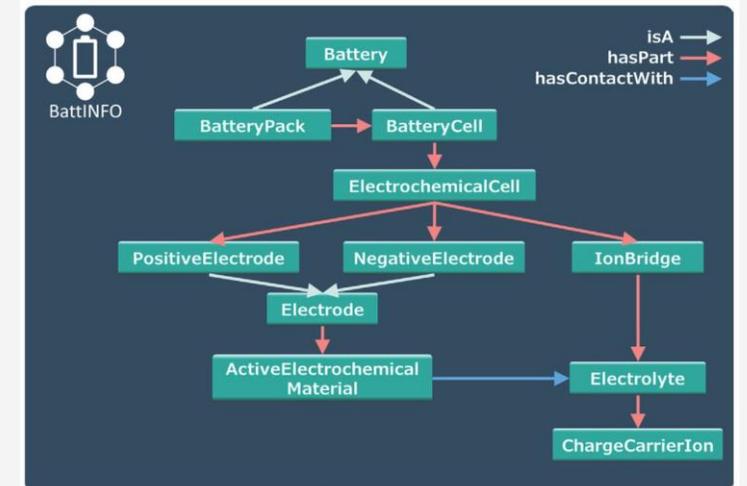
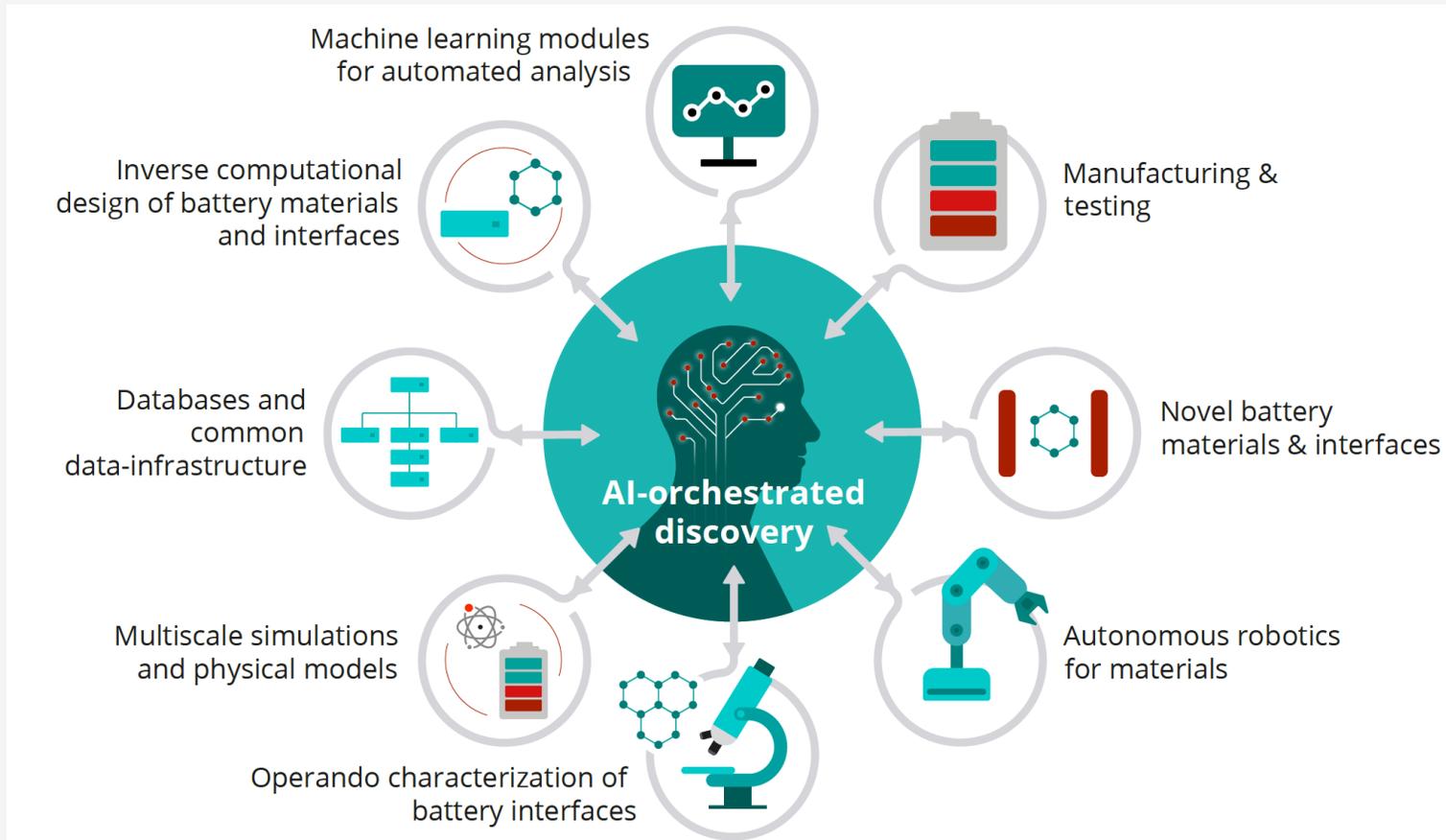
**Semantic data for battery innovation**

Simon Stier  
Head of Digital Transformation  
Fraunhofer ISC

# Materials Acceleration Platforms (MAPs)



# BIG-MAP: Battery Interface Genome Materials Acceleration Platform



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



# FAIR Linked Data

- **How?**

- Using unique identifiers
- Using common vocabulary
- Mapping terms to quantities & items
- Use Open Formats, Licenses, etc.

## QUDT

Quantity, Unit, Dimension and  
Types Ontology



## EMMO

Elementary Multiperspective  
Material Ontology

Unambiguous description of the content !

**Example:**  
Bio-Logic EIS spectrum

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

unit:HZ  
emmo:Frequency

unit:OHM  
emmo:ElectricImpedance

unit:SEC  
emmo:Time

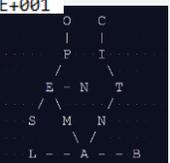
unit:MilliA  
emmo:ElectricCurrent

unit:V  
emmo:ElectricPotential

<https://big-map.github.io/BattINFO/getstarted.html>

Dr. Simon Stier

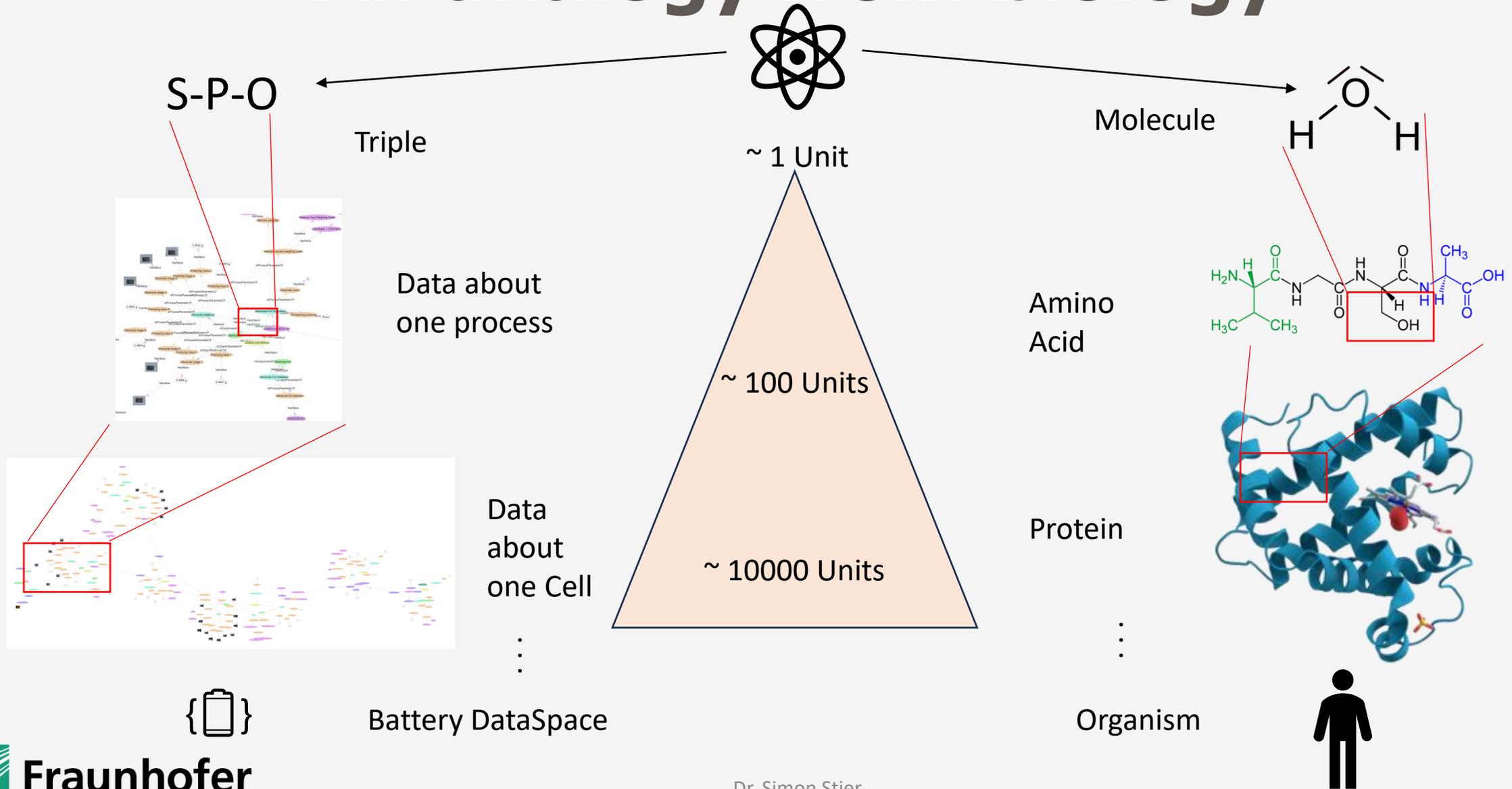
Head of Digital Transformation @ Fraunhofer ISC

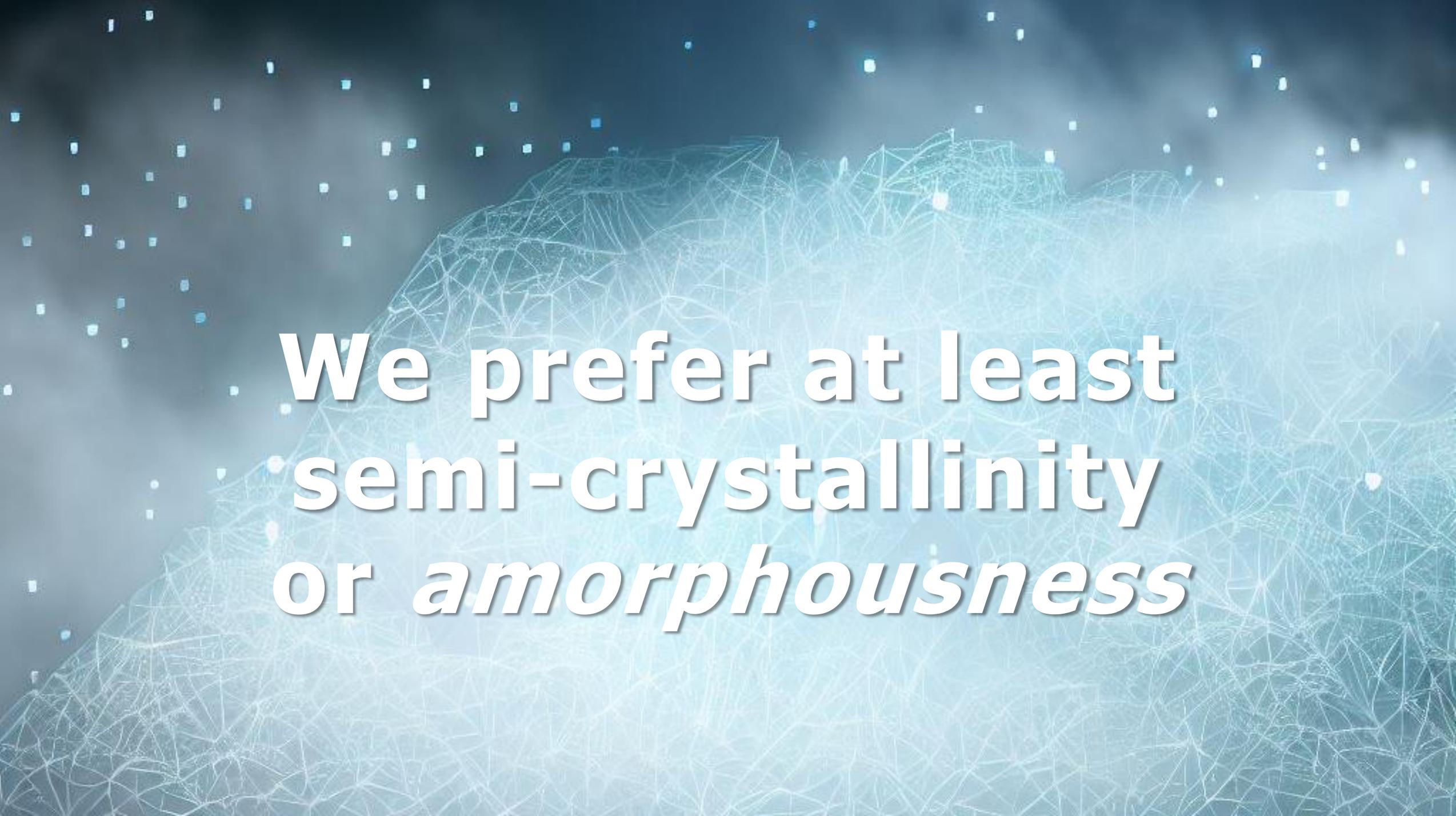




# **RDF as atomistic view on information**

# An analogy from biology





**We prefer at least  
semi-crystallinity  
or *amorphousness***

# An Object-Oriented view on the Graph

```
ex:DataModelShape
  sh:NodeShape ;
  sh:targetClass ex:DataModel ;
  sh:property [
    sh:path ex:p1;
    sh:datatype xsd:string ;
  ] ;
  sh:property [
    sh:path ex:p2 ;
    sh:class ex:AnotherModel ;
  ] ;
]
```

```
{
  "$id": "DataModel",
  "properties": {
    "param1": {"type": "string"},
    "param2": {"$ref": "AnotherModel"}
  }
}
```

```
ex:DataModel rdf:type owl:Class ;
  rdfs:subClassOf ex:Superclass ;
  rdfs:subClassOf [
    rdf:type owl:Restriction ;
    owl:onProperty ex:p2 ;
    owl:someValuesFrom ex:AnotherModel ;
  ] .
```

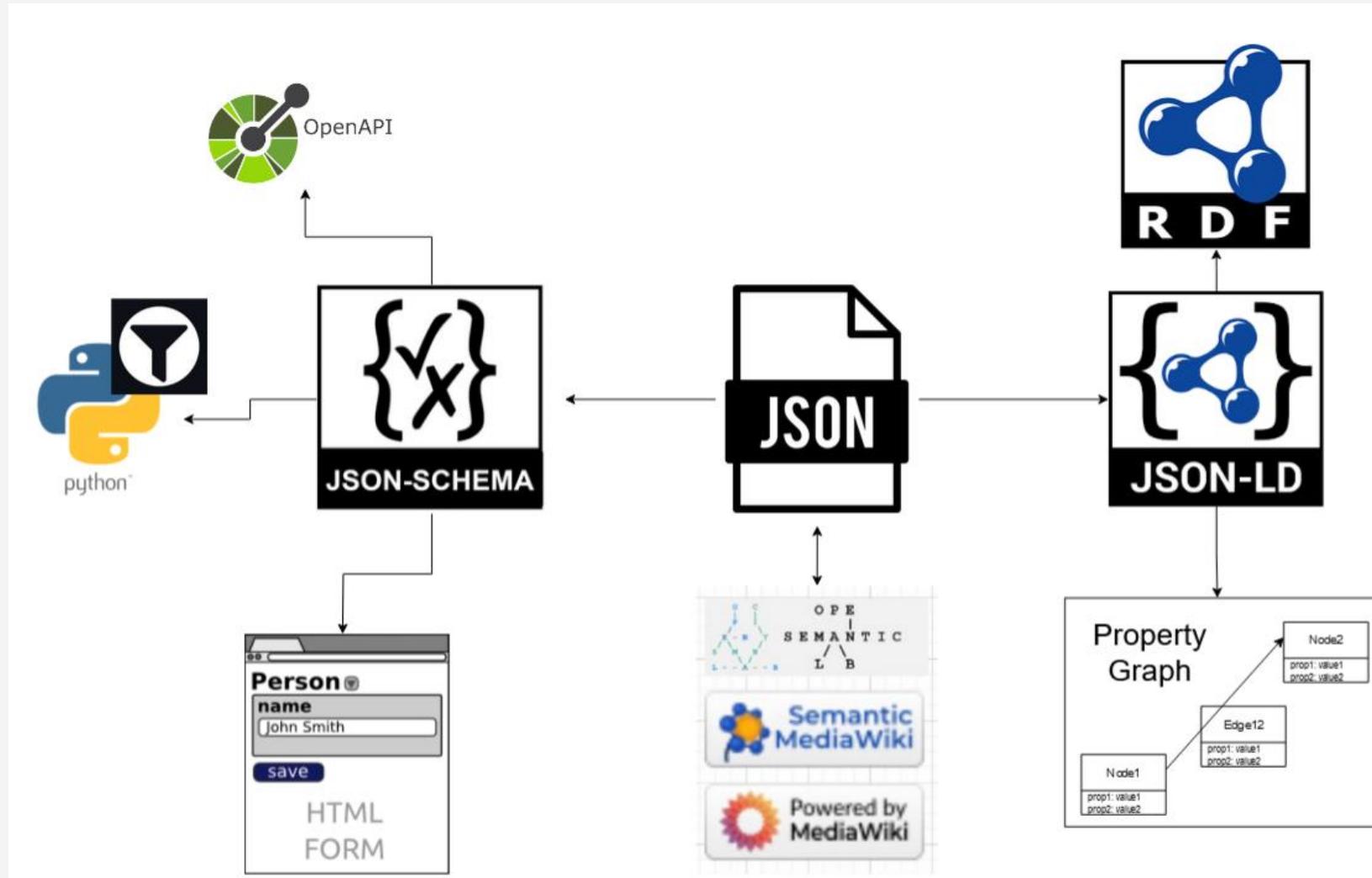


```
class DataModel(Superclass):
  param1: str
  param2: AnotherModel
```

```
class DataModelController(DataModel):
  def calc(self):
    res = self.param
```



# Combining established technologies



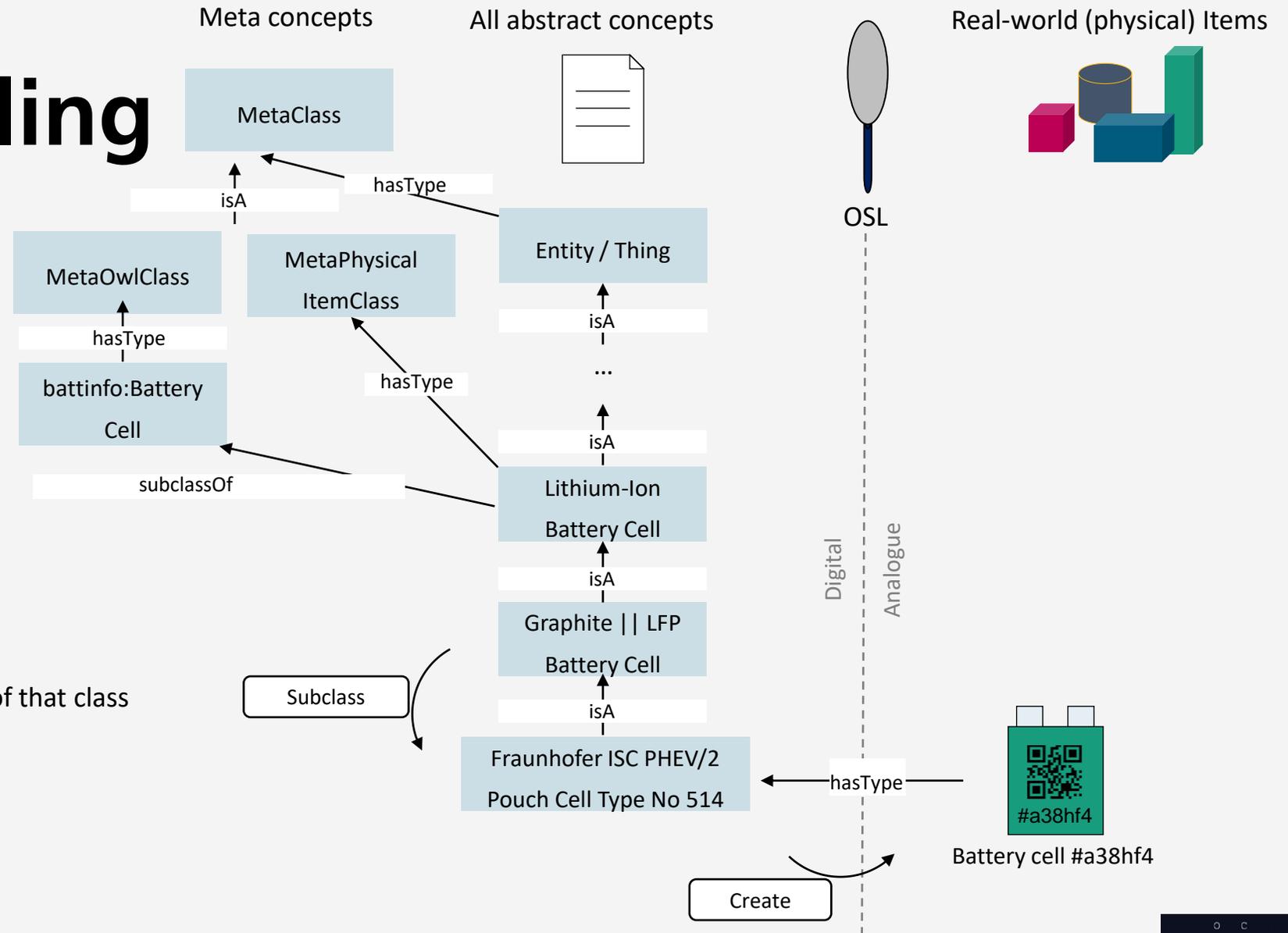
<https://oo-ld.github.io/playground/>



# Data Modelling

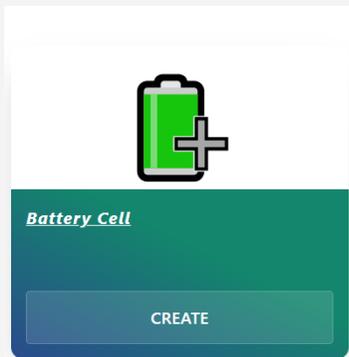
## Commonly (subconsciously) used concept

- Object
  - Basic unit of OO
  - Can be anything
  - Has a Type
  - Has an ID
  
- Class / Category
  - Type: Object
  - User-defined data type
  - Properties that are common to all objects of that class
  - Hierarchy and Inheritance
  
- Instance / Item
  - Type: <Some Category>
  - Properties from its class



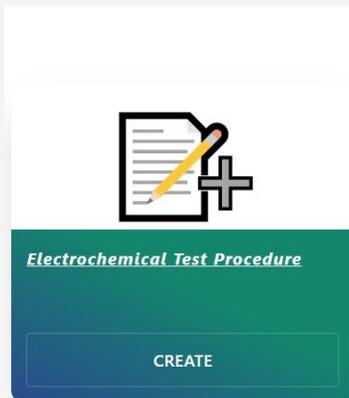
# Linked Data Schemas

Common  
Repositories



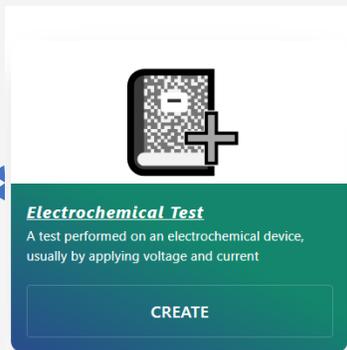
**Battery Cell**

CREATE



**Electrochemical Test Procedure**

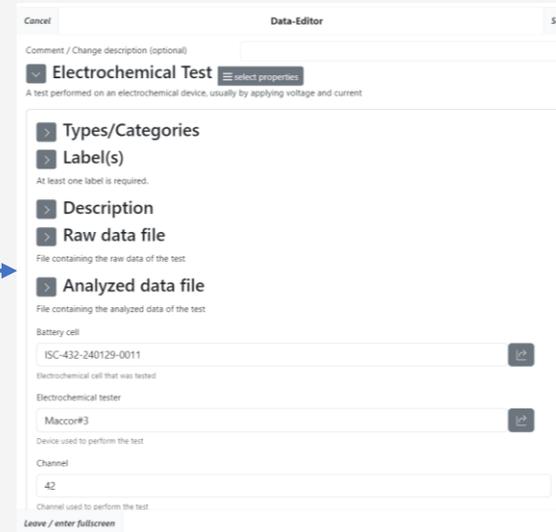
CREATE



**Electrochemical Test**

A test performed on an electrochemical device, usually by applying voltage and current

CREATE



**Electrochemical Test**

A test performed on an electrochemical device, usually by applying voltage and current

**Types/Categories**

**Label(s)**  
At least one label is required.

**Description**

**Raw data file**  
File containing the raw data of the test

**Analyzed data file**  
File containing the analyzed data of the test

Battery cell  
ISC-432-240129-0011

Electrochemical cell that was tested

Electrochemical tester  
Maccor#3

Device used to perform the test

Channel  
42

Channel used to perform the test

... and send to digital workflows

```

1= {}
2= {
3  "type": [
4  ],
5  "battery_cell_dut": "Item:OSW6dc0d2fd2a6a4a14bfff380f3a37be1d",
6  "tester": "Item:OSW3c0298bf657c47ef9ea2d0b6553f255d",
7  "channel": 42,
8  "test_procedure": {
9    "subcategory_select": "Category:OSWcb168c1ad3c7467bb4ed740381771928",
10   "instance_select": "Item:OSW1e0c880fcaa94f5ca3e58ca9c91ed028"
11  },
12  "test_temperature": 25,
13  "test_humidity": 50,
14  "environmental_test_chamber": "Item:OSWec7661418e654a429d044a524a144480",
15  "raw_data_files": [],
16  "analyzed_data_files": [],
17  "uuid": "50996a4d-6272-4509-b178-f7c6969b7054",
18  "label": [
19  {
20    "text": "Demo #2",
21    "lang": "en"
22  },
23  ],
24  "description": [
25  {
26    "text": "A test case for the BIG-MAP Workshop",
27    "lang": "en"
28  },
29  ],
30  "name": "Demo2"
31  }

```

independent  
schemas ...

... Combined to application  
specific structures

What you see

What you create in the background



# OpenSemanticLab as MAP ELN



**MapColorMixingRequest**  
A MAP experiment to create and characterize a food color mixture

CREATE

Comment / Change description (optional)

**MapColorMixingRequest**

Types/Categories

Label(s)

At least one label is required.

Title: [title of the entry] Lang code: en

Description

Requested fractions

Specify the amount of each so or for the mixture

red_fraction	0.33
green_fraction	0.33
blue_fraction	0.33

REST-API

only green for video

Description

Instrument

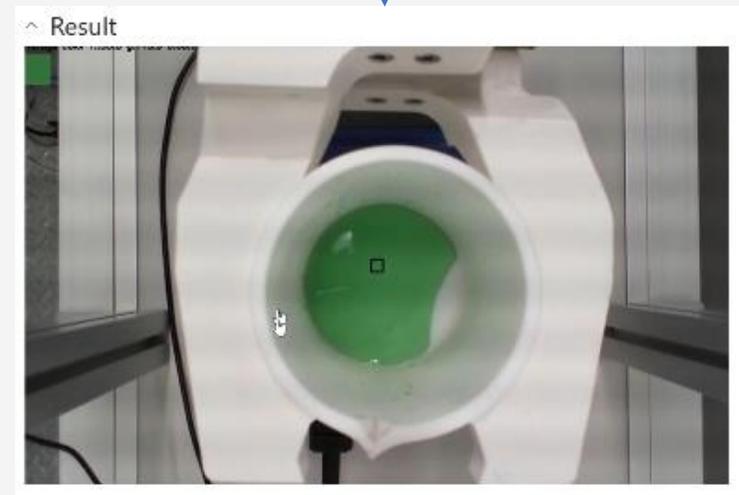


Result

Process Graph

Metadata

Label	only green for video
Machine compatible name	only green for video
Statements (pending)	
Statements (processing)	
Keywords	Item
Type(s)/Category(x)	Info
Process	
FinalizeRequest	
MapColorMixingRequest	
Workflow Runs	
Requested fractions	Mod. 0, Green, 0.5, Ultra. 0



Prefect



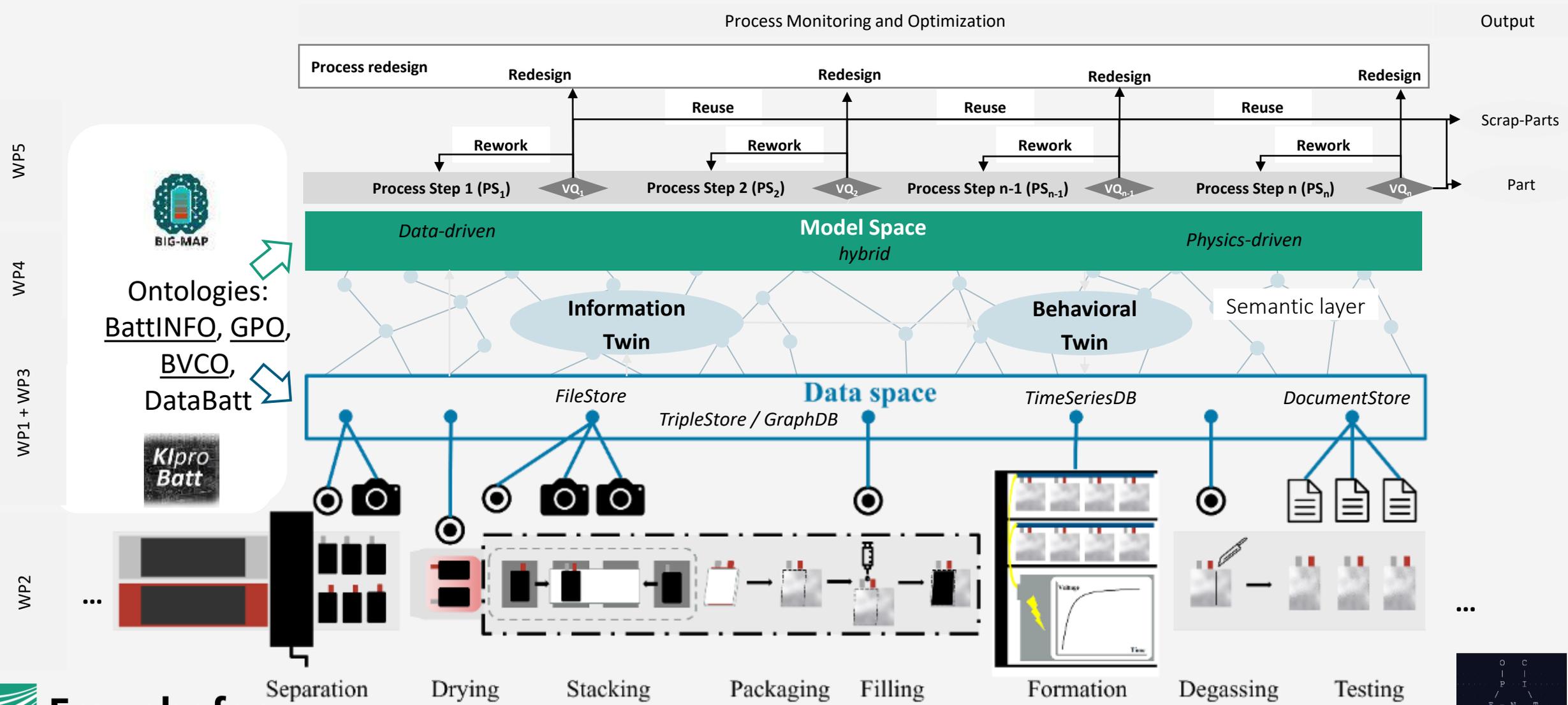
BIG-MAP Archive



<https://github.com/OpenSemanticLab>

<https://doi.org/10.5281/zenodo.8110654>

# Usecase: Comprehensive Semantic Information Structure in the Battery Value Chain



# Domain specific Knowledge Graphs

Electrode foil

Separation

Drying

Filling

Formation

AI Image Segmentation

Stacking

Battery cell

EoL-Test

**Cell manufacturing/Stacking**

**Description**

**Production process**

- Separated electrode sheets are stacked in a repeating cycle of anode, separator, cathode, separator, etc.
- Classic variant of stacking is the so-called Z-folding
- Anode and cathode sheets are inserted alternately from the left and right into the z-shaped folded separator; separator is used as endless tape and cut off after the stacking process is completed
- Finalized cell stack is fixed with adhesive tape
- Sheets are transported and positioned by vacuum grippers
- Depending on cell specification, the cell stack consists of a specific number of individual layers

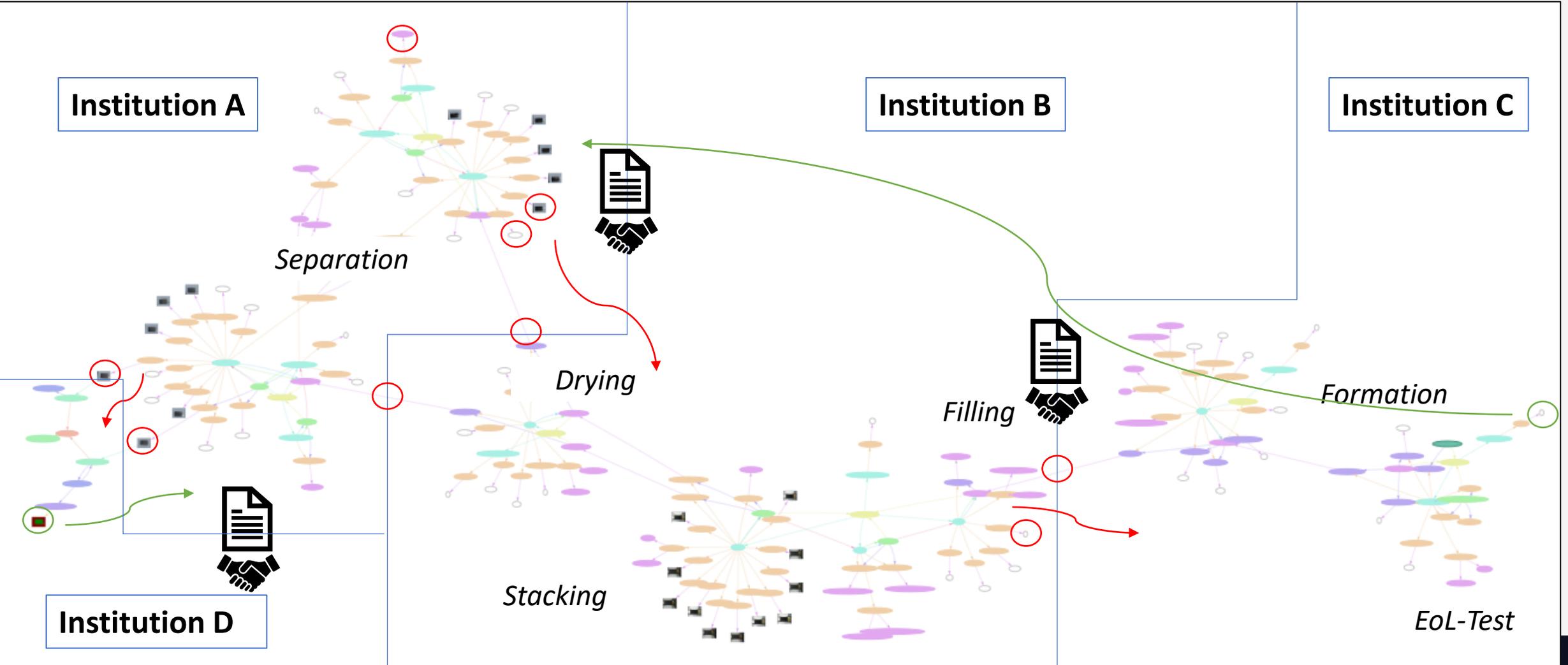
**Process parameters & requirements**

**Legend:**

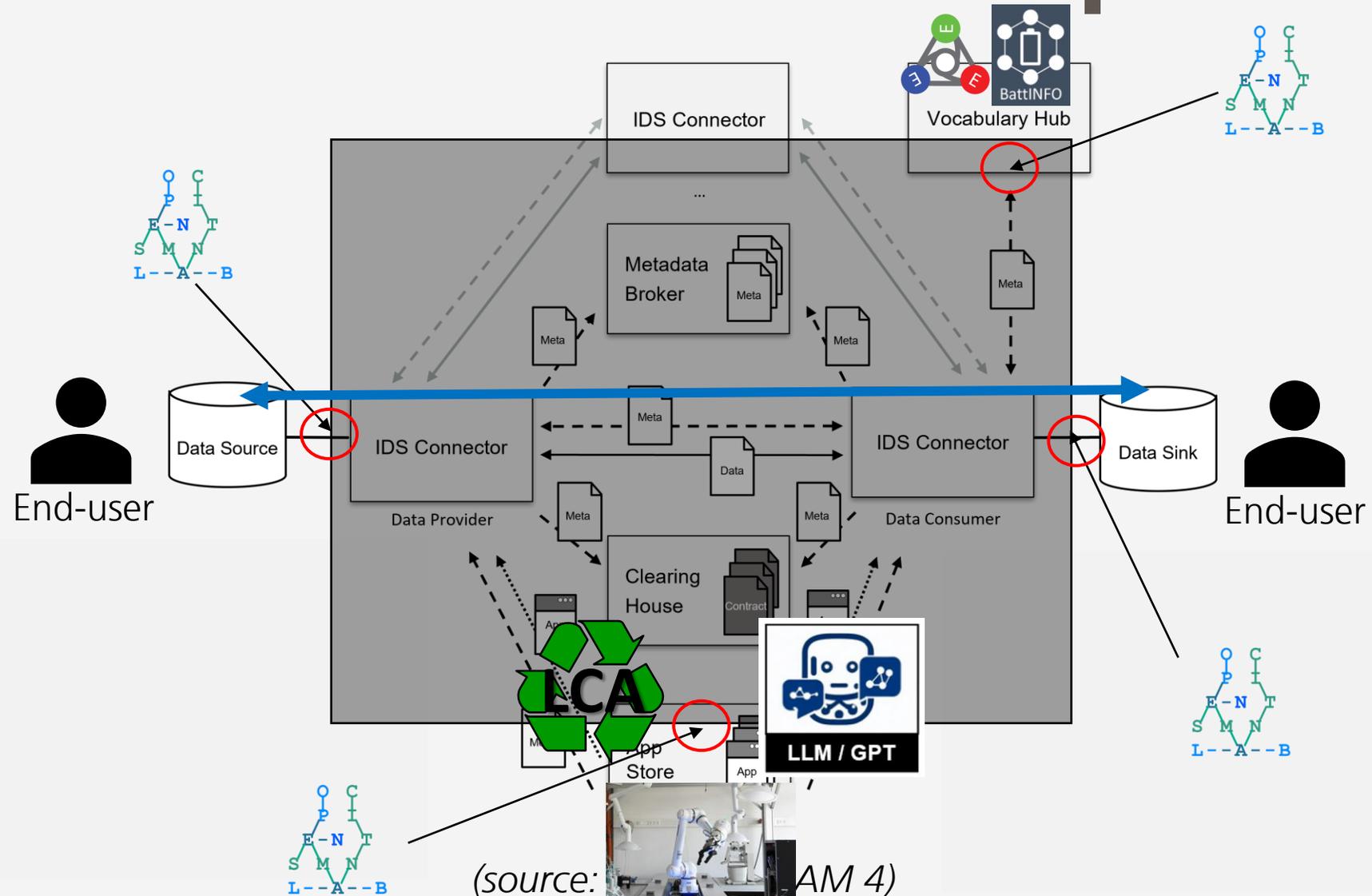
- Has part
- Has successor
- Has educt
- Has product



# Data space along the value chain



# Towards Material Data Spaces



(source: AM 4)

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# Thank you for your attention!

Contact:

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+49 931 4100 661

Fraunhofer ISC, Neunerplatz 2, Würzburg

More Information: [isc.fraunhofer.de/digitale-transformation](https://isc.fraunhofer.de/digitale-transformation)  
[github.com/OpenSemanticLab](https://github.com/OpenSemanticLab)



# ISC *Digital*