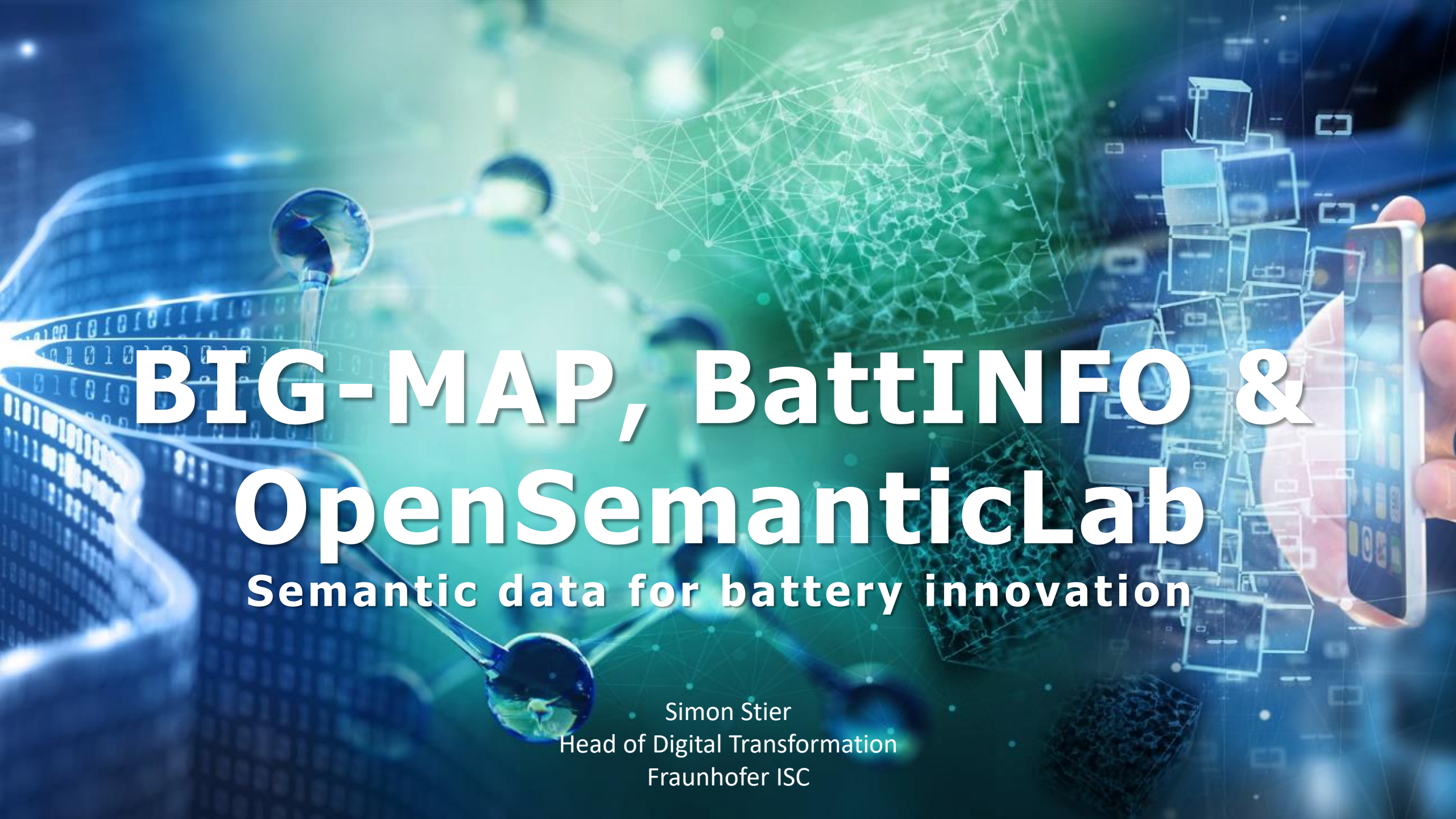
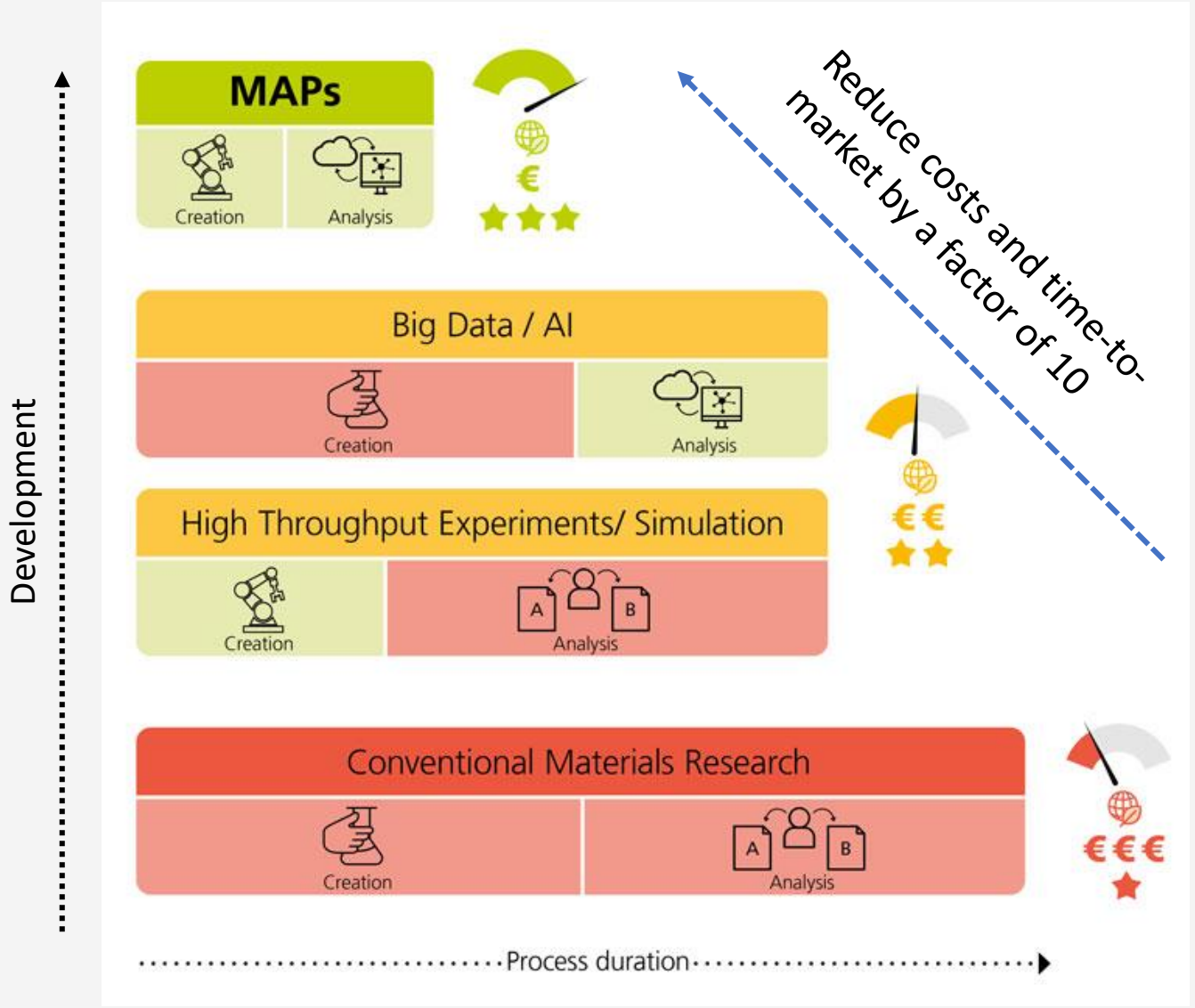


BIG-MAP, BattINFO & OpenSemanticLab

Semantic data for battery innovation

Simon Stier
Head of Digital Transformation
Fraunhofer ISC

Materials Acceleration Platforms (MAPs)



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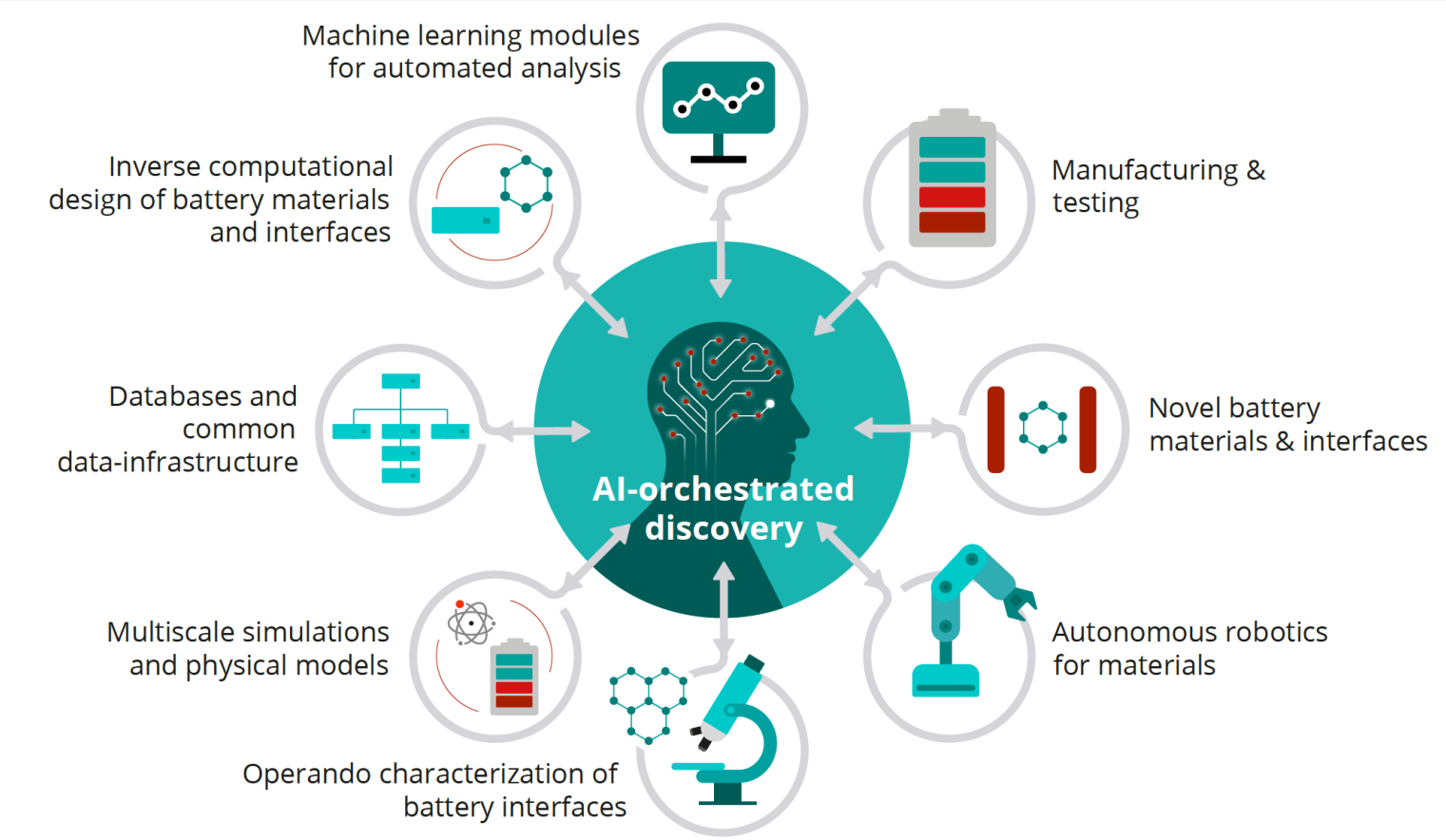
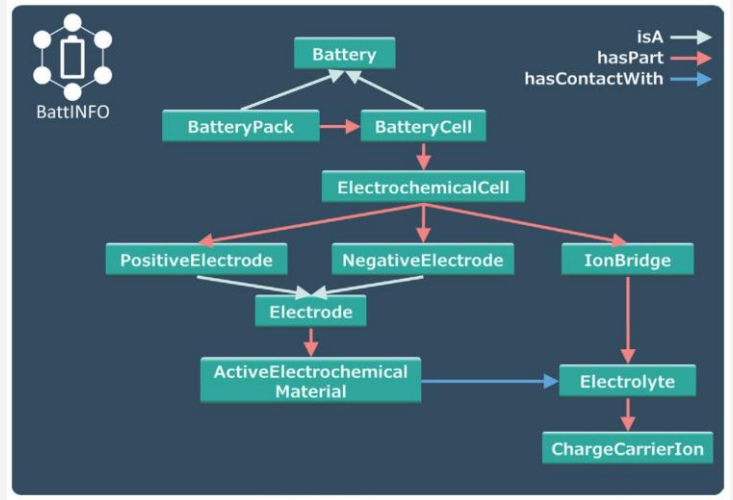
BIG-MAP: Battery Interface Genome Materials Acceleration Platform





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

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FAIR Linked Data

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

QUDT
Quantity, Unit, Dimenson and Types Ontology

EMMO
Elementary Multiperspective Material Ontology

Unambigious description of the content !

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

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

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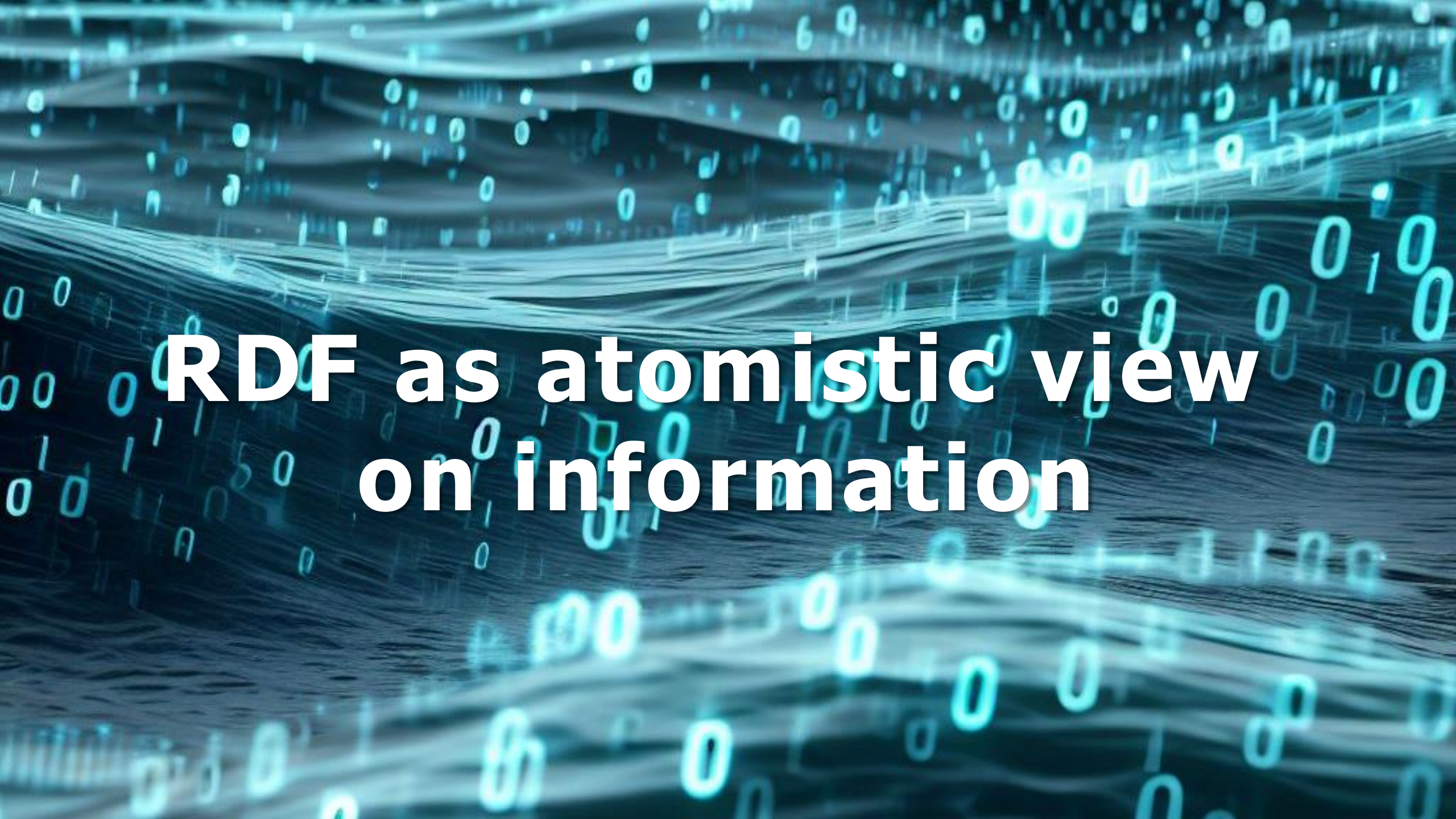
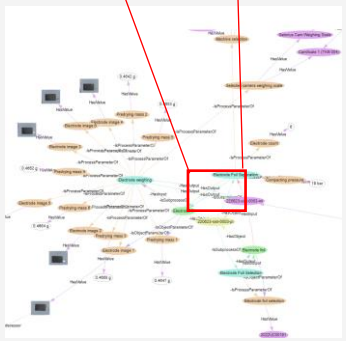

RDF as atomistic view
on information

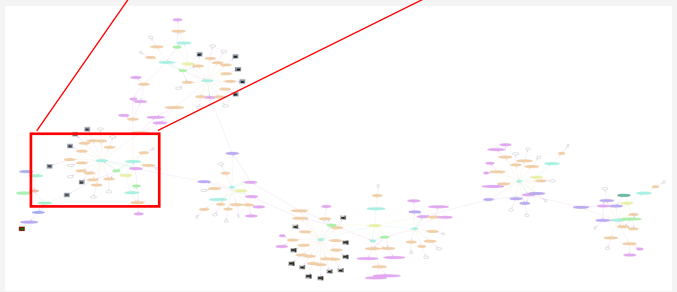
An analogy from biology

S-P-O

Triple



Data about one process



Data about one Cell

⋮

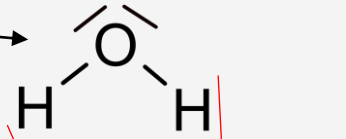
Battery DataSpace

~ 1 Unit

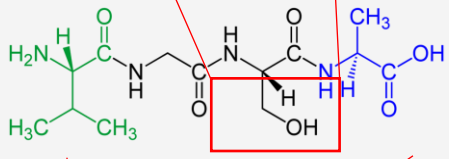
~ 100 Units

~ 10000 Units

Molecule



Amino Acid



Protein

⋮

Organism

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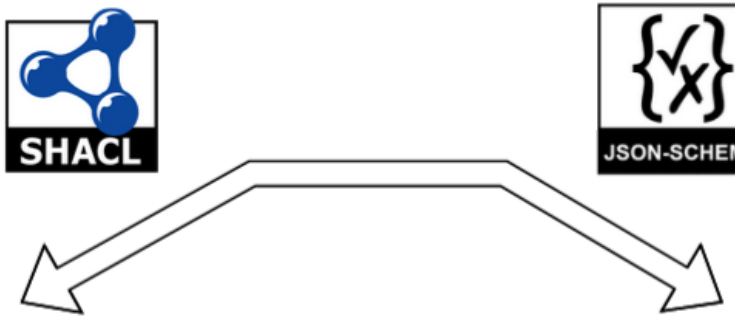
We prefer at least
semi-crystallinity
or *amorphousness*

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
```

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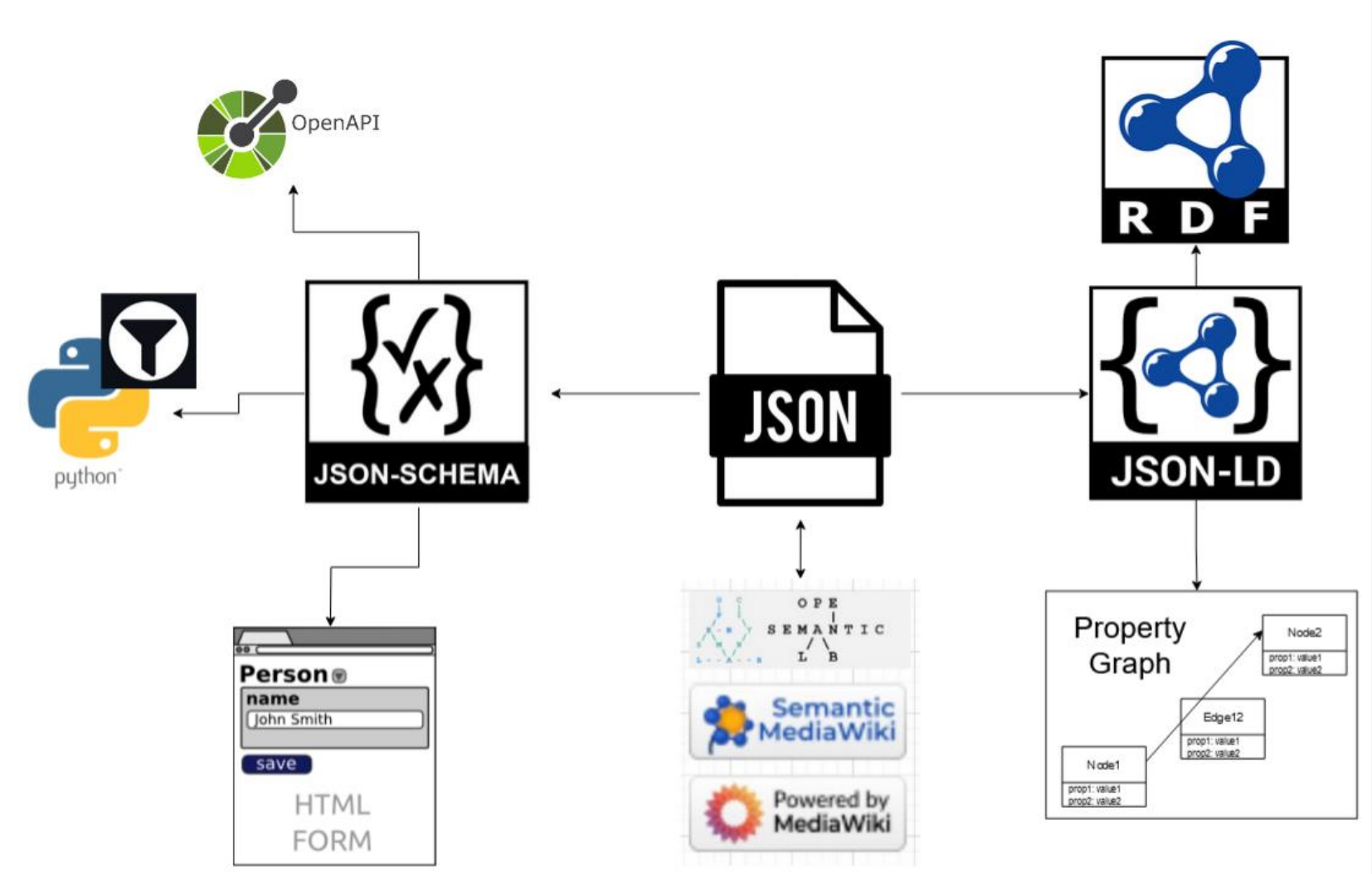
Combining established technologies



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

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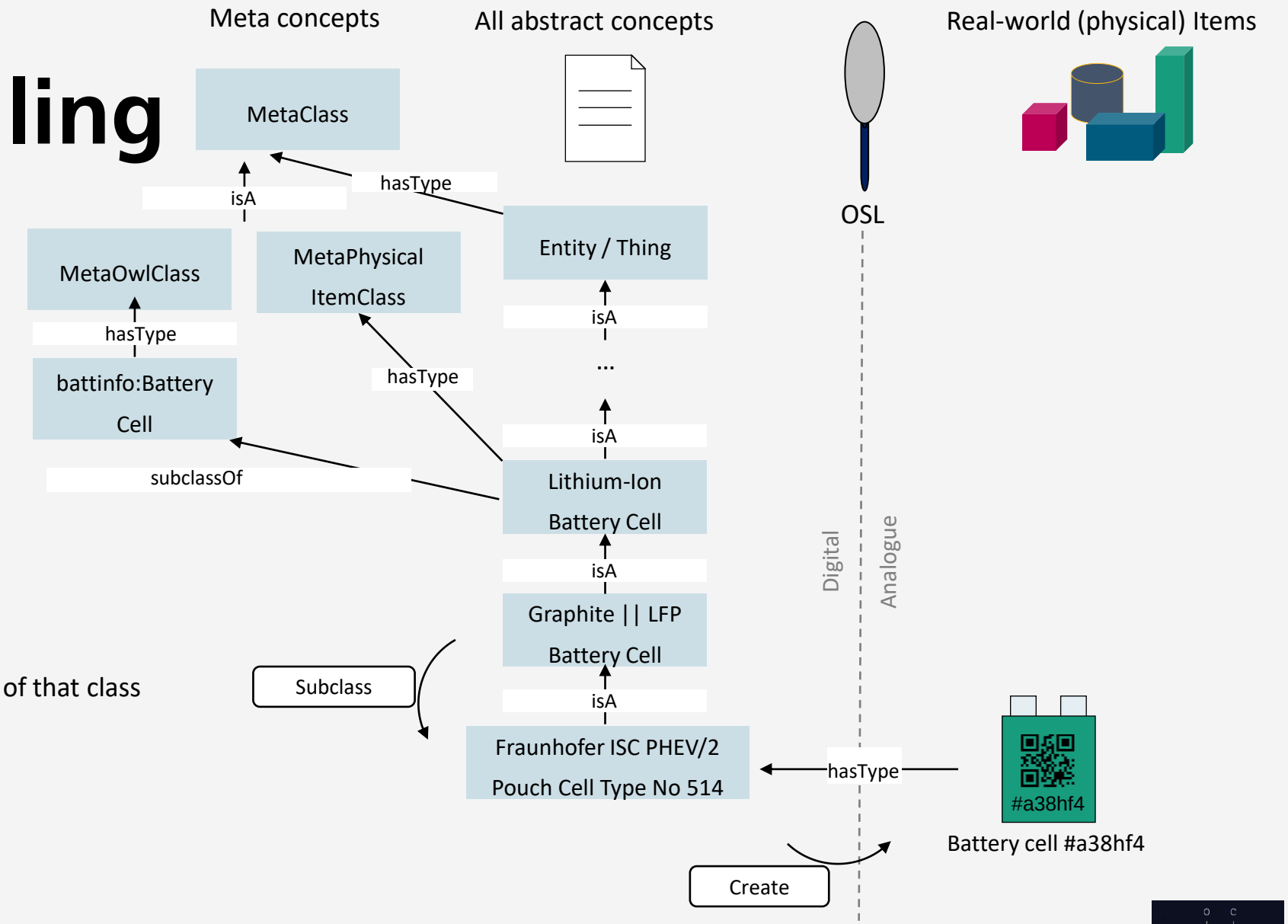
Data Modelling



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

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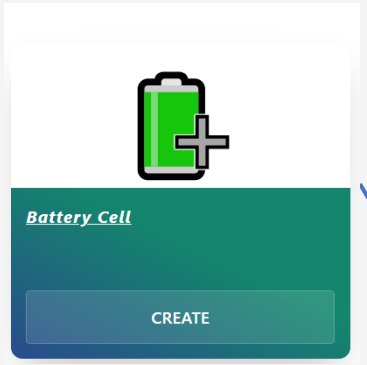
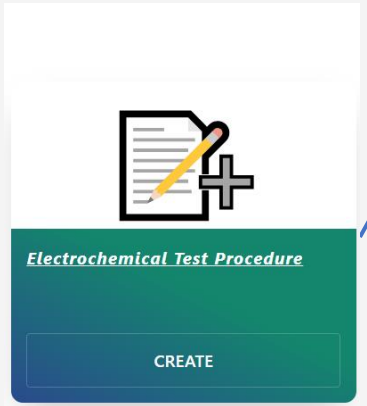
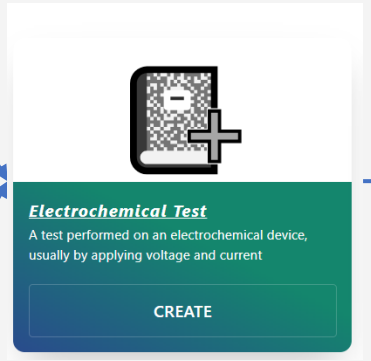
Linked Data Schemas

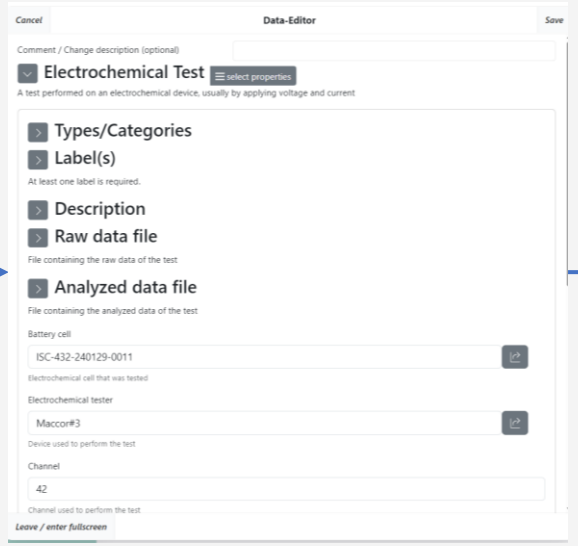
- … and send to digital workflows

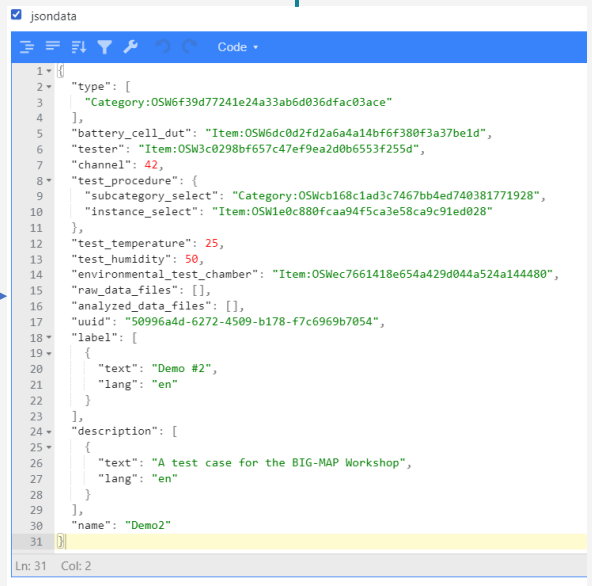
Common Repositories











- independent schemas ...
- … Combined to application specific structures
- What you see
- What you create in the background

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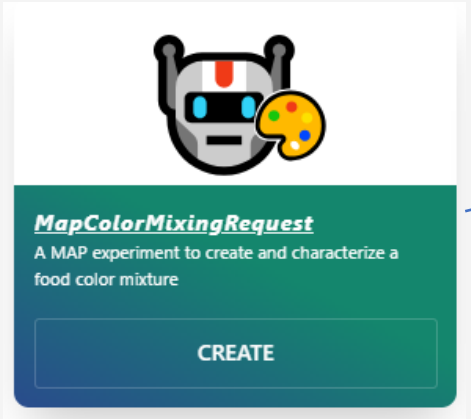
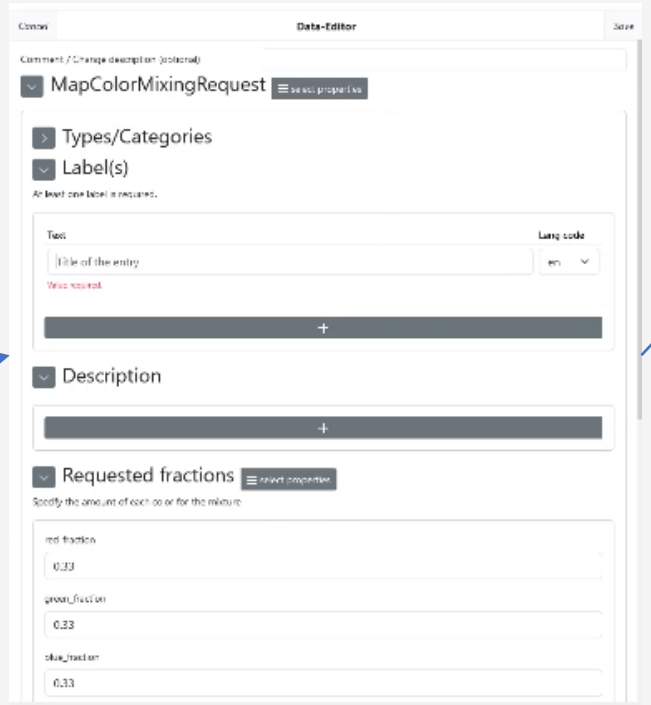
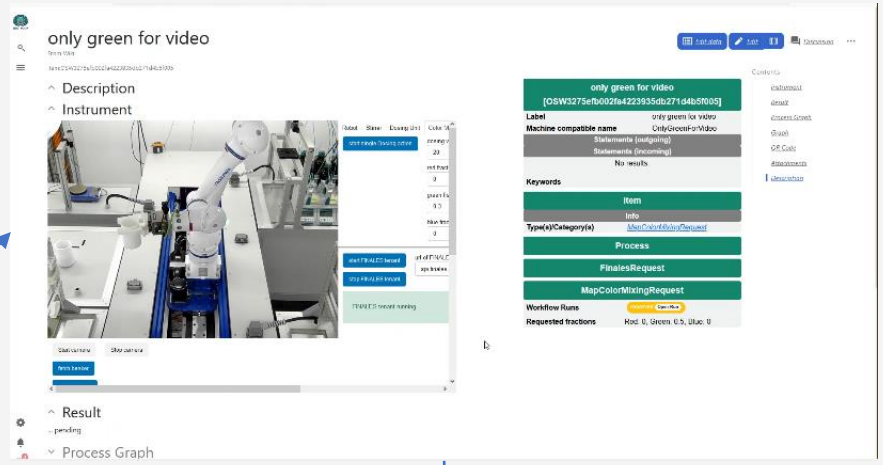
OpenSemanticLab as MAP ELN





REST-API



Prefect

BIG-MAP Archive

https://github.com/OpenSemanticLab

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

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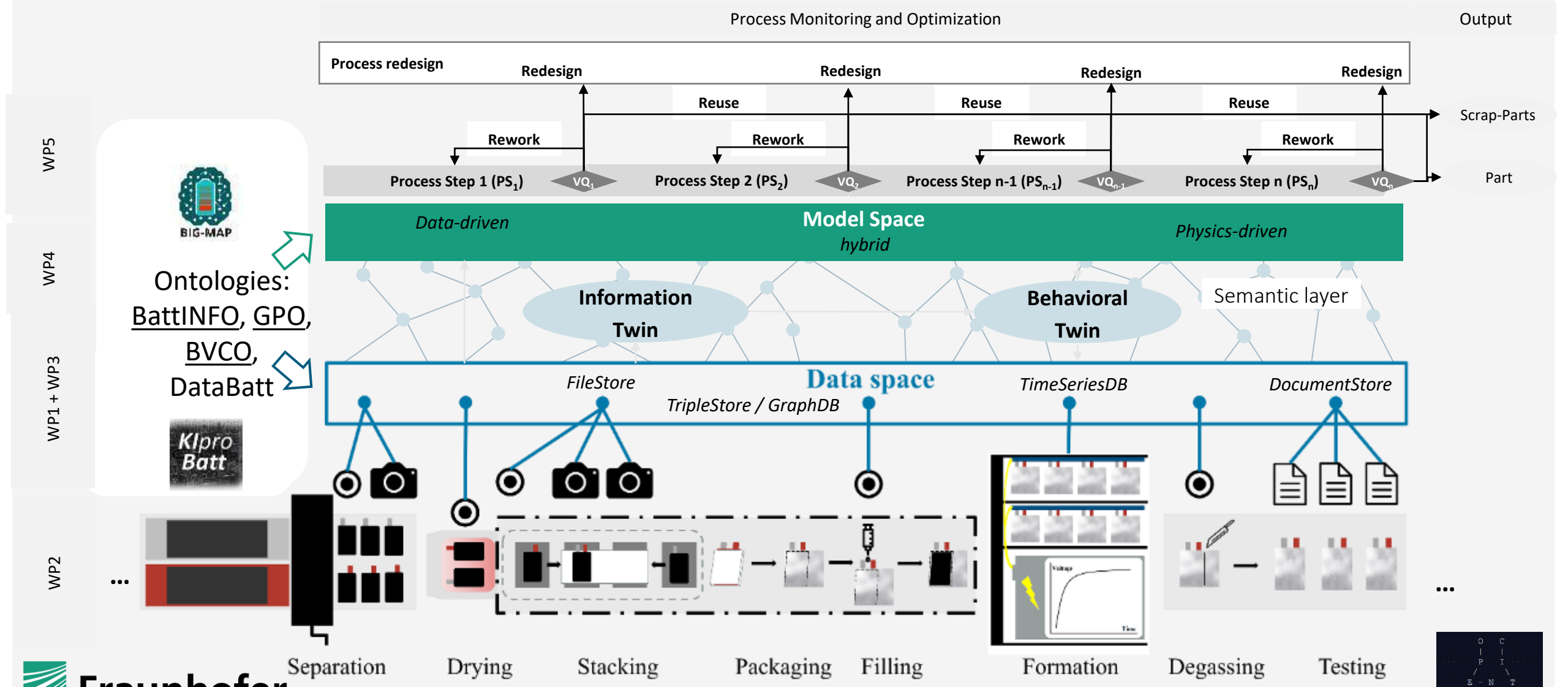
Usecase: Comprehensive Semantic Information Structure in the Battery Value Chain



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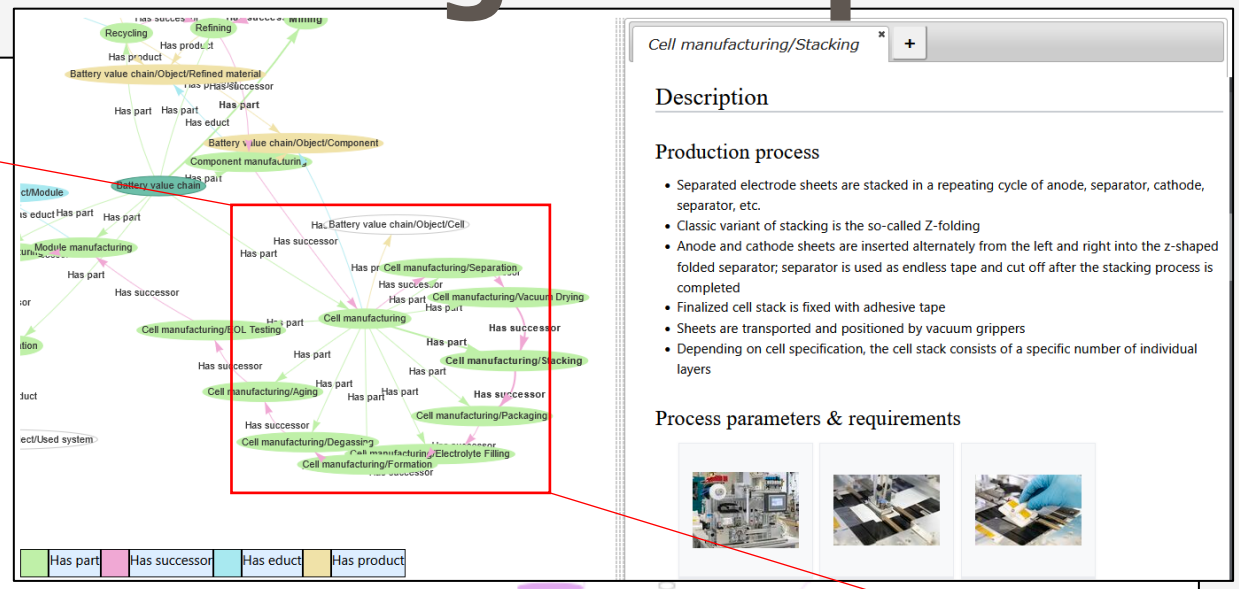
Domain specific Knowledge Graphs

Electrode foil



Separation

AI Image Segmentation

Drying

Stacking

Filling

Formation

Battery cell

EoL-Test

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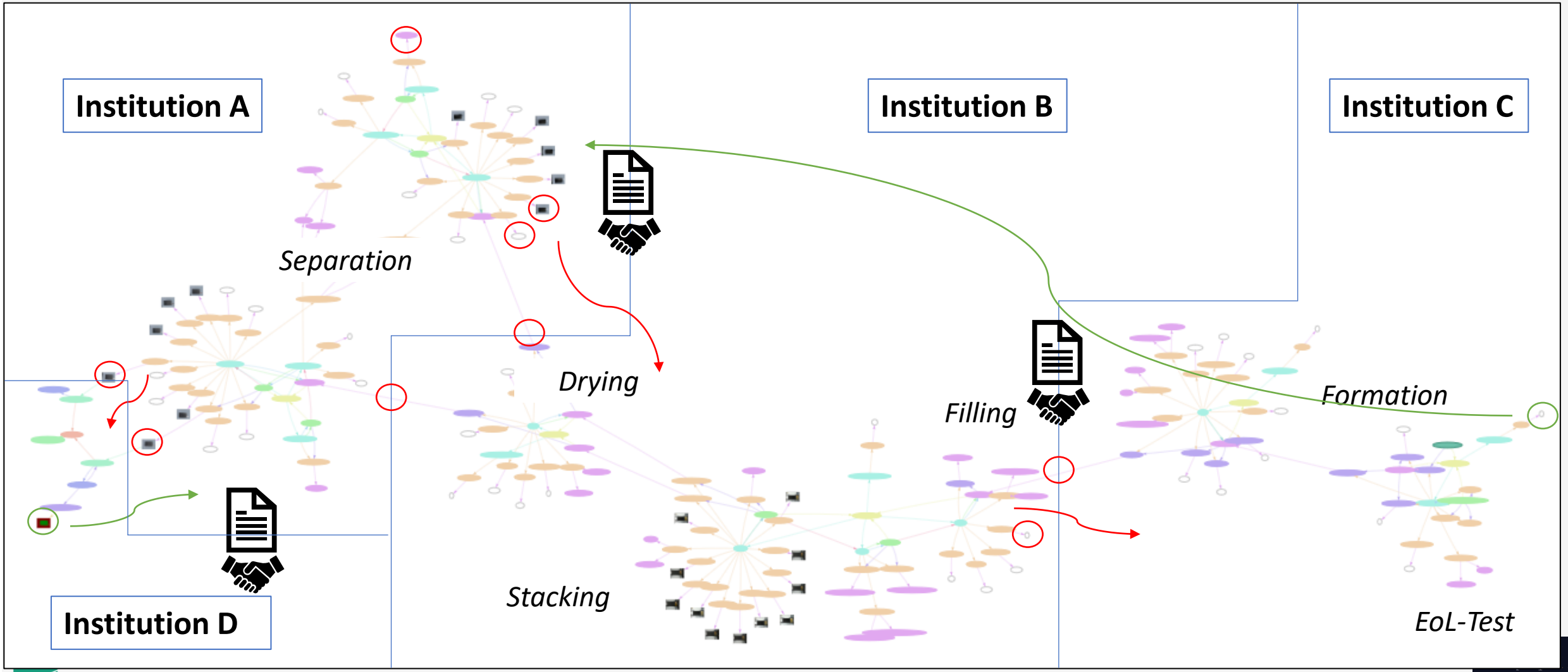
Data space along the value chain



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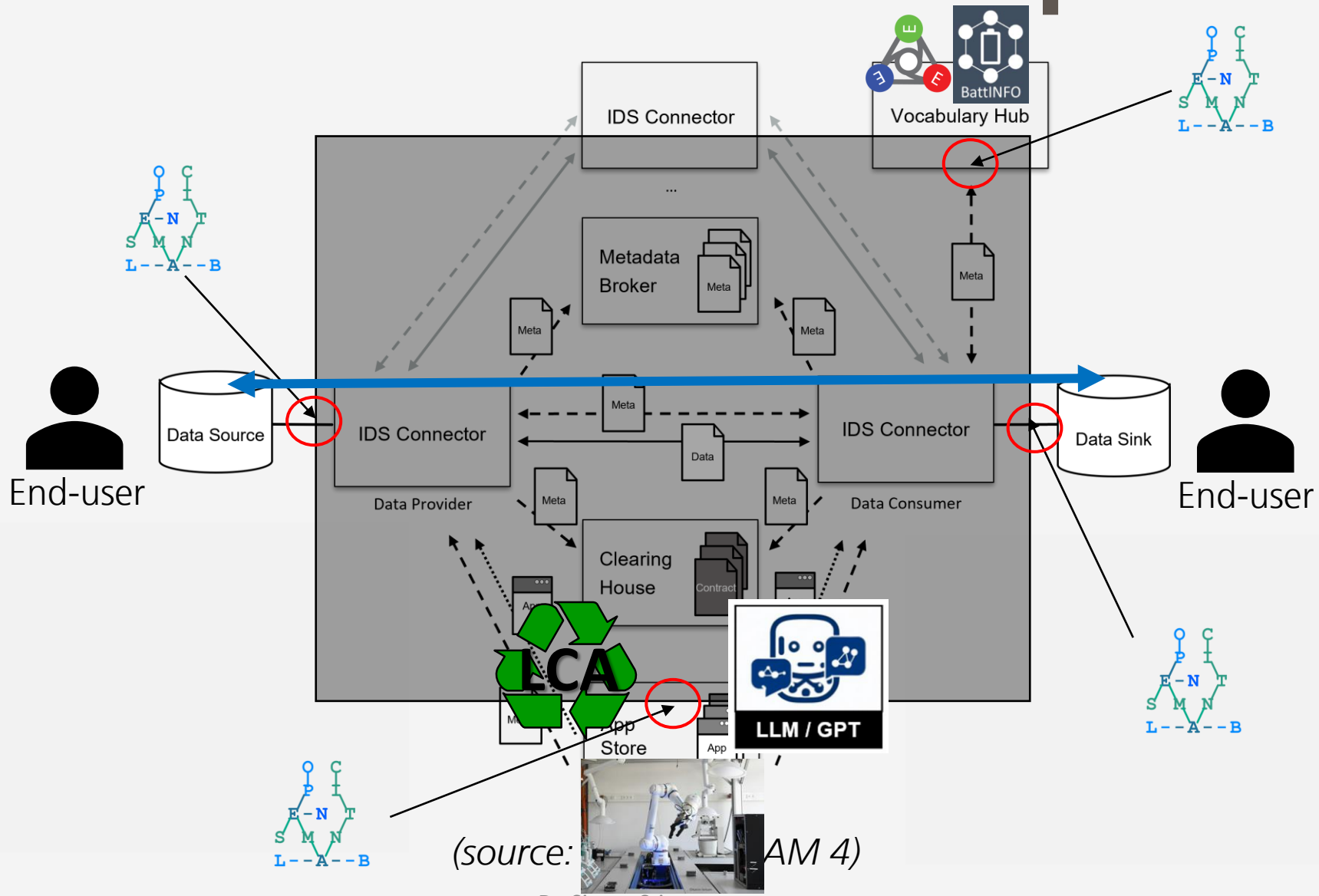
Towards Material Data Spaces



(source: AM 4)

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Thank you for your attention!

More Information: isc.fraunhofer.de/digitale-transformation
github.com/OpenSemanticLab

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