FEMS 2025 EUROMAT

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EMMO: an ontology based on universal materials science concepts

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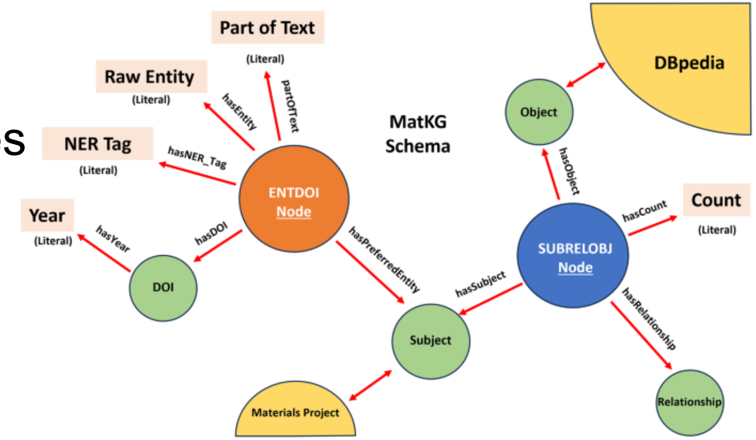
Abstract

- The task of building a 'materials science knowledge graph' is intriguing but also appears daunting. However, in materials science we can build on fundamental physical science principles and foundations. That is how the EMMO ontology has been constructed from the bottom up. The paper will discuss these foundational requirements in relation to the ISO standard for Top Level Ontologies, and how materials science desiderata are fulfilled by EMMO. Based on these solid foundations, examples of the EMMO discipline and domain ontologies will be showcased. In particular, we highlight the CHAMEO ontology for materials characterisation, which underlies the updated "CHADA" CWA 17815:2025. Finally the application of CHAMEO to industrial applications including battery testing and automotive coatings will be demonstrated.

A Materials Science Knowledge Graph

- Repository of entities and relationships extracted from scientific literature.
- **Formulated based on statistical metrics**, >70,000 entities and 5.4 million unique triples
- Largest Materials Science KG to date
- **Cannot distinguish “correlation” and “causation”,** e.g. a material that is commonly used during a synthesis method and a material synthesized.
- **Lacks underlying ontology**



Venugopal, V., Olivetti, E. MatKG: An autonomously generated knowledge graph in Material Science. *Sci Data* **11**, 217 (2024). https://doi.org/10.1038/s41597-024-03039-z

Let's talk about commitments

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Knowledge Graphs, Schema not really committed…

- Weak semantics → limited interoperability
- Semantic drift → inconsistency, duplication
- Retrofits → attempts to add ontology later
- Example: **Fast Healthcare Interoperability Resources (FHIR)** (USA)
    - FHIR “Patient” is a resource definition
    - FHIR “Observation” is a structured payload, not a commitment about the nature of observation

  Has since undergone ontological retrofitting

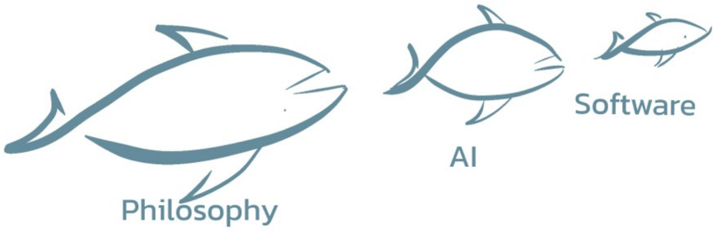
Source: J. Bittner, When Standards Fail to Ontologize, August 2025
https://www.linkedin.com/pulse/when-standards-fail-ontologize-j-bittner-lr8ye/

Ontologies

- Conceptualisation of a domain
- Explicit and formal
- **Commitments: axioms, assertions about things and constraints.**
- Conforms to a logical framework (e.g. First Order Logic, Description Logic)
- Logic reasoner algorithms can check consistency and make inferences.

"Philosophy eats AI" due to teleology, epistemology, ontology

https://www.forbes.com/sites/josipamajic/2025/05/22/software-ate-the-world-ai-ate-software-and-now-philosophy-is-eating-ai/



Top Level Ontologies and their benefits

Quoting from J.Bittner: SemanticallySpeaking:

- Make data actionable
- Reduced integration costs: avoid spending millions reconciling incompatible schemas later.
- Compliance and auditability: Regulations and rules can be encoded as axioms, enabling automated compliance checks instead of manual reviews.
- Agentic systems and AI safety: provide the logical constraints that keep LLMs and AI agents from hallucinating.
- Longevity: While schemas drift with technology cycles, ontologies endure. Standards built on ontologies remain relevant for decades.

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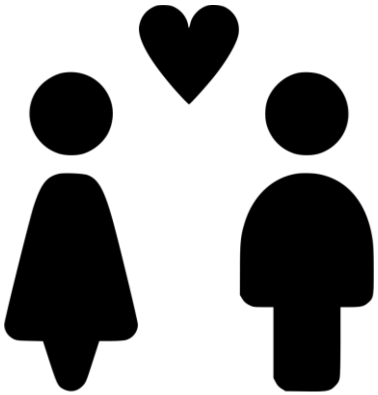
The right one?

- What do I commit to?



Top Level Ontologies: ISO/IEC 21838-1

Information technology — Top-level ontologies (TLO) — Part 1: Requirements

- **Domain neutrality**
- **A clear stance on**
  - **Space and time**
  - **Qualities and quantities**
  - **Parthood, Location, Constitution, Time and Change, and Events and Processes**
  - **Classifications and Mathematical, Informational, Social, & Mental Entities**
  - **Causation and scale & granularity**
- **Formal requirements:** formal languages etc

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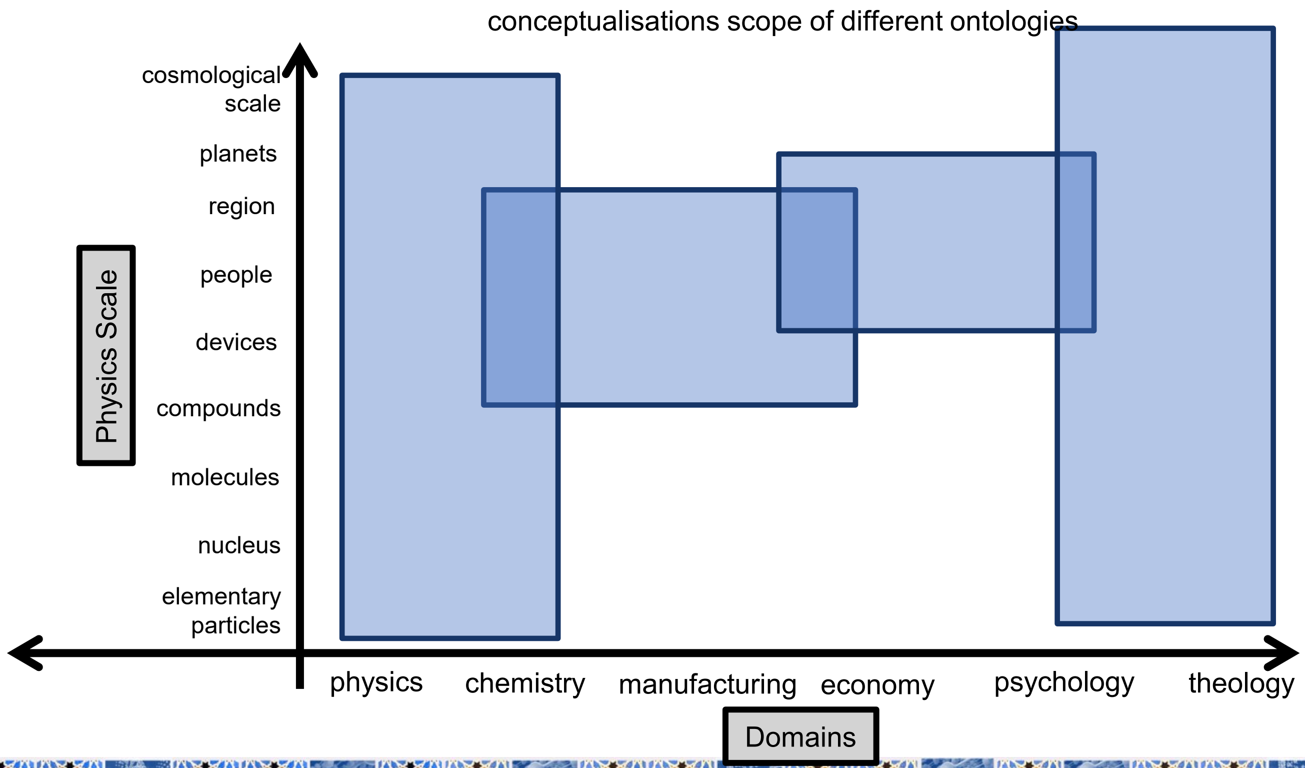
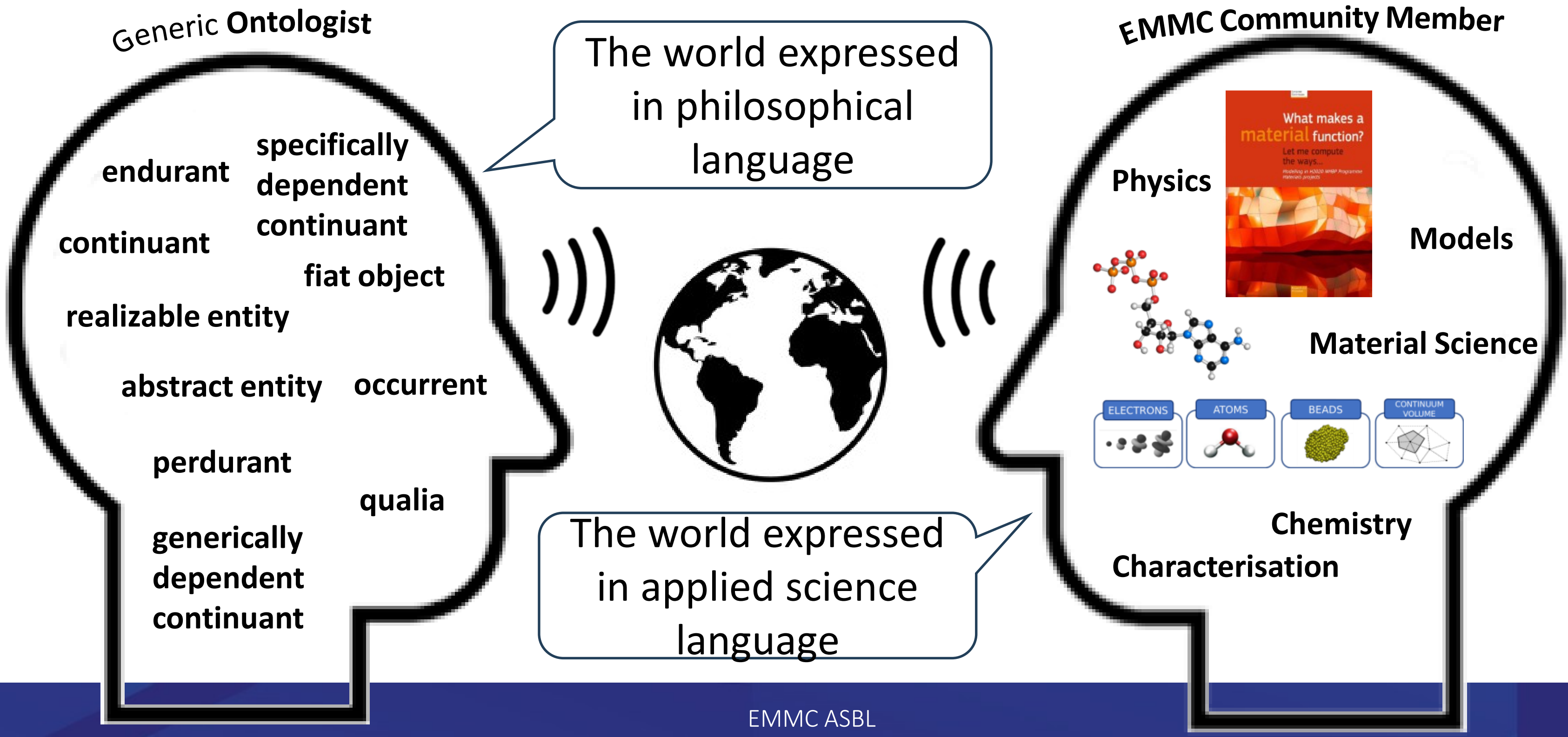
Domain neutrality

Ontologies (incl TLOs) display varying degrees of suitability in different contexts and given different pragmatic goals/use cases.



Why a new foundational ontology for materials science?



Desirable TLO stances for Materials Science

Conceptual Requirement	**Desirable Design Choice**
Space & Time	- Unitary treatment - Separation of measured time and ontological constraints
Qualities and Quantities	- Providing means to represent the subjectivity of observation - Identification of a property with specific measuring or calculating procedures, in accordance with ISO 10303-45:201 & metrology
Classifications and Mathematical, Informational, Social, & Mental Entities	No ontological commitments or strictly reduced to/grounded in Physical Entities
Parthood, Location, Constitution, Time and Change, and Events and Processes	Favoring “reductionist” approaches and extensional criteria of identity: - Adoption of an Extensional Mereology - Identification of entities and location (supersubstantivalism/relational theory of space-time) - Perdurantist approach to Perdurance in time - No substantial ontological distinction between events and objects
Causality	- Direct support through a relation or axiomatic constraints - Adoption of a productive notion with a physical interpretation
Scale and granularity	- Direct support for the representation of the same entity at different scales - Reductionistic approach taking into account scientific pluralism

Credit: Francesco Zaccharini, Univ Bologna

EMMO Foundations

Everything is made of indivisible **discrete quantum elements** as suggested by SMP(**reductionism**, **mereology**)

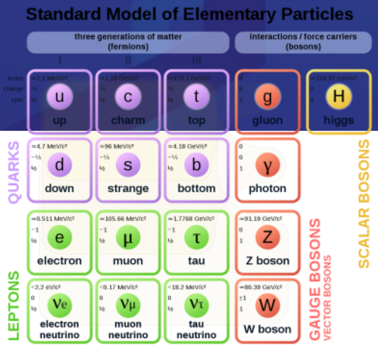
Must be coherent with **special relativity** (**causality**)

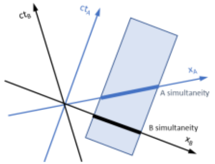
Must be coherent with **quantum mechanics** and **QFT** (**mereocausality**)

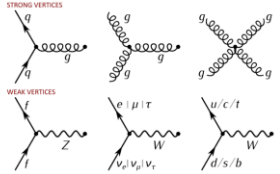
Must be coherent with **conservation laws**, i.e., every change in an entity requires an interaction with at least another entity (**4D**)

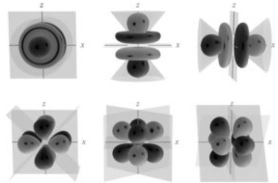
Nothing exists if doesn't interact causally with another entity, i.e. **abstract objects do not exist** (**physicalism, nominalism**)

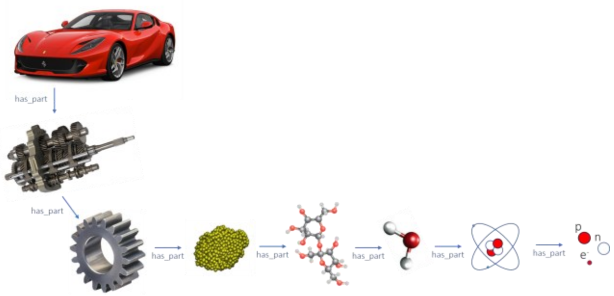
Properties are not inherent to things, but are bounded to a specific observer and observation mechanism (**semiotic approach**)











EMMO Backbone and Perspectives

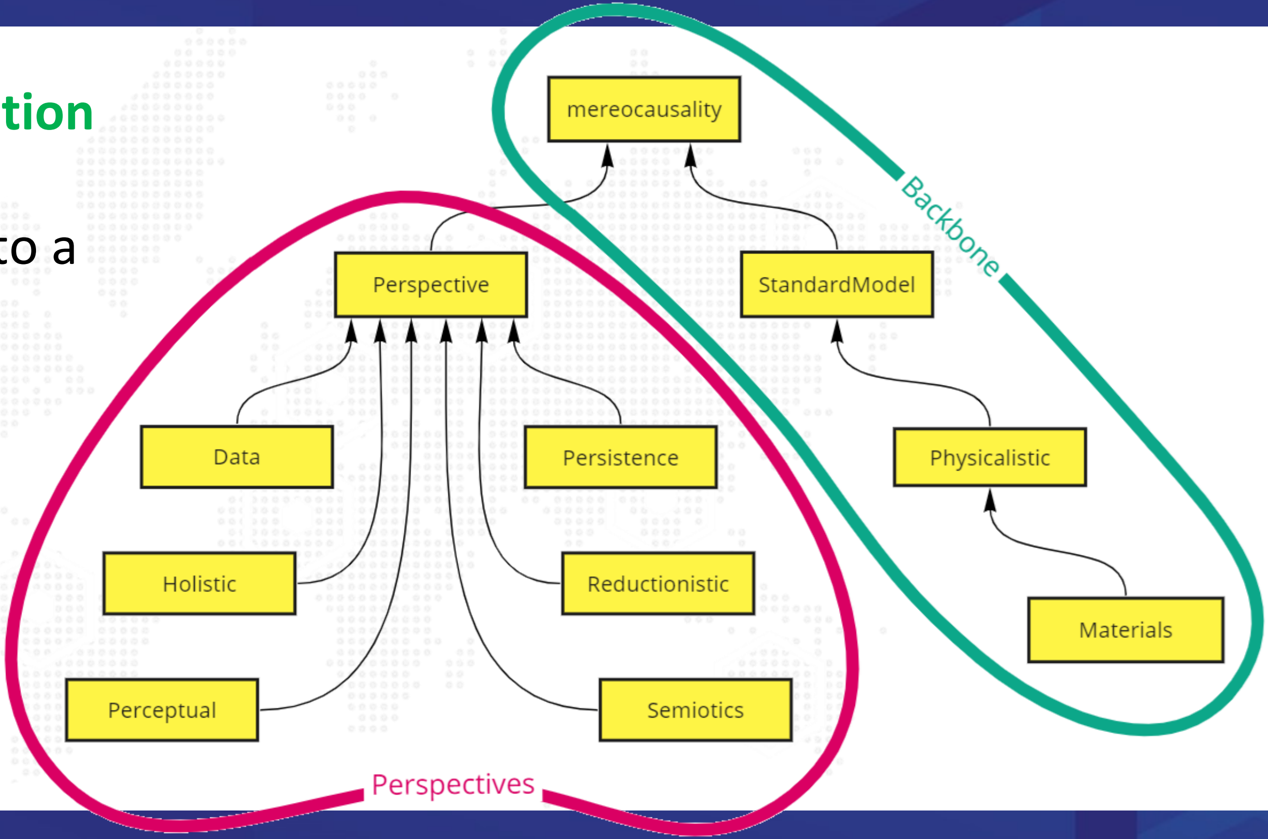
Physics-based representation modules:

Anything can be reduced to a "material" nature

and

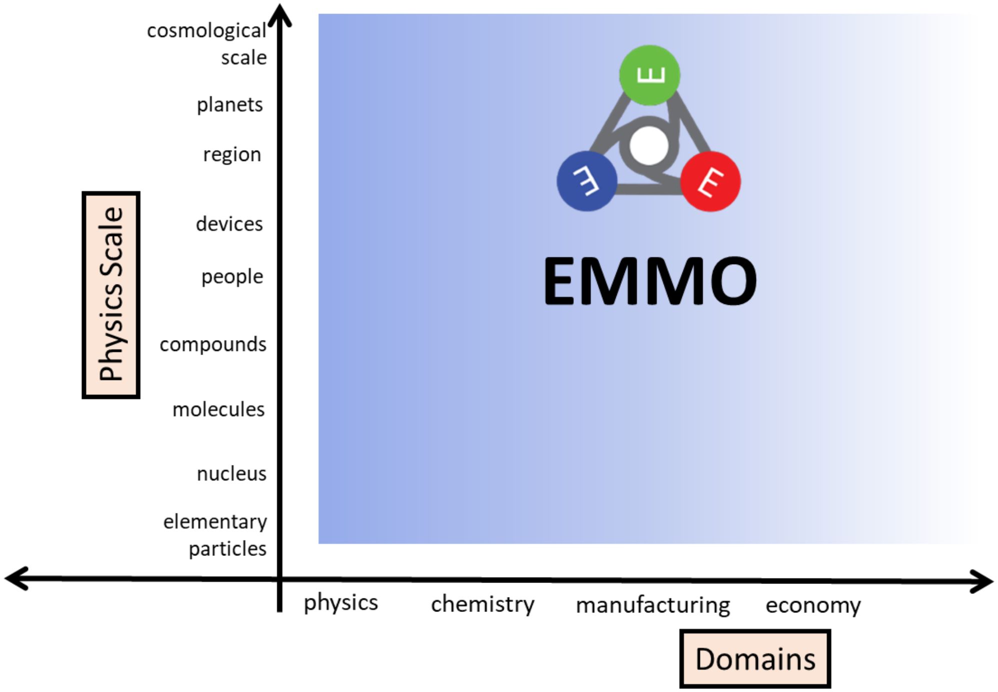
Generic representation modules (Perspectives)

Things can be described in different "common-sense" ways



EMMO: from standard model to materials

EMMO achieves complete **multiscale** representational capabilities with solid foundations in physics



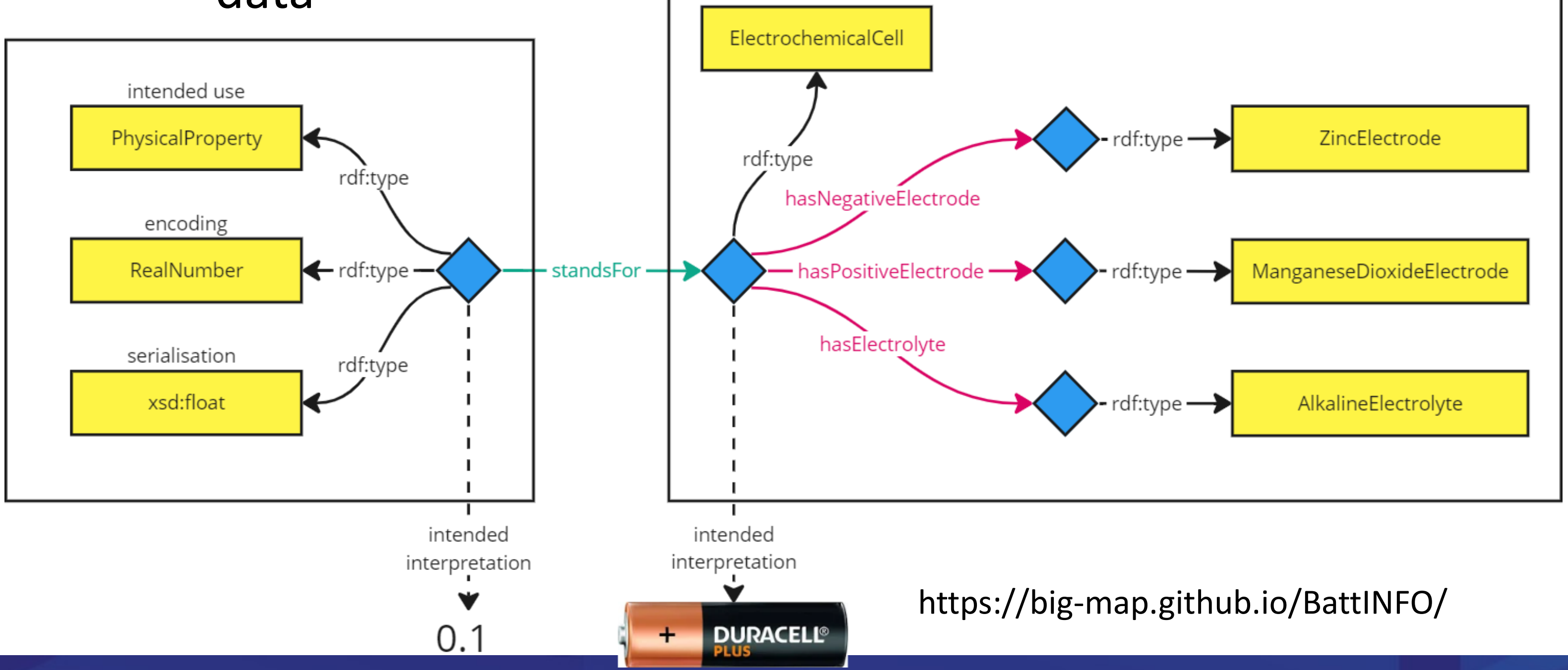
Clear separation of concerns

Battery Ontology
- Based on **EMMO**
- Representing batteries cells, materials, components, methods and properties

information

data

physical entity (mereocausality, no data)



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

EMMO: 3 prime principles for all relations

Mereology: parthood, “spatial”
Causality: incl time sequence
Semiotics: “signs”
“model for”, “property of”, “name of” etc

- EMMORelation
  - causal
  - mereological
  - semiotical

- DOLCERelation
  - constantConstituentOf
  - constantlyOverlaps
  - constantlySpatiallyLocatedAt
  - constantQualeOf
  - overlaps
  - presentAt
  - qualeOf
  - specificallyDependsOn

- BFORelation
  - concretizes at some time
  - continuant part of at some time
  - environs
  - exists at
  - first instant of
  - generically depends on at some time
  - has continuant part at some time
  - has first instant
  - has history
  - has last instant
  - has material basis at some time
  - has occurrent part
  - has participant at some time
  - has realization
  - history of
  - is carrier of at some time
  - is concretized by at some time
  - last instant of
  - located in at some time
  - location of at some time
  - material basis of at some time
  - occupies spatial region at some time
  - occupies spatiotemporal region
  - occupies temporal region
  - occurrent part of
  - occurs in
  - participates in at some time
  - preceded by
  - precedes
  - realizes
  - spatially projects onto at some time
  - specifically depended on by
  - specifically depends on
  - temporally projects onto

They proved to be so **powerful** that every relation (object property) concept can be placed under them.

EMMO complies with ISO/IEC 21838-1

Information technology — Top-level ontologies (TLO) — Part 1: **Requirements**

Domain neutrality: Based on scientific principles and analytic philosophy

Logics: EMMO is available at the Top Level in First Order Logic as well

A clear stance on all ISO standard requirements such as

- **Space and time**: practically 4-dimensional
- **Qualities and quantities**
- **Parthood, Location, Constitution, Time and Change, and Events and Processes**
- **Classifications and Mathematical, Informational, Social, & Mental Entities**
- **Causation and scale & granularity** have been individuated as especially important topics a TLO tailored for MSE should focus on

- Further details to be published!

Battery Ontologies Ecosystem in EMMO

EMMO Top
(Mereocausality)

EMMO Perspectives
Persistence - Holistic - Contrast - Semiotics - ...

EMMO Reference
Standard Model/Physicalistic - Agency - Data/Information - Workflow -

EMMO Disciplines
Matter/Chemistry/Materials - Manufacturing - Metrology - Properties - Models - Maths - ....

Chemical Substance (battery) | Battery (whole) | Electrochemistry | CHAMEO | Battery Value Chain

CHEMS — Chemical Substance Domain Ontology
BATTERY — Battery Domain Ontology
ECHO — Electrochemistry Domain Ontology
CHAMEO

Example

Causal Structure

Process (Persistence)

Agent Driven Process, IntentionalProcess

Manufacturing, Materials Processing ISO and DIN standards

ElectroCoating

BIG-MAP

Plus alignment with: Semantic Sensor Network Ontology

OGC Making location count.

W3C

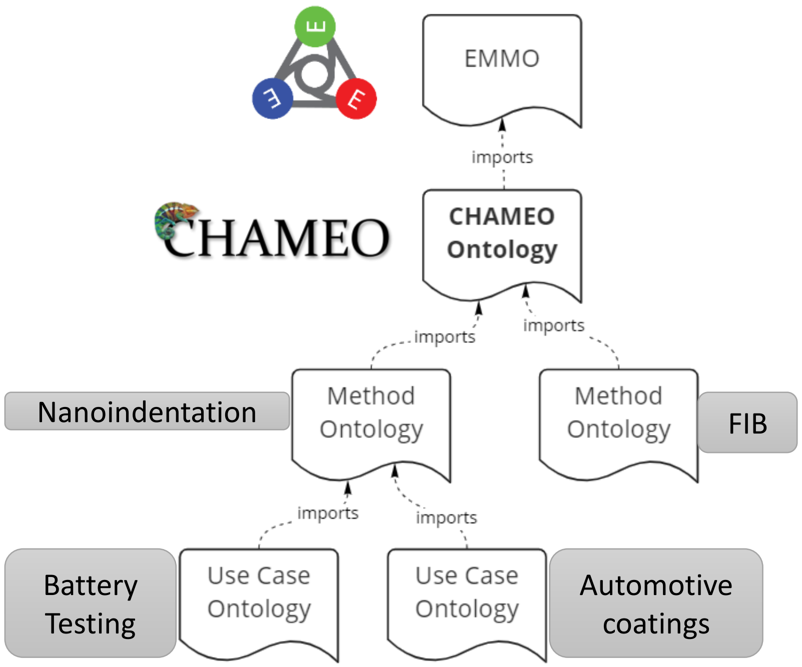
References
[1] Battery Cell Assembly Twin (BatCAT) http://www.batcat.info/
[2] Elementary Multiperspective Material Ontology, https://github.com/emmo-repo/emmo
[3] Characterisation Methodology Domain Ontology (CHAMEO), https://github.com/emmo-repo/domain-characterisation-methodology
[4] Electrochemistry Ontology https://github.com/emmo-repo/domain-electrochemistry
[5] Battery Domain Ontology, https://emmo-repo.github.io/domain-battery/index.html
[6] Semantic Sensor Network Ontology, https://www.w3.org/TR/vocab-ssn/
[7] Chemical Substance Ontology, https://github.com/emmo-repo/domain-chemical-substance
[8] Battery Value Chain Ontology, https://github.com/Battery-Value-Chain-Ontology/ontology

BatCAT Battery Cell Assembly Twin

Materials Characterisation

Aligned with a CEN Workshop Agreement: Materials characterizaton - Terminology and structured documentaton

https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/RI/2025/cwa17815_2025.pdf



What is in CHAMEO?

Material/Batch

Sample

- Dimensions
- Structure (e.g. layers)
- Material's physical and chemical composition
- Hazard

Characterisation procedures

- Sample extraction
- Sample preparation
- Sample inspection
- Calibration process
- Measurement system adjustment
- Characterisation measurement process
- Data preparation
- Data post-processing
- Data validation

Operator

Laboratory

Instrument

Environment, Parameters

Level of expertise

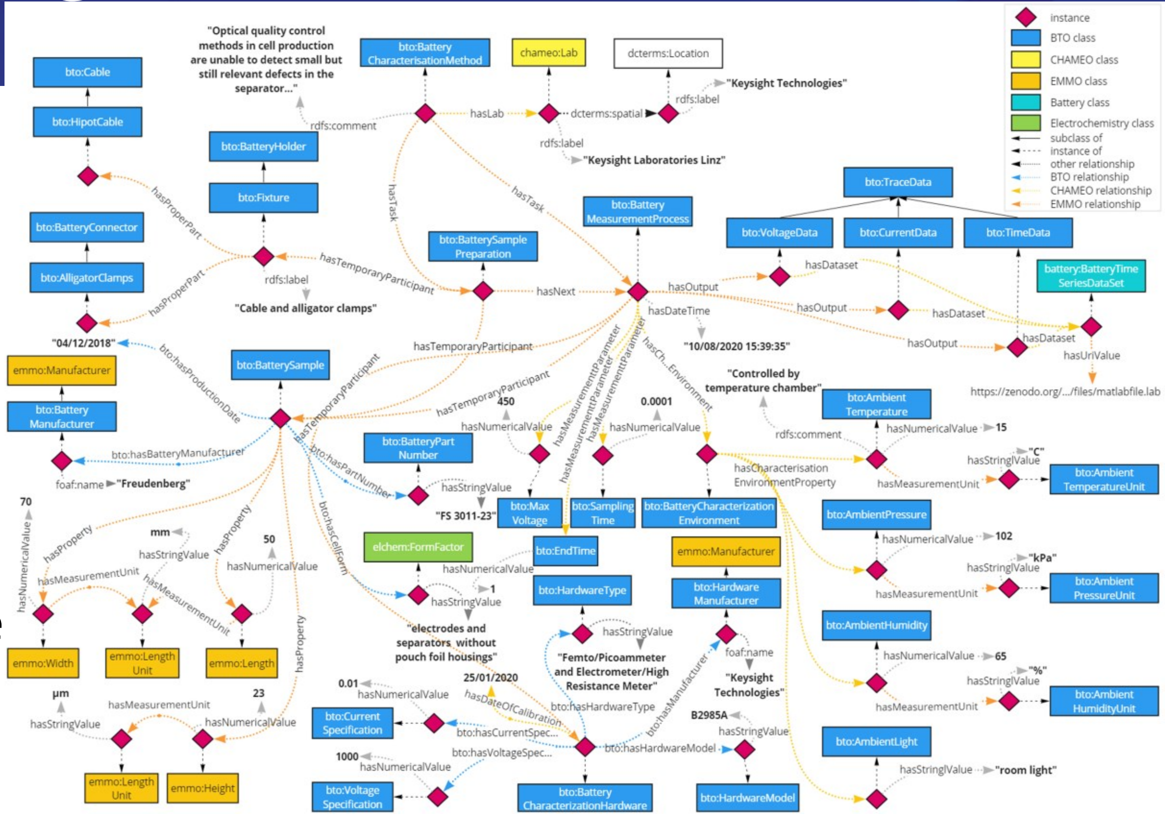
Characterisation Data

- Calibration data
- Raw data
- Primary data
- Secondary data
- Characterisation property

nanoMECommons

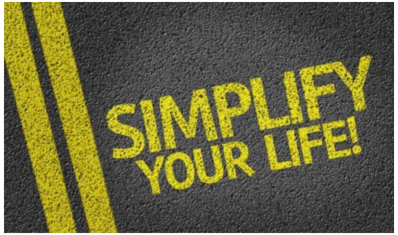
Battery Testing Use Case

- Unified structure for organising knowledge and data in battery testing and battery quality control.
- Supports a range of electrical battery cell tests, including impedance spectroscopy, self-discharge, and high-voltage

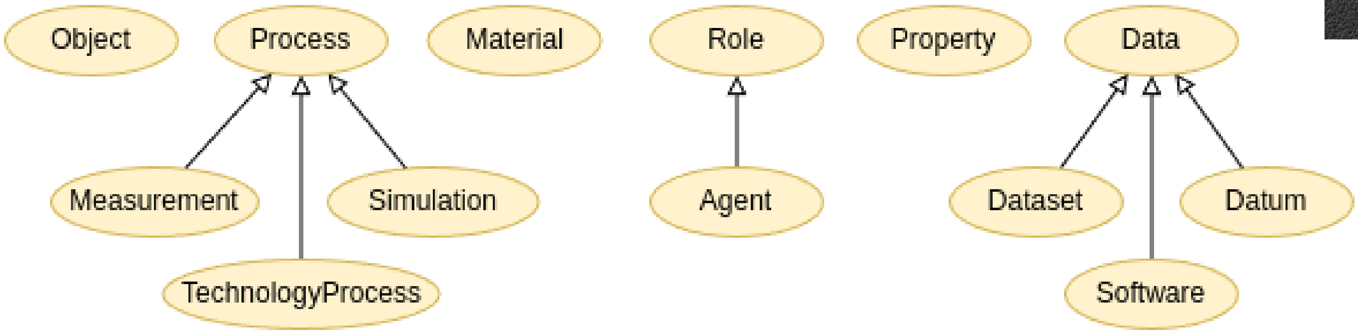


Battery testing ontology: An EMMO-based semantic framework for representing knowledge in battery testing and battery quality control Computers in Industry, https://www.sciencedirect.com/science/article/pii/S0166361524001313

Reducing complexity for applications: ELITE



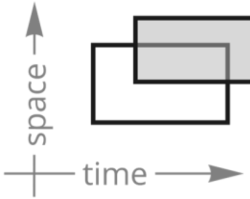
- Retains the most common mid-level concepts
- Interoperable with complete EMMO (same IRIs)



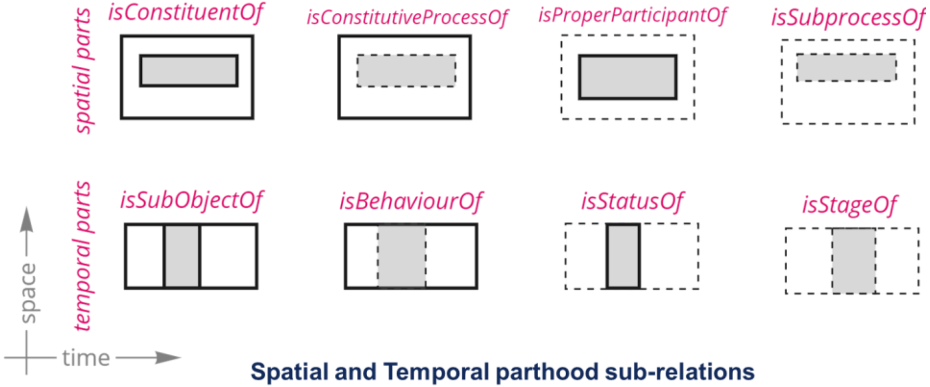
https://github.com/emmo-repo/EMMO/wiki/guidelines-development

emmo-lite	https://w3id.org/emmo/emmo-lite	Selected leaf classes and properties for rapid development and deployment in graph databases.

EMMO toolbox of Object Properties

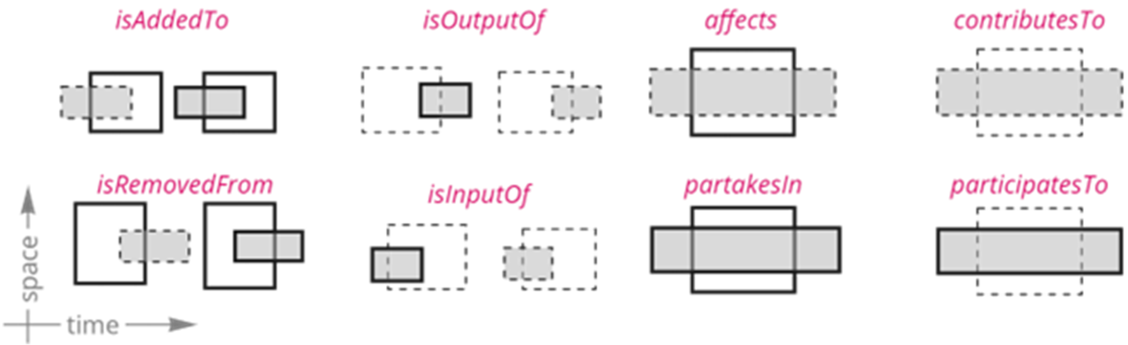


4D approach and **space/time** graphical representation of entities.



Spatial and Temporal parthood sub-relations

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

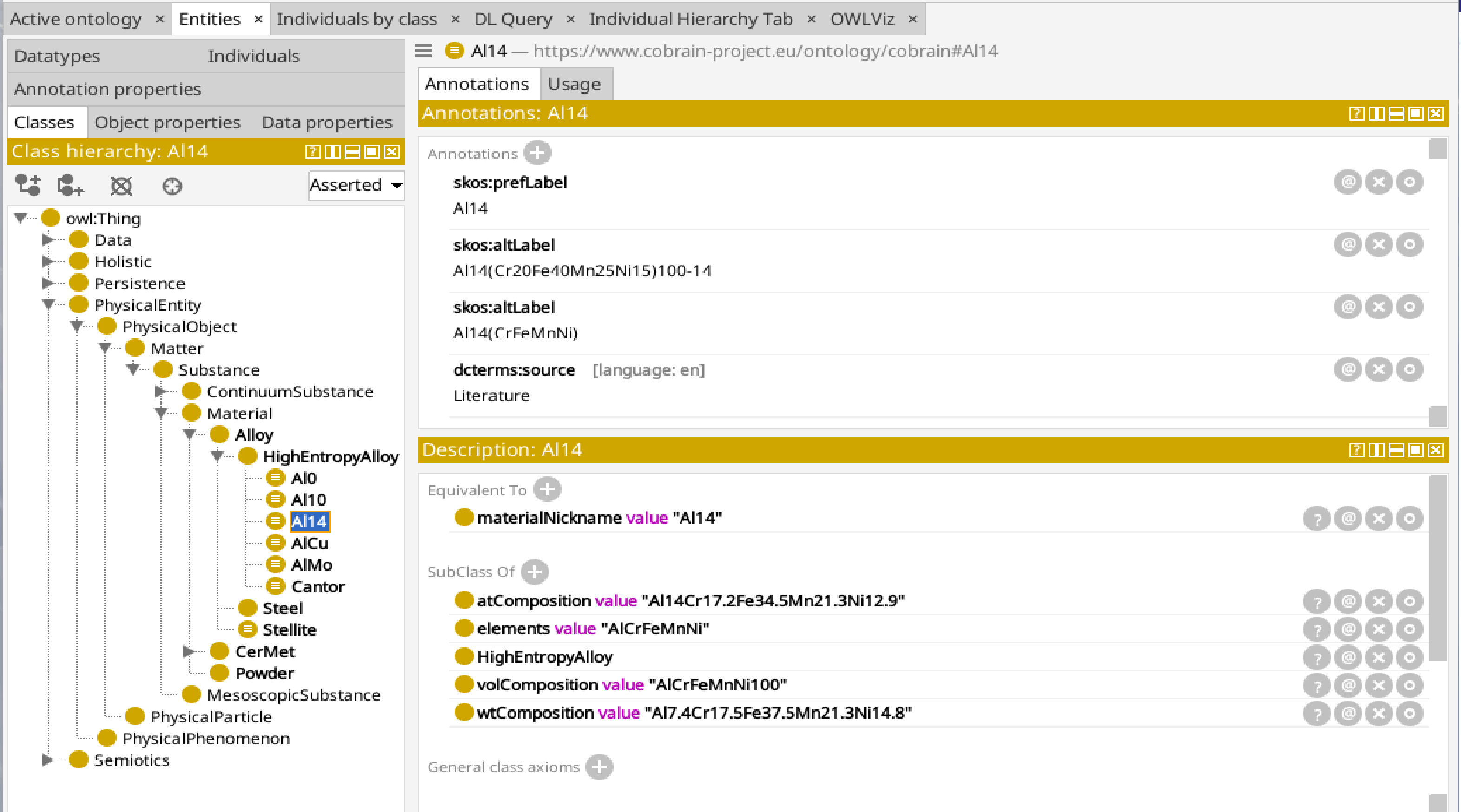


Proper overlap sub-relations (continuous line standing for objects, dashed line for processes, and relations going from the grey to the white boxes)

ELITE application, examples

- CoBrain project
- Similar approach in BatCAT project
- Connect-NM: European Nuclear Materials Knowledge Base
- Student projects, e.g. on Fukushima accident (Univ Bologna)

CoBRAIN


Active ontology
Entities
Individuals by class
DL Query
Individual Hierarchy Tab
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Individuals
Annotation properties
Classes
Object properties
Data properties
Class hierarchy: Al14
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AlCu
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Cantor
Steel
Stellite
CerMet
Powder
MesoscopicSubstance
PhysicalParticle
PhysicalPhenomenon
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Literature
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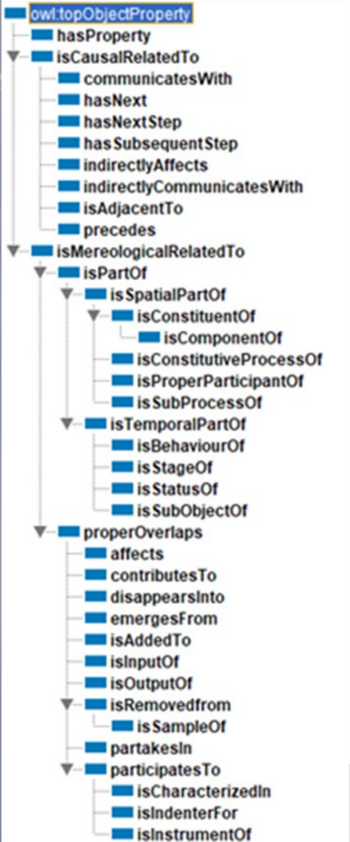
elements value "AlCrFeMnNi"
HighEntropyAlloy
volComposition value "AlCrFeMnNi100"
wtComposition value "Al7.4Cr17.5Fe37.5Mn21.3Ni14.8"
General class axioms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isProperParticipantOf
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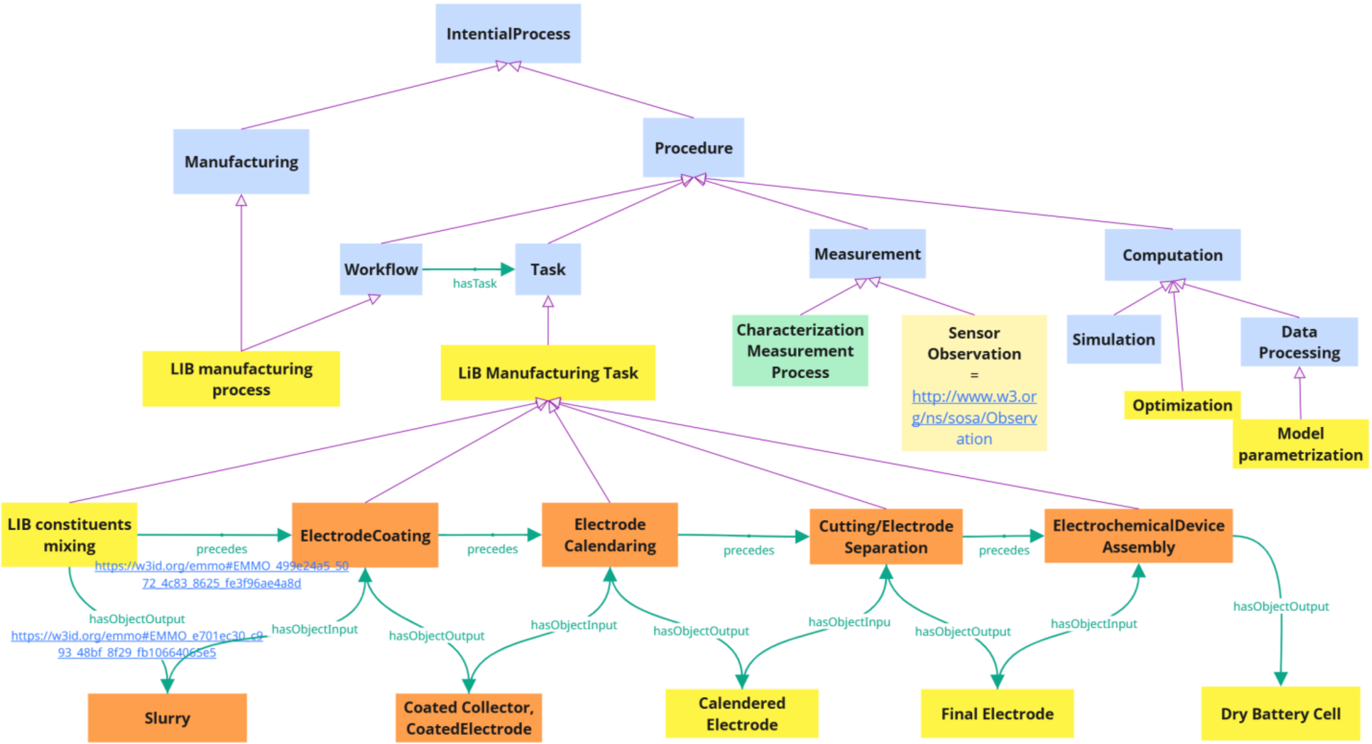
isInstrumentOf

Battery Cell Assembly Digital Twin (BatCAT)



BatCAT
Battery Cell Assembly Twin

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Conclusions

- **Commitment pays off in the long run.**
- **EMMO**: based on scientific world-view, commitment to a material-based world, with common-sensical Perspectives
- A growing **ecosystem** of Discipline and Domain ontologies
- **ELITE** makes it more user-friendly, while keeping the foundations.

Thanks to EMMO developers and projects

https://emmc.eu/emmo/

The EMMO **core development group**:

- Emanuele Ghedini (UNIBO)
- Gerhard Goldbeck (GCL)
- Jesper Friis (SINTEF)
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- Georg Schmitz (ACCESS)
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- Otello Roscioni (ex-GCL)

And many more…

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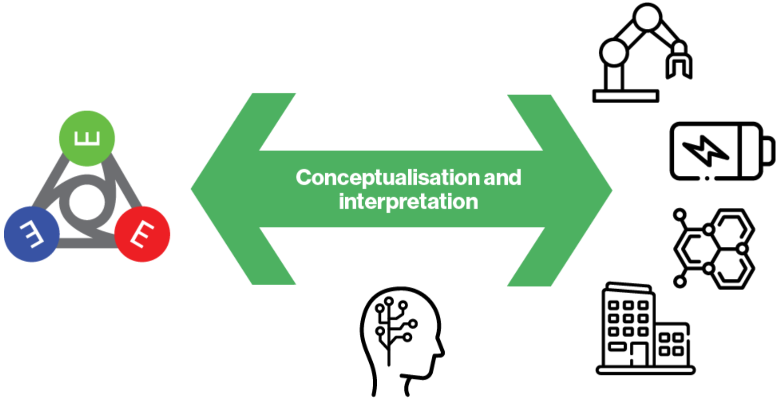
Semantic Materials

SemanticMaterials

- A team of EMMO authors and experts
- Technology partners
- **Semantic Materials Workshop 2025**
  - 10 November, 2025
  - Cambridge



https://semanticmaterials.com

SemanticMaterials

Thank you!