Materials data documentation:

how to improve interoperability in a complex field of many perspectives

FIRST INTERNATIONAL SYMPOSIUM FOR MATERIALS R&D DATA,
Nano Korea 2022

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Projects and Initiatives involved

The European
Materials Modelling Council

Ontology Ecosystem

Open Translation Environment

Harmonisation of characterization protocols

Material Modelling Innovation Platform

Open Simulation Platform

Materials Modelling Marketplaces

Industrial Data Marketplace

Challenges and industrial requirements

Requirement for materials, process and product

Industry requires

"unique way of representing materials, processing and the according devices"

- Deeper understanding
- Precise manipulation of respective influences

Faster Development and Innovation Cycles

Underpinning Digitalisation

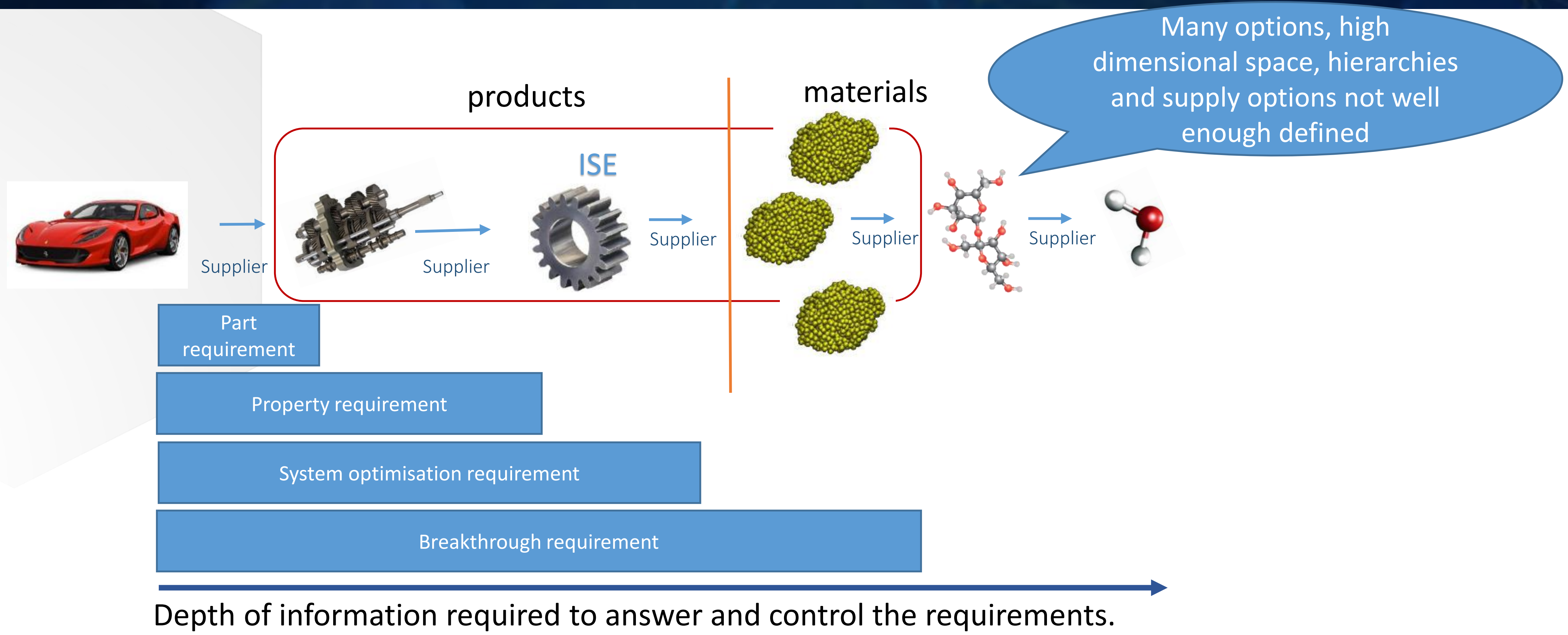
Enhanced Collaboration

Insights, improved decisions, reduced risk of failure

Predictive Science: data, smarter experimentation

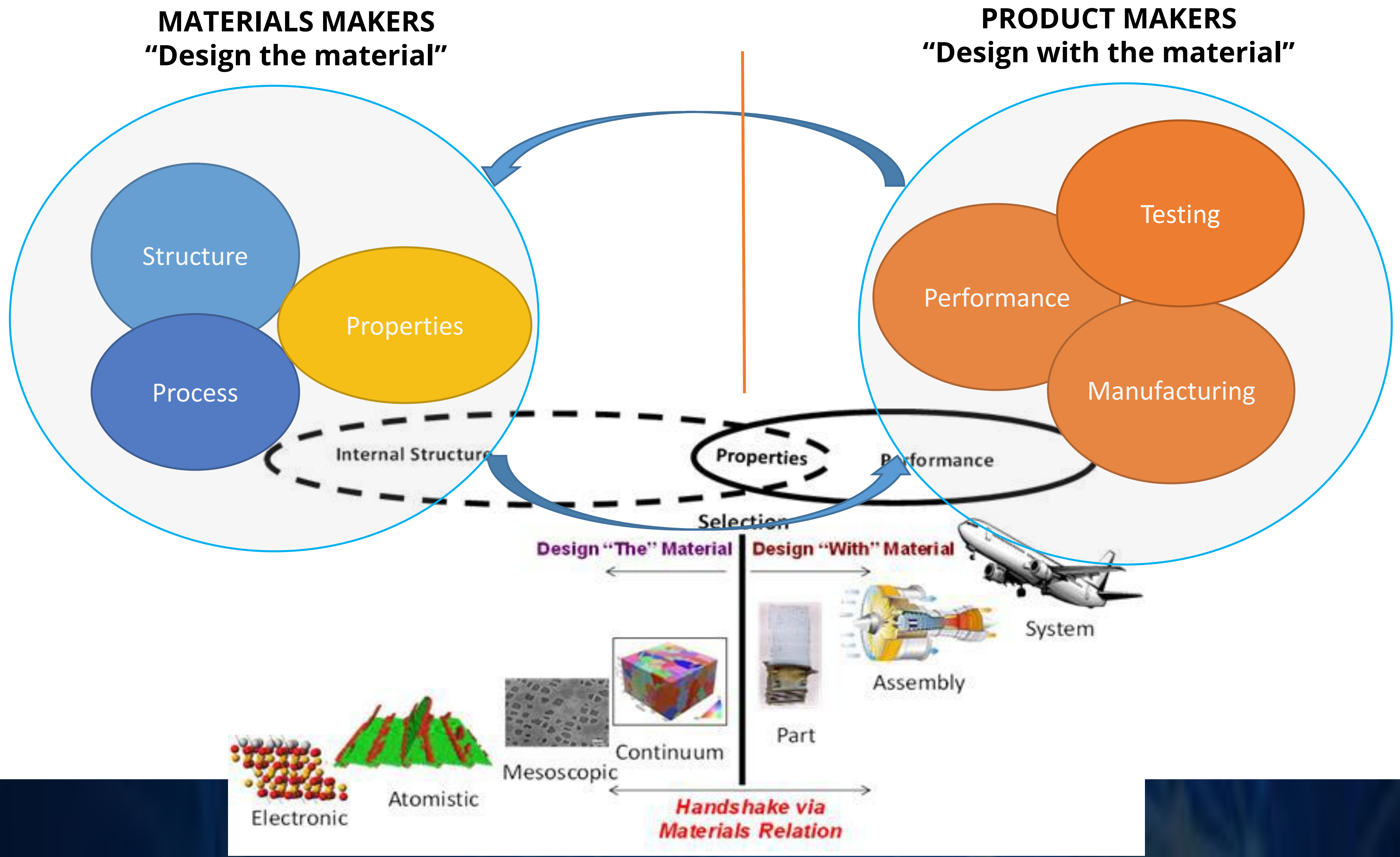
Requires rich materials knowledge capture as well as data interoperability

Knowledge based materials integrate depth of design, sustainability and support breakthroughs



Move to more complex requirements (and controlling the related risks!) requires deeper, shared data model

Materials vs Products development
Pluralism challenge: coexistence of different views

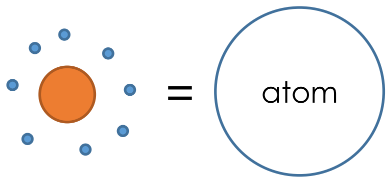


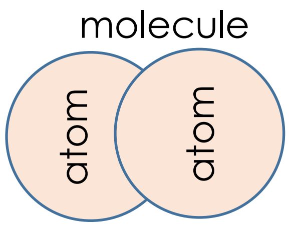
Plurasim challenges, e.g. Chemistry vs Physics

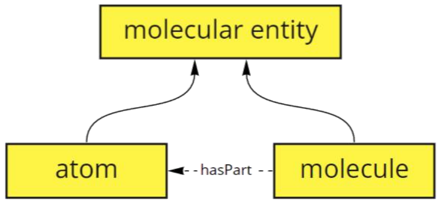
IUPAC Definitions (Chemistry)

An Atom is a nucleus of Z positive charge and Z electrons

A Molecule is an electrically neutral entity consisting of more than one atom



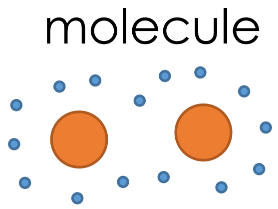


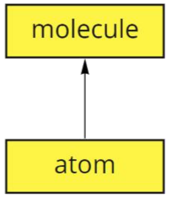


Chemical-Physics Definitions

A Molecule is an electrically neutral entity consisting of nuclei and electrons

NB: no atom involved here: atom is a singular type of molecule



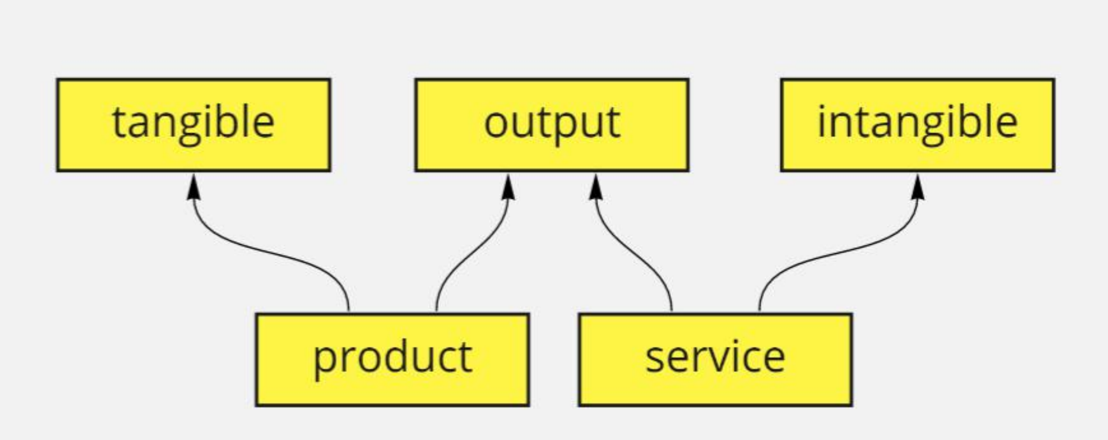


Chemistry and Chemical-Physics are two different approaches the lead to a **different definitions of atoms and molecules** and hence different parthood relations between their concepts.

Pluralism: Product definition in ISO standards

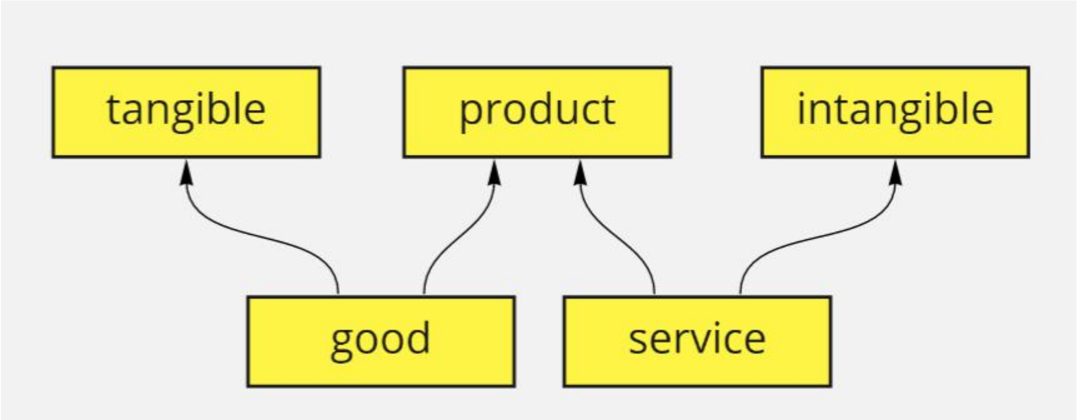
ISO 9000
Quality management systems

Process perspective



Role perspective

ISO 14040
Environmental management — Life cycle assessment



The definitions of **product** in ISO 9000 and ISO 14040 **are somewhat incompatible**, and for an ontology embracing one ISO means that the other ISO will be no more representable.

Challenge and Status Quo

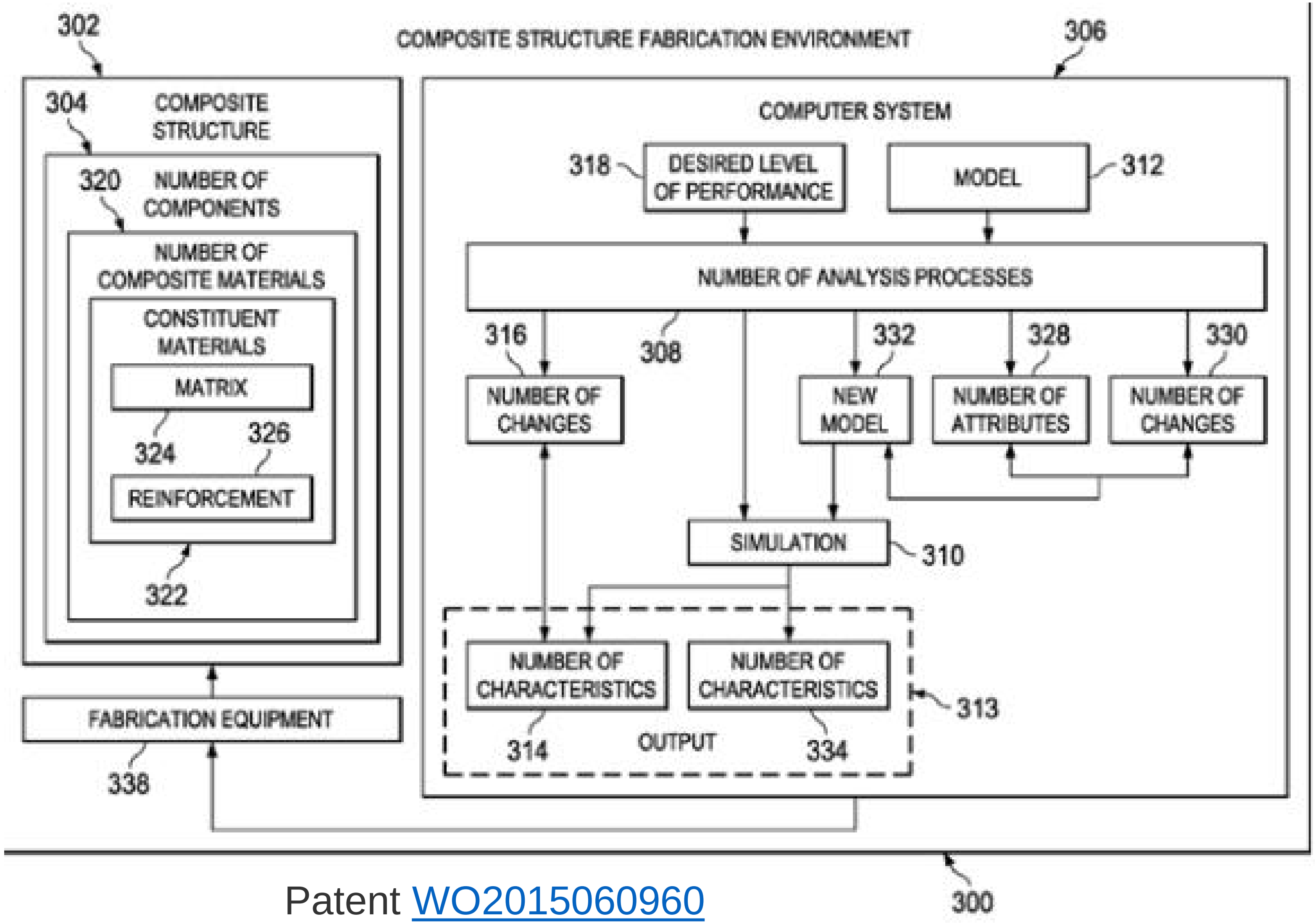
- Materials and product development draws on
  - Multiple expertise in multiple (sub-) domains
  - Multiple information and data resources
- Each domain has its own language and ways of handling data
- Lack of a common representation system

Need to organise data by materials science foundational principles!
Need to recognise the plurality of perspectives!

Overcoming the challenges

Boeing patent: Product Chemical Profile System (2014)

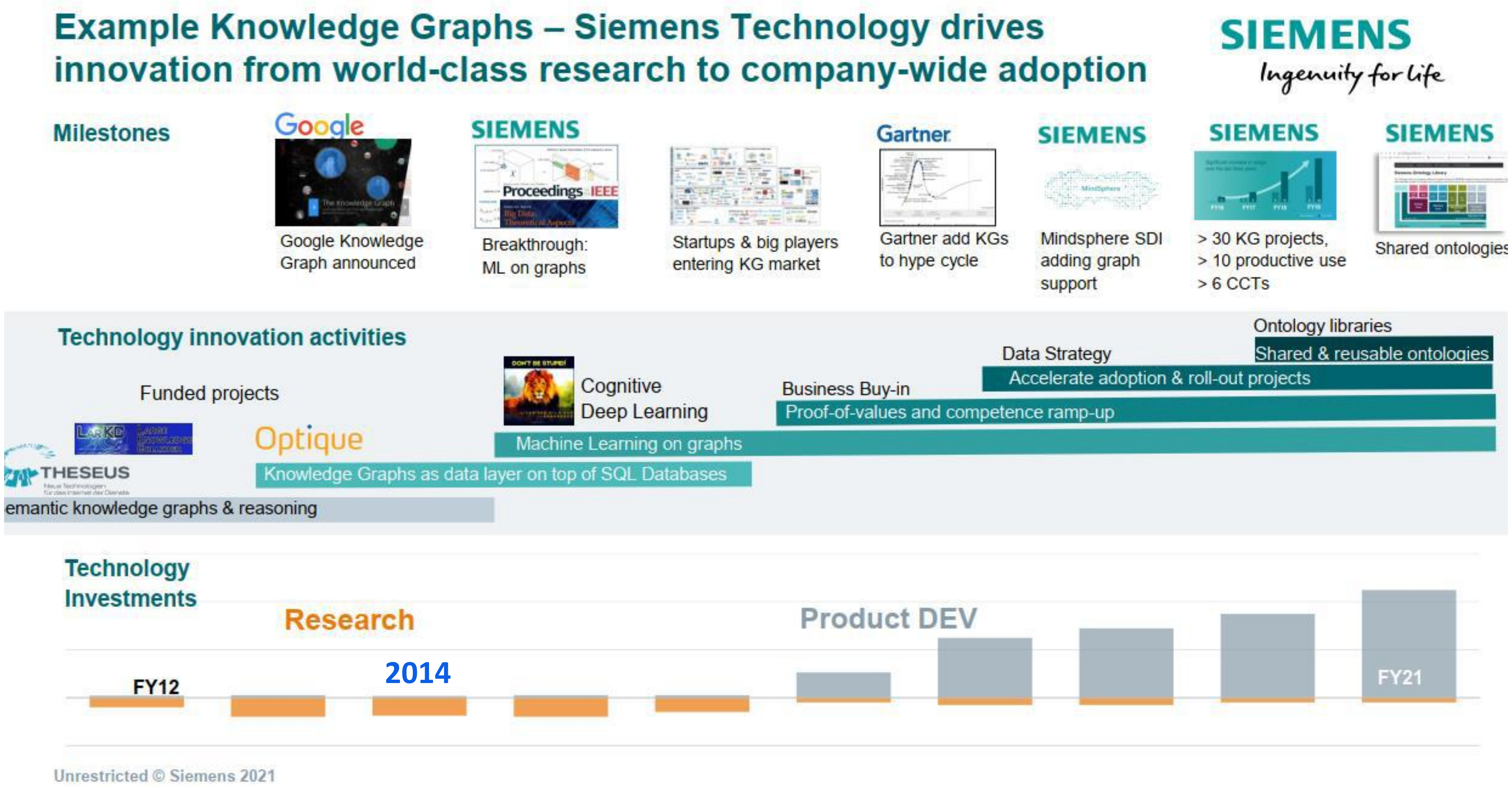
- A system that is able to pull together and **query all levels of information about a product down to the chemistry level**
- "A **product-to-chemical continuum** is generated …. to traverse the product-to-chemical continuum through the callout-context pathway segments that **span the plurality of levels**."



Patent [WO2015060960](WO2015060960)

https://materialsmodelling.com/boeing-is-moving-ahead-with-integrating-chemistry-and-materials-modelling-into-the-product-life-cycle/

Learning, reasoning, Semantic Web technologies

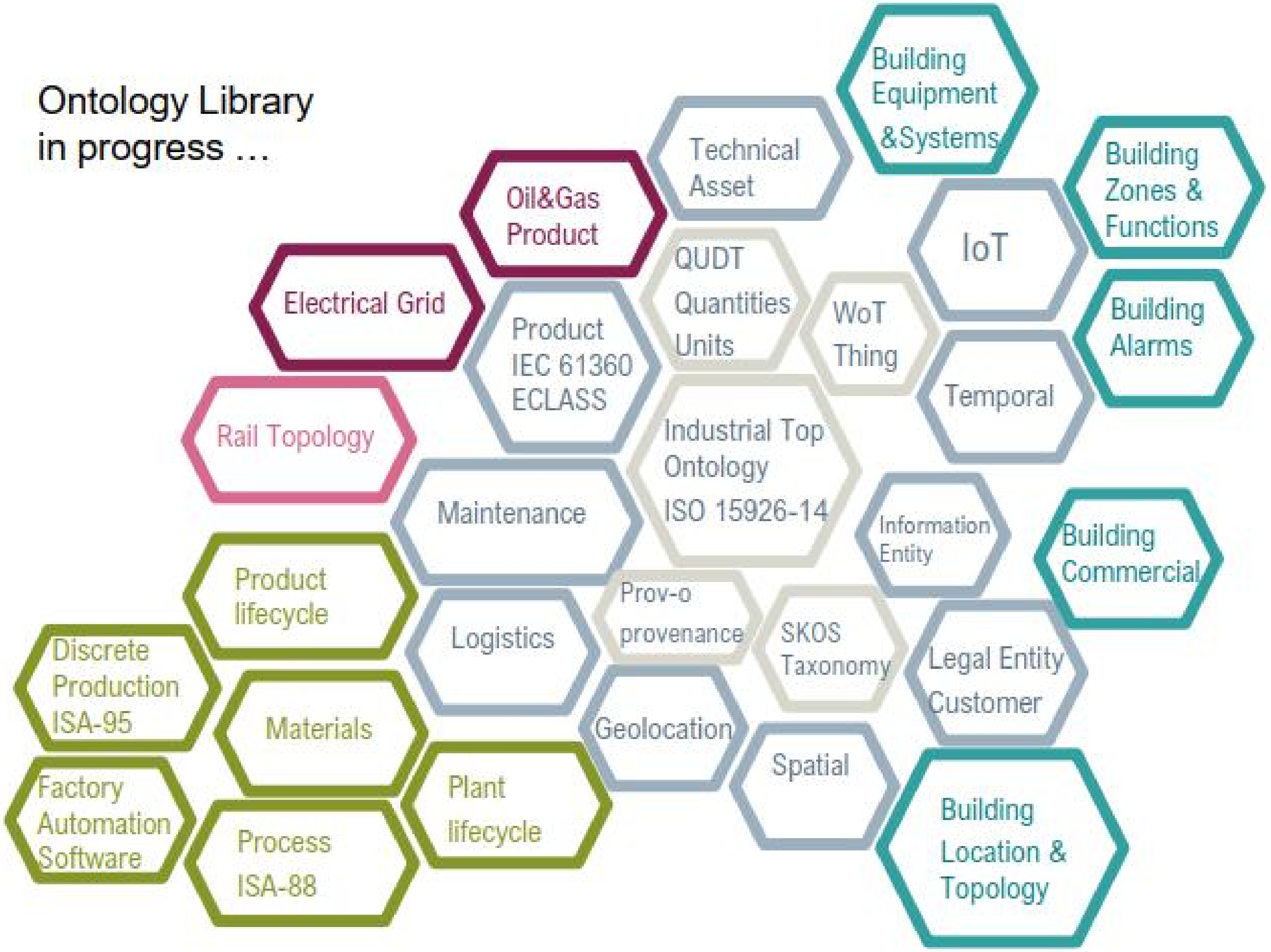


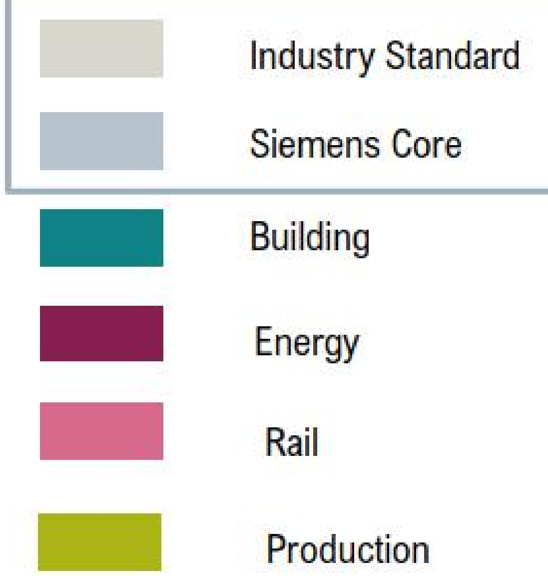
Industrial Ontologies @ Siemens, Dr. Maja Miličić Brandt, Siemens Technology, Semantics and Reasoning, OntoCommons DORIC-MM Worksho, 7 June 2021

Ongoing Initiative: Shared Ontology Guidelines, Upper-Ontology and Siemens-wide Ontology Publication Platform

SIEMENS
Ingenuity for life

Ontology Library
in progress …





A growing core ensures model quality and interoperability!!!

Harmonised data documentation through ontologies

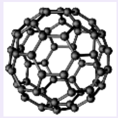
Cooperation with existing intiatives

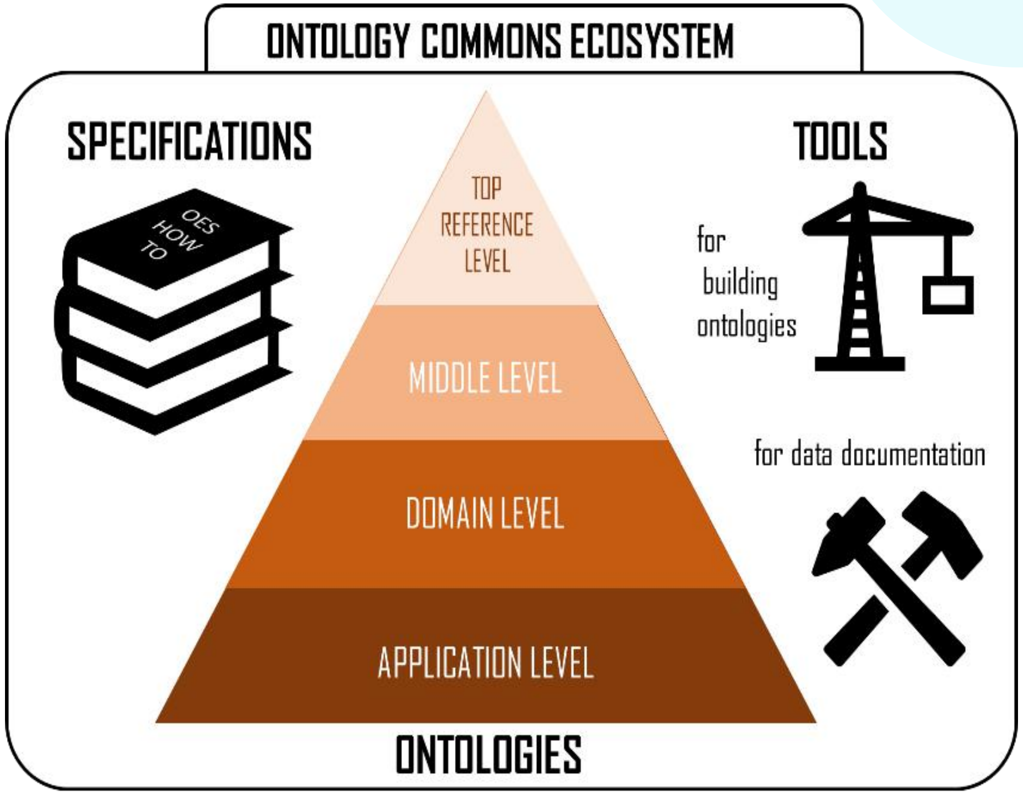
Ontology Commons EcoSystem

- Foundation for data documentation
- Requirements and specifications
- Set of ontologies as a part of the EcoSystem
- EcoSystem tools

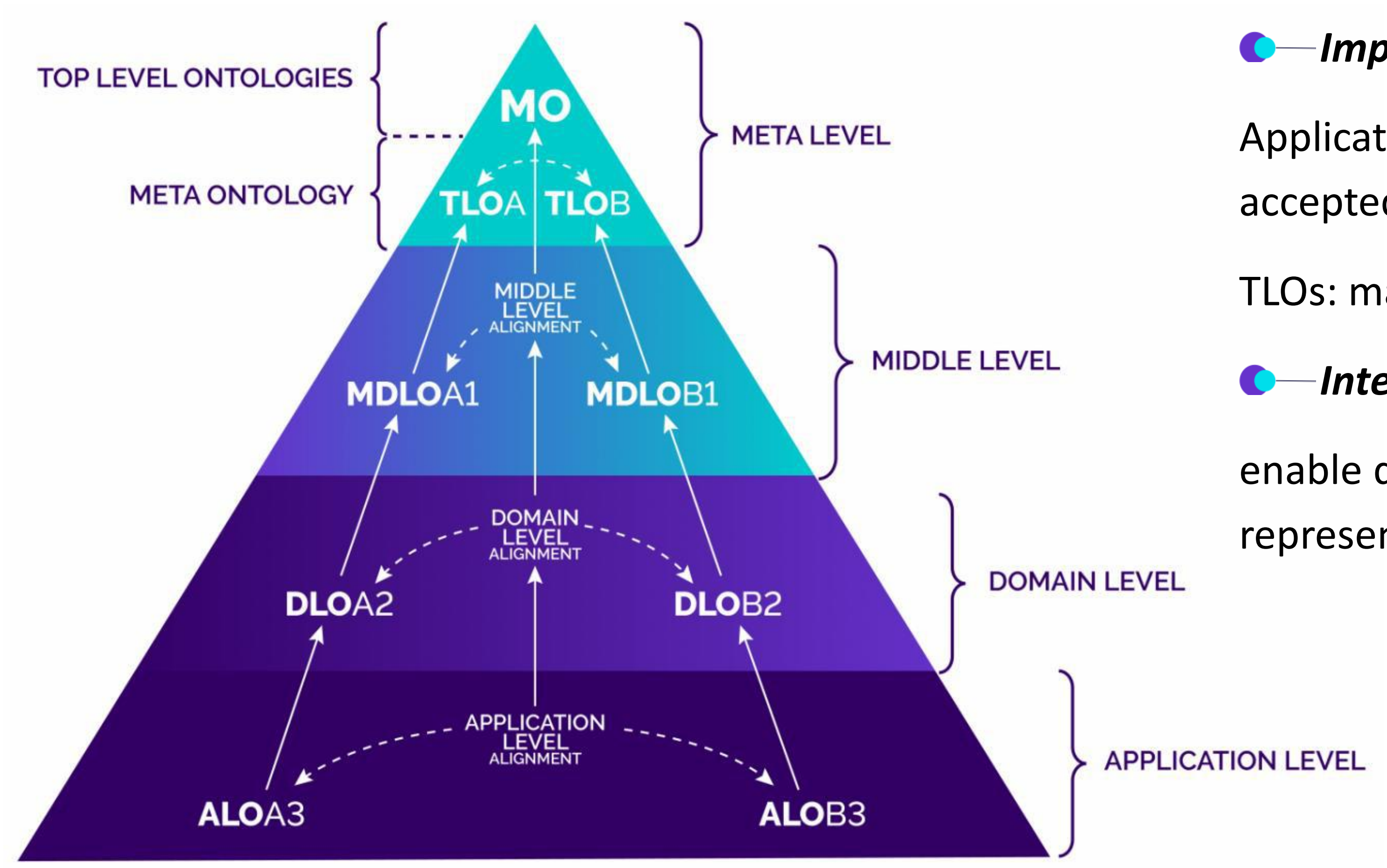
Demonstrators

- Materials and Manufacturing applications



Interoperability in OntoCommons



- ***Improve vertical alignment:***

Application and Domain ontologies based on widely accepted TLO/MLOs

TLOs: mainly ***BFO, DOLCE, EMMO***

- ***Inter-ontology interoperability:***

enable data sharing between different semantic representations of data from different TLOs

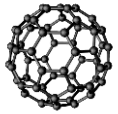
OntoCommons Stakeholders

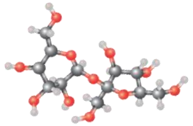
Manufacturing

Aerospace
Automotive
Electronics
Energy
Personal Goods
Parts manufacturing and supply

DOMAIN EXPERT THEORETICAL SCIENTIST DOMAIN SUBJECT EXPERT	**ONTOLOGIST** PHILOSOPHER LOGICIAN SEMANTIC WEB EXPERT	**IMPLEMENTER** ONTOLOGY DEVELOPMENT EXPERT REASONING EXPERT GRAPH DATABASE PROVIDER INTEROPERABILITY SPECIALIST	**INDUSTRIAL STAKEHOLDER** MANUFACTURER DATA PROVIDER INDUSTRIAL RESEARCHER BUSINESS DEVELOPER	**BUSINESS ECOSYSTEMS STAKEHOLDER** CROSS-DOMAIN DEVELOPER CROSS-DOMAIN ENTREPRENEUR CROSS-DOMAIN INVESTOR

Materials





Materials suppliers
Chemicals

Standardisation

ONTO COMMONS
ONTOLOGY-DRIVEN DATA DOCUMENTATION FOR INDUSTRY COMMONS

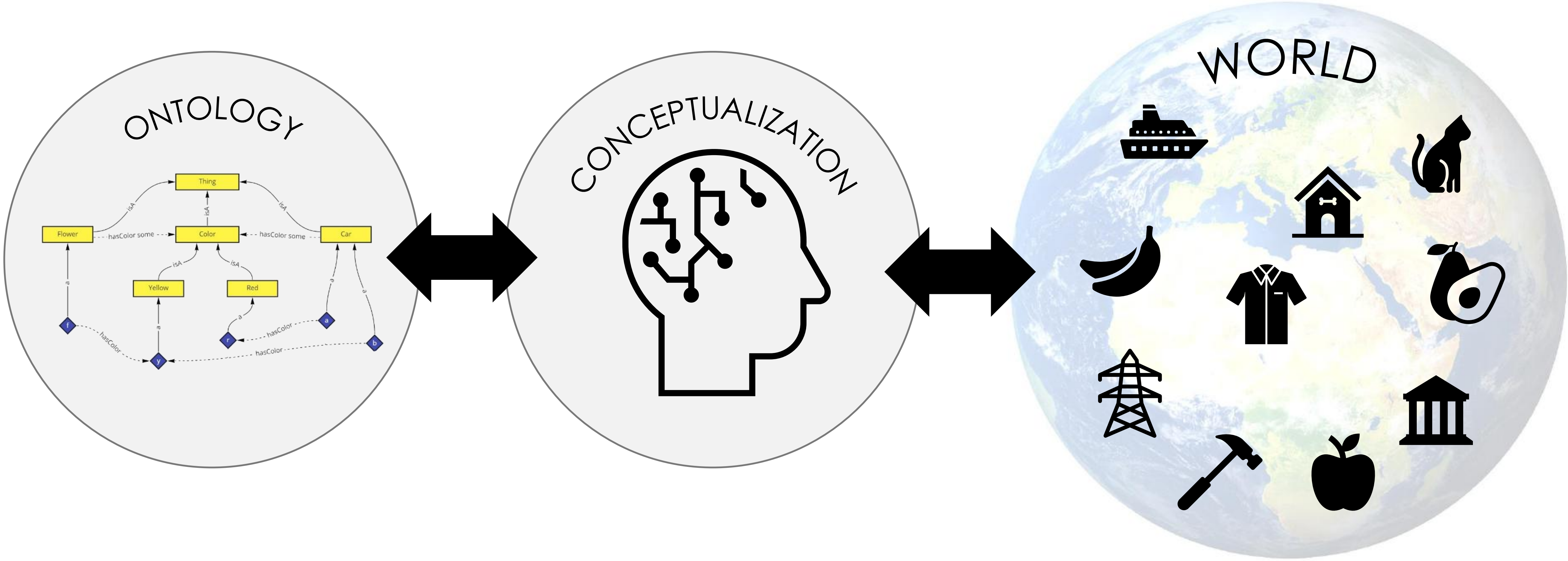
The OntoCommons Demonstrators

Home /

https://ontocommons.eu/ontocommons-demonstrators

- AIRBUS DESIGN AND MANUFACTURING
- BOSCH MANUFACTURING
- AIBEL PROCUREMENT
- TRIBOLOGICAL CHARACTERISATION
- DIGITAL MATERIALS MARKETPLACES
- OAS PRODUCT SERVICE SYSTEM
- FRAUNHOFER QUALITY
- IRES NANO-MATERIALS
- ONTOLOGY-BASED MAINTENANCE
- ELVAHALCOR METAL INDUSTRY
- SIEMENS DIGITAL MANUFACTURING
- BASAJAUN
- CHEMICAL PRODUCT LIFE CYCLE
- ONBOARD MAINTENANCE SYSTEM
- AUTOMOTIVE OPERATORS' SAFETY
- FOOD KNOWLEDGE GRAPH
- INDUSTRIAL INTERNET OF THINGS
- IKEA KNOWLEDGE GRAPH
- MATERIALS DATABASES INTEGRATION
- MATERIALS CHARACTERISATION ONTOLOGY
- LUBRICANT DESIGNER
- SOLUTION FOR SOILLESS CULTURE NUTRIENT

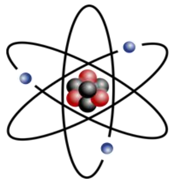
A New Language to Talk to Machines



Physics uses **Quantities** (numbers) to model the world

Ontologies use **Concepts** to build a **(onto)-logical representation** of the world

Universal language



PHYSICS

$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ MATH

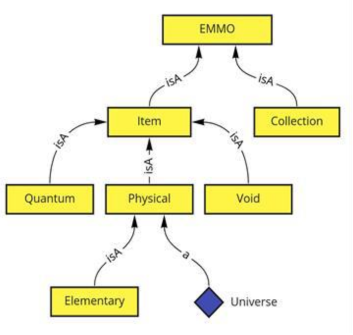
Math has been the key for the highest achievements in **Physics**

(e.g. Newton, Maxwell, Einstein, Schrodinger, Standard Model)

Ontologies can be the key for a quantum leap in **Industry**

(e.g. pervasive digitalization, knowledge sharing, Industry 4.0 to 5.0)

INDUSTRY



ONTOLOGY

- **document data**
- infer **new knowledge** (e.g. resoners)
- support **AI** (e.g. ontology assisted AI)

EMMO ontology

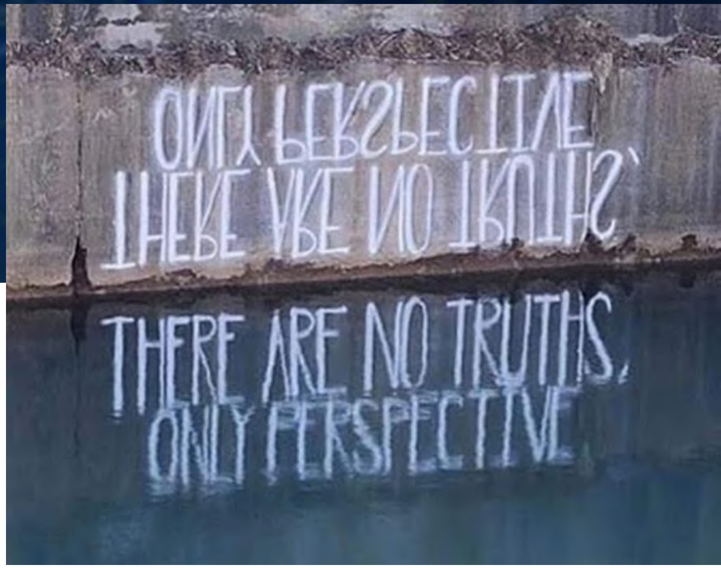
Elementary Multiperspective Material Ontology

A knowledge management framework for applied sciences and engineering

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

- Based on fundamental science principles well known and agreed by applied science community
- Integrates data science (W3C) and pure logics/philosophy
- Pluralism: embrace a diversity of views in a single framework
- Materialist: no abstract concepts: everything we know is based on some observation
- Mereocausality: well defined relations between entities
- Semiosis: ‘signs’ communicate meaning (e.g. model stands for real object)
- Able to represent quantum to engineering systems

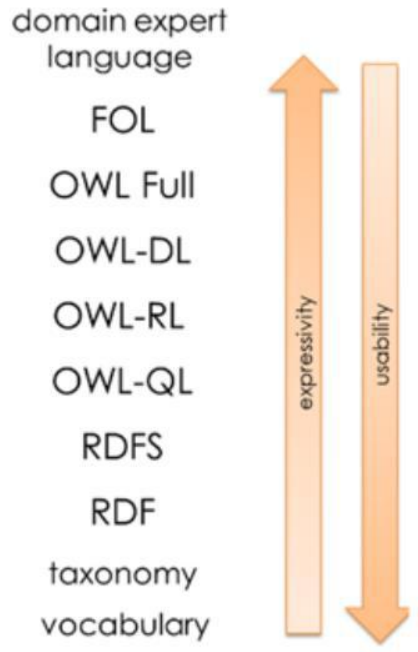
EMMO Approach



- **Project** existing and new knowledge onto data
  - Facilitates capturing expert **knowledge, not just data**

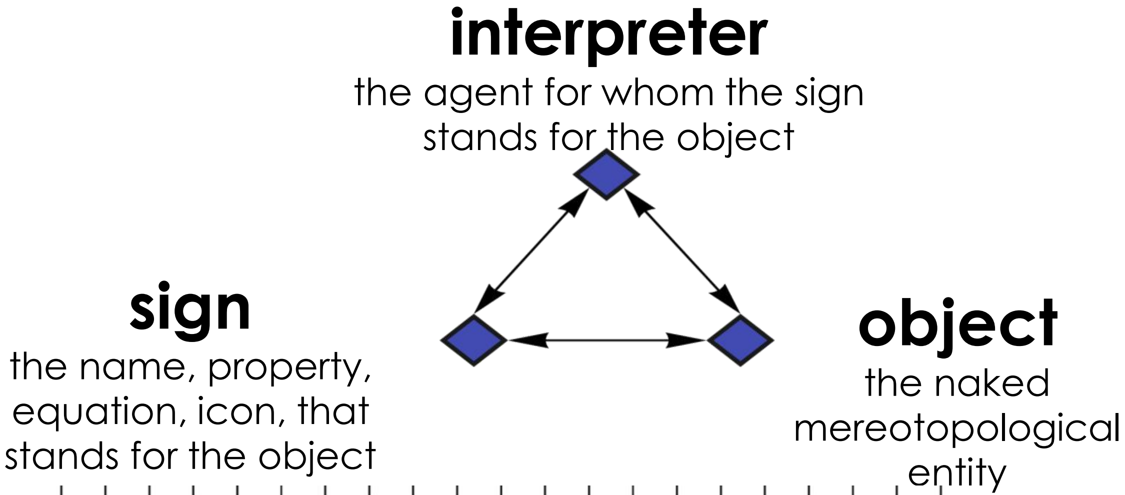
- No absolute definitions of the ontological nature of objects excepts for the Universe and the single indivisible quantum elements

- Scalable approach to knowledge representation

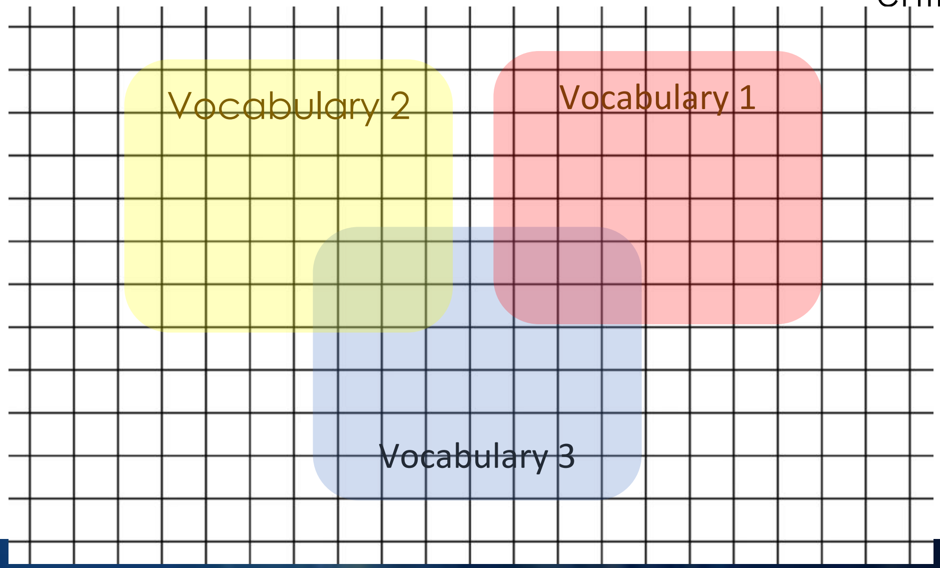


EMMO PLURALISM

Semiotic approach to knowledge representation **(in-ontology pluralism)**



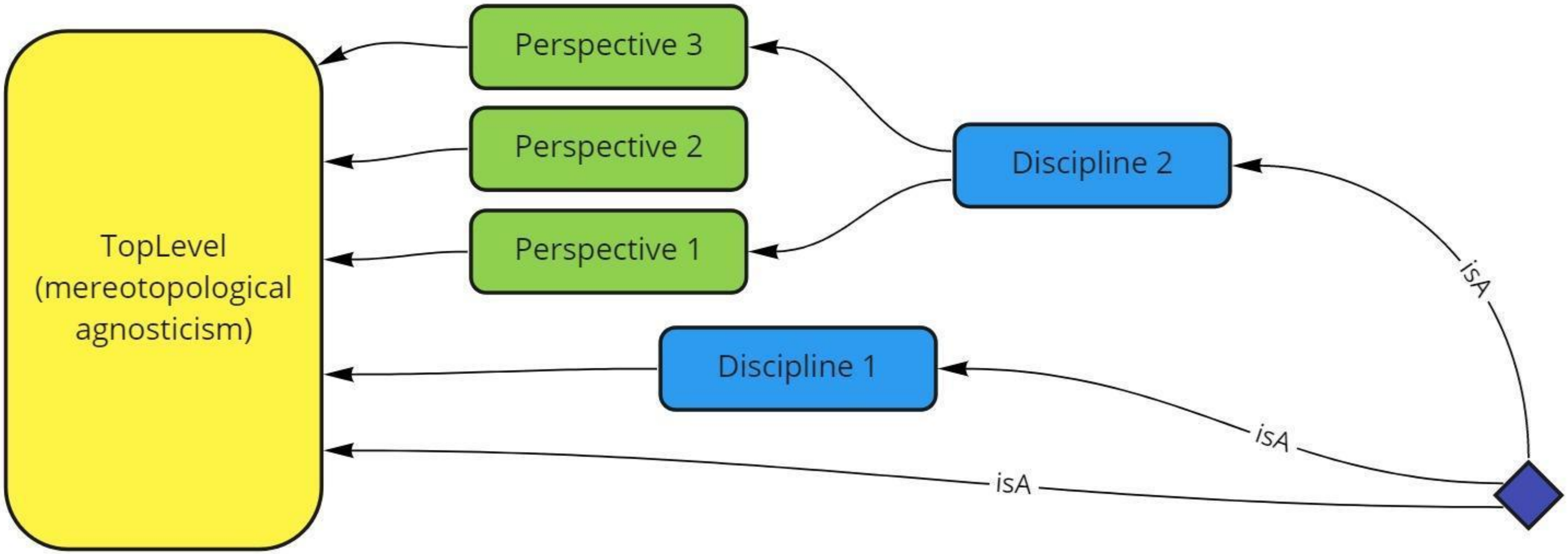
Perspectives in EMMO (outside ontology pluralism)



AGNOSTICS ONTOLOGY FRAMEWORK

EMMO Environment Structure

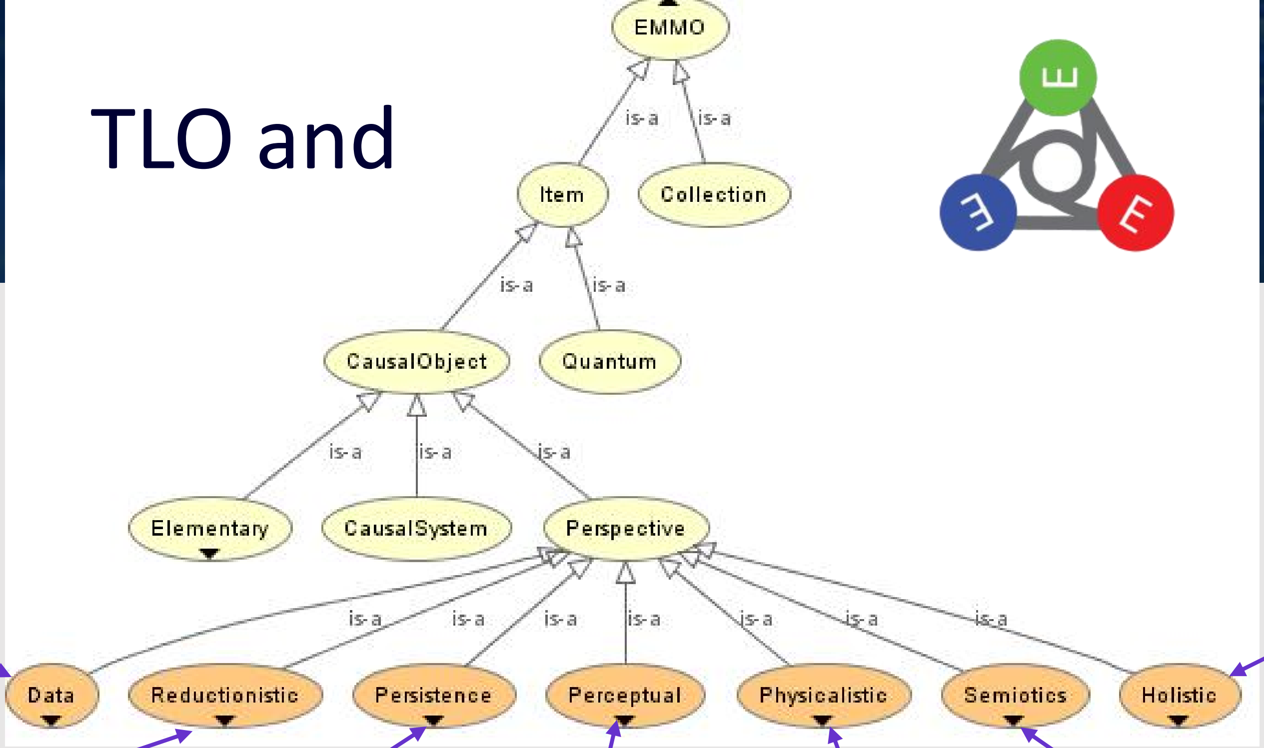
General Perspective Concepts
(ontological pluralism -> MLO, covering axioms)



Mereotopology
(parthood, causality)

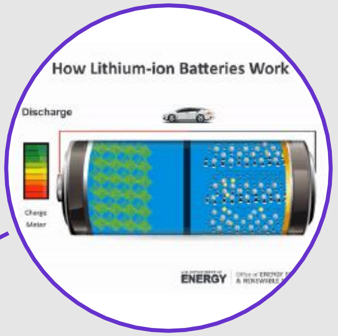
Practical Disciplines
(domain and application pluralism -> DLO, no covering axioms)

EMMO TLO and Perspectives



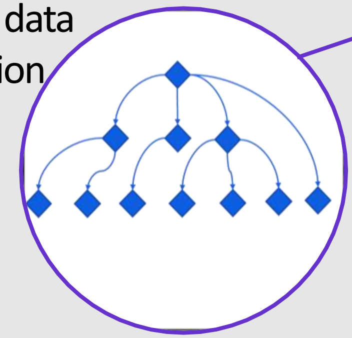
Data

- Contrasts
- Encoded data
- Information



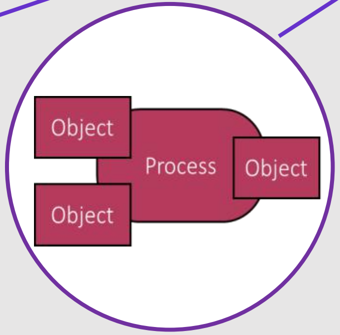
Holistic

- Whole
- Parts (roles)



Reductionistic

- Direct parthood
- Countability
- Ordering

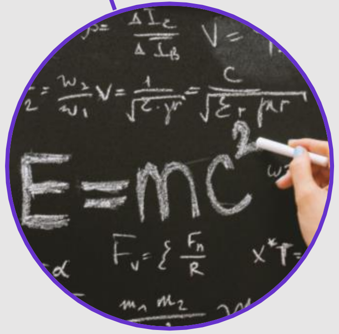


Persistence

- Process
- Objects

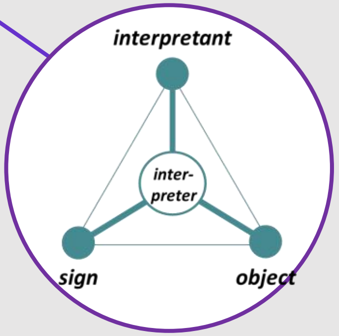
Perceptual

- Audio
- Visual
- Olfactory etc



Physicalistic

- Matter
- Field
- Material

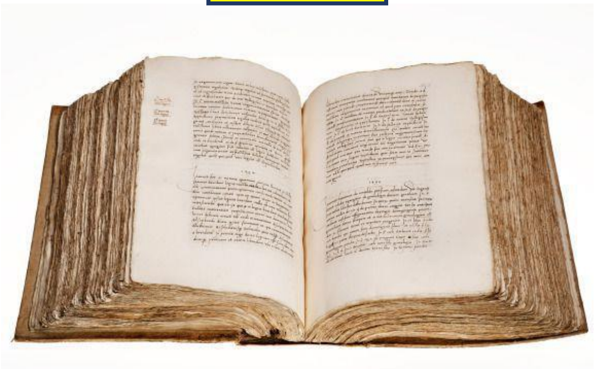


Semiotics

- Signs
- Models
- Properties

Multiperspective

Book



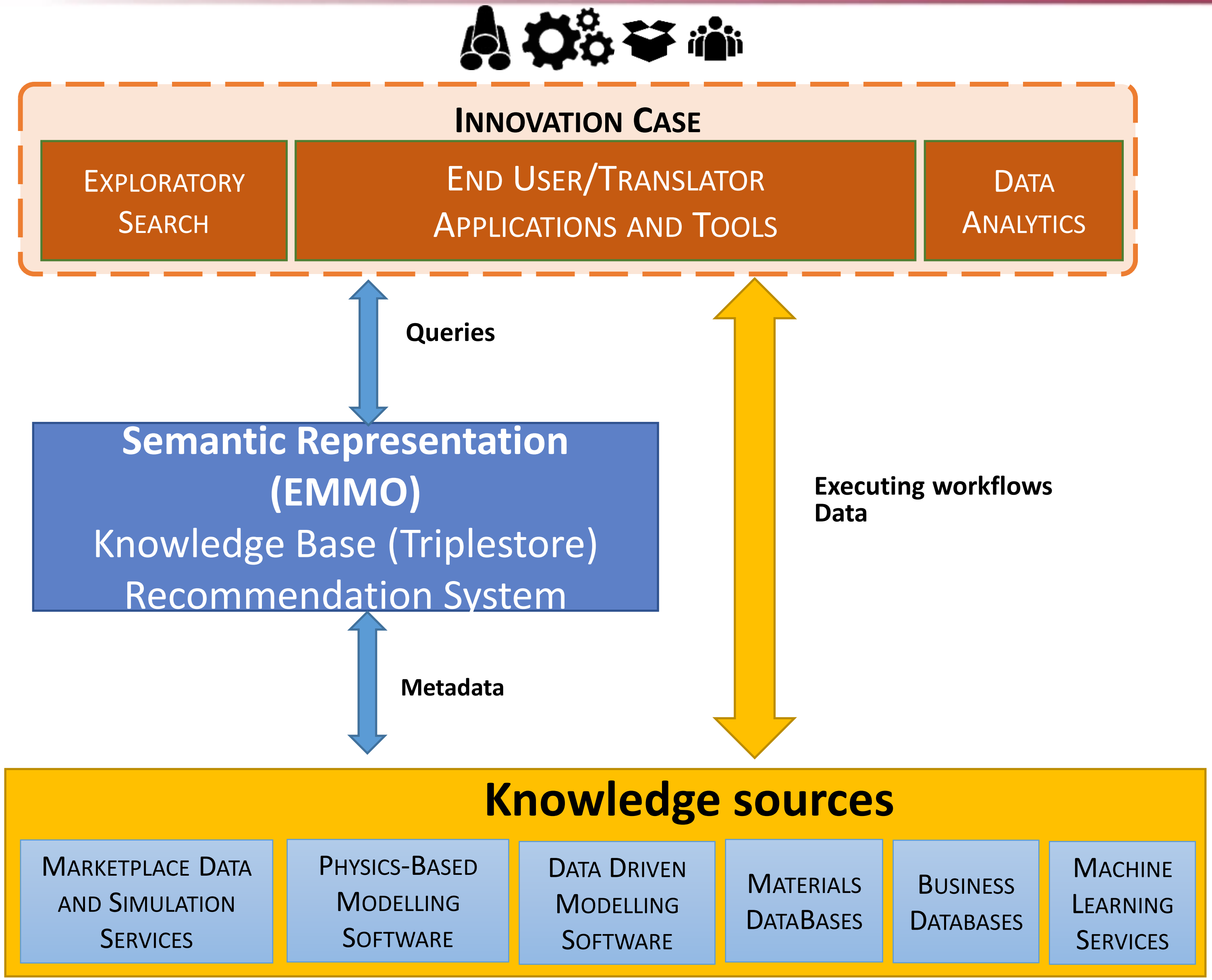
Physicalistc
A solid which is an aggregate of organic and inorganic molecules

Holistic	Persistence
A whole and an object	

Physicalistic	Reductionistic
A hierarchy of physical entities book -> pages -> paper -> fiber -> …	

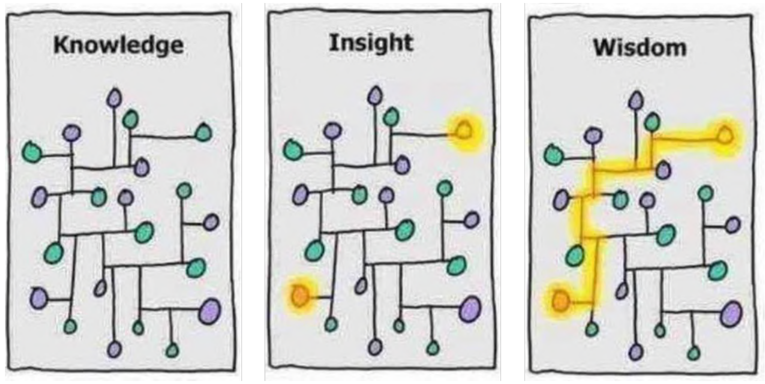
Semiotics
A sign that stands e.g. for the life of a person

Symbolic	Reductionistic
A hierarchy of book -> chapters -> paragraphs -> words -> symbols	



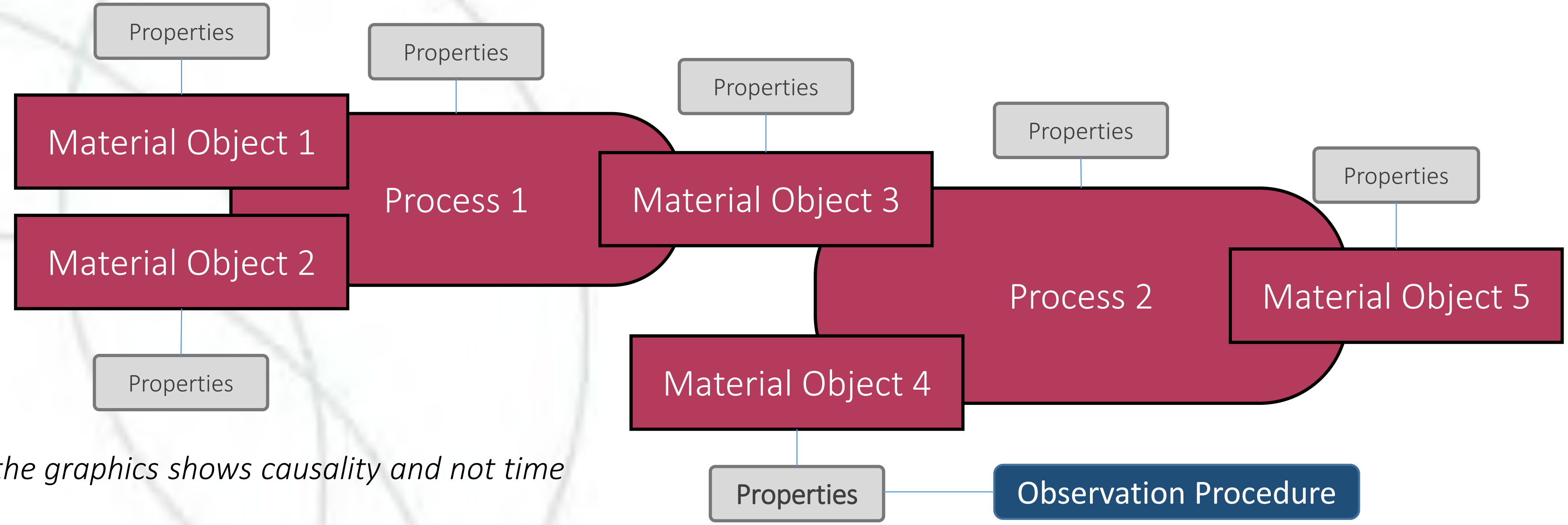
Connecting innovation case KPIs to relevant knowledge sources via:

- Formalising innovation case
- Representing in ontology
- Connections made by reasoning and knowledge graph exploration



- Providing End User Apps and Tools

Innovation Case: Causality



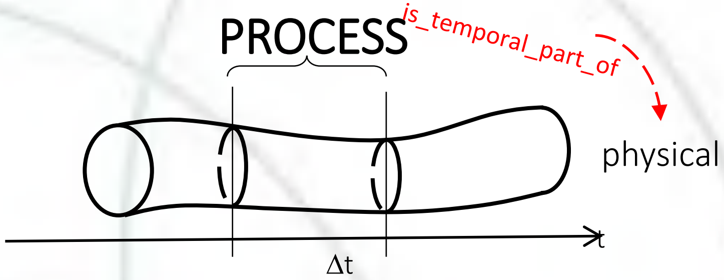
Note that the graphics shows causality and not time

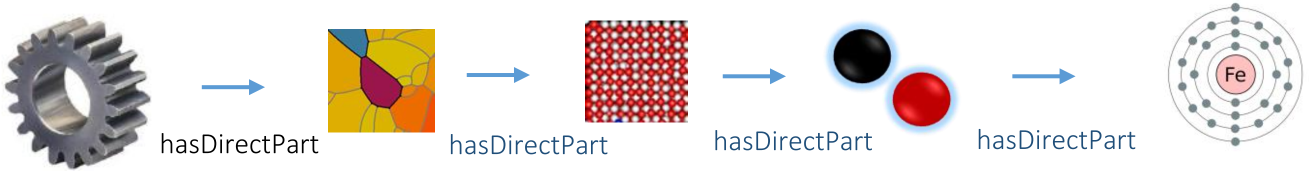
The innovation case identifying all the **entities** that play a **role,** meaning:

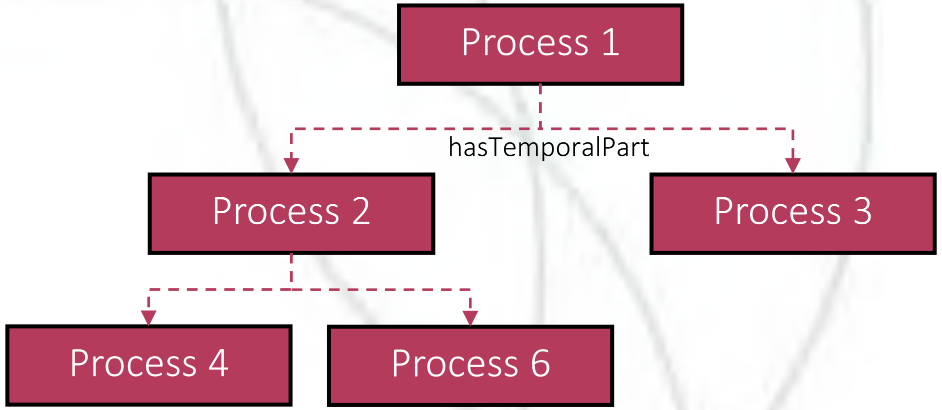
- There is some causality / interaction
- their properties/behaviour are of importance
- there are knowledge sources (data, measurement, model) for them

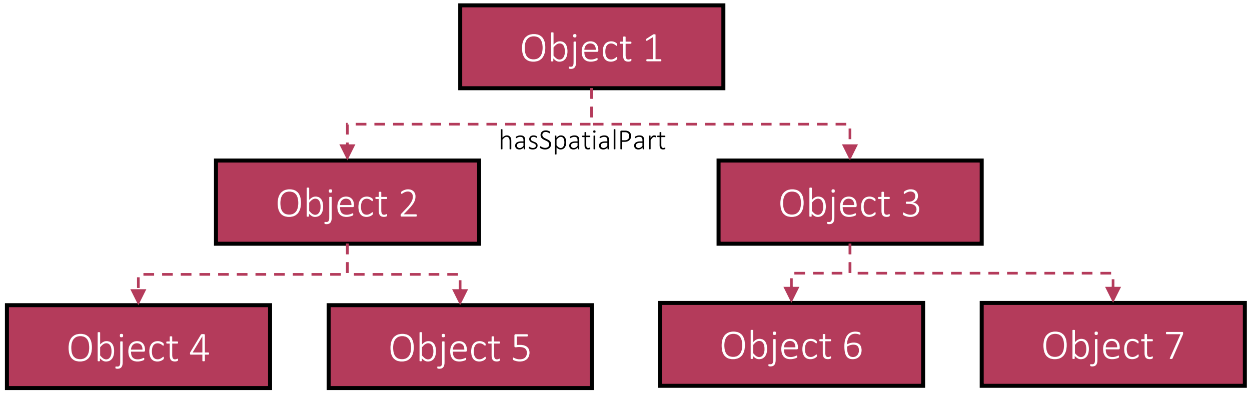
Materials and Process Entities are represented as EMMO classes

Innovation Case: Parthoods









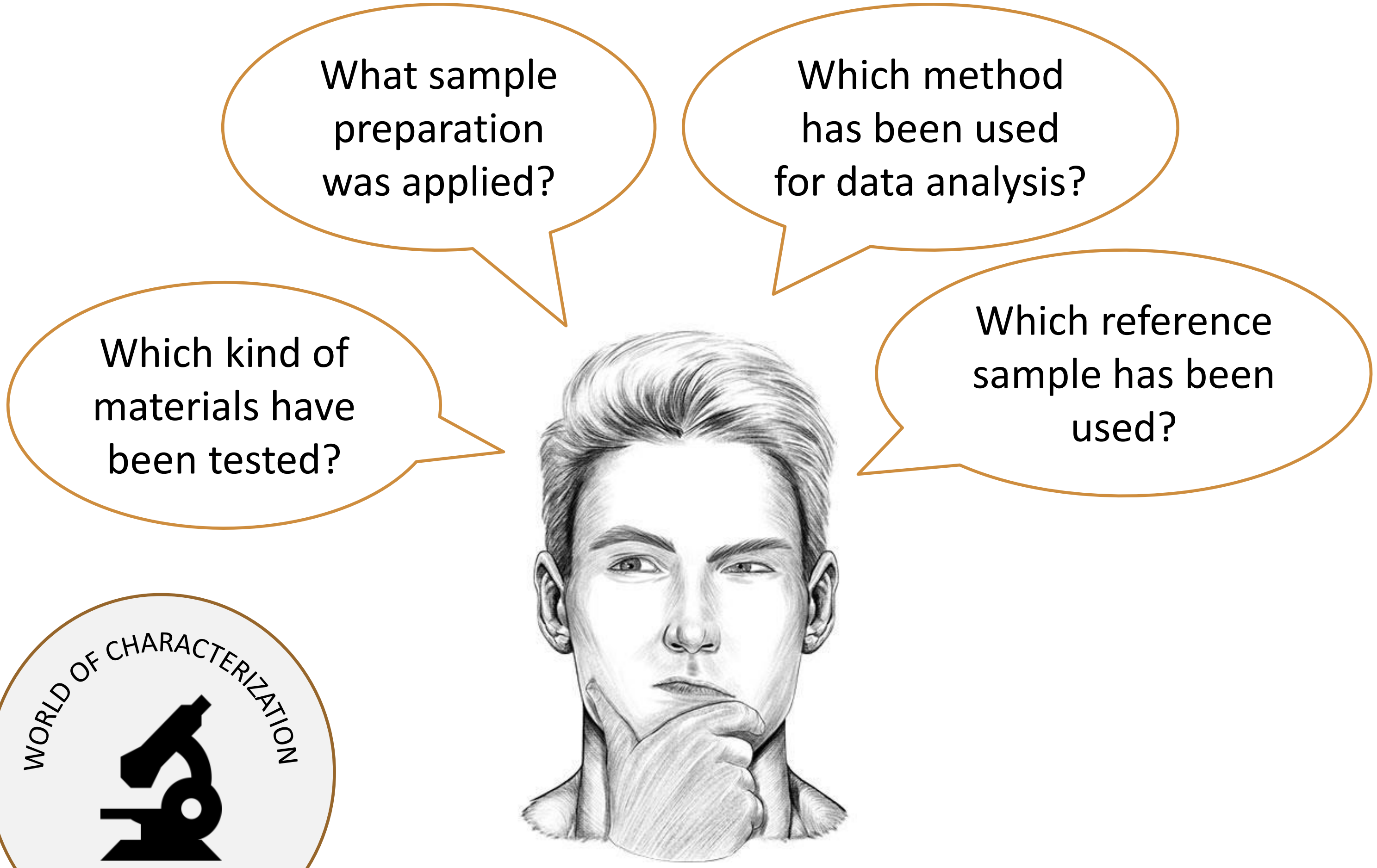
The Innovation Case may have different levels of detail, both in space and time.

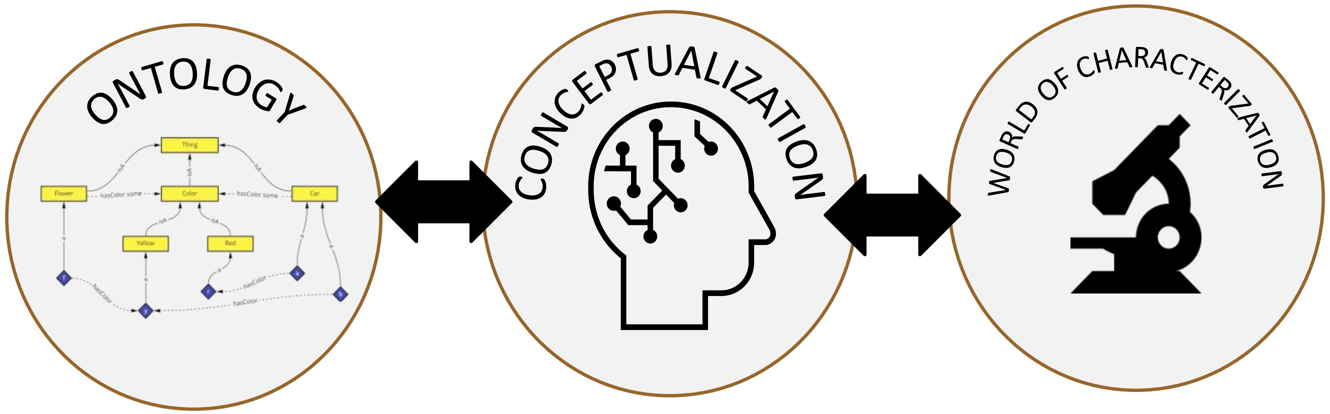
Can be expressed by means of Parthoods

OntoTrans ArcelorMittal Application Case

Characterisation Domain Ontology

- Objectives:
  1) Machine readable
  2) Interoperable
  3) Enable users to query characterisation knowledge





This project is supported by the European Union under the HORIZON2020 Framework Programme Grant Agreement no. 952869.

Mapping to EMMO Perspectives

Characterisation entities are either about

◦ Objects (e.g. instrument) and Processes (e.g. measurement)	PERSISTENCE
◦ Materials (e.g. Sample)	PHYSICALISTIC
◦ Roles (e.g. Sample holder)	HOLISTIC
◦ Properties (e.g. Environment: T,p etc)	SEMIOTIC

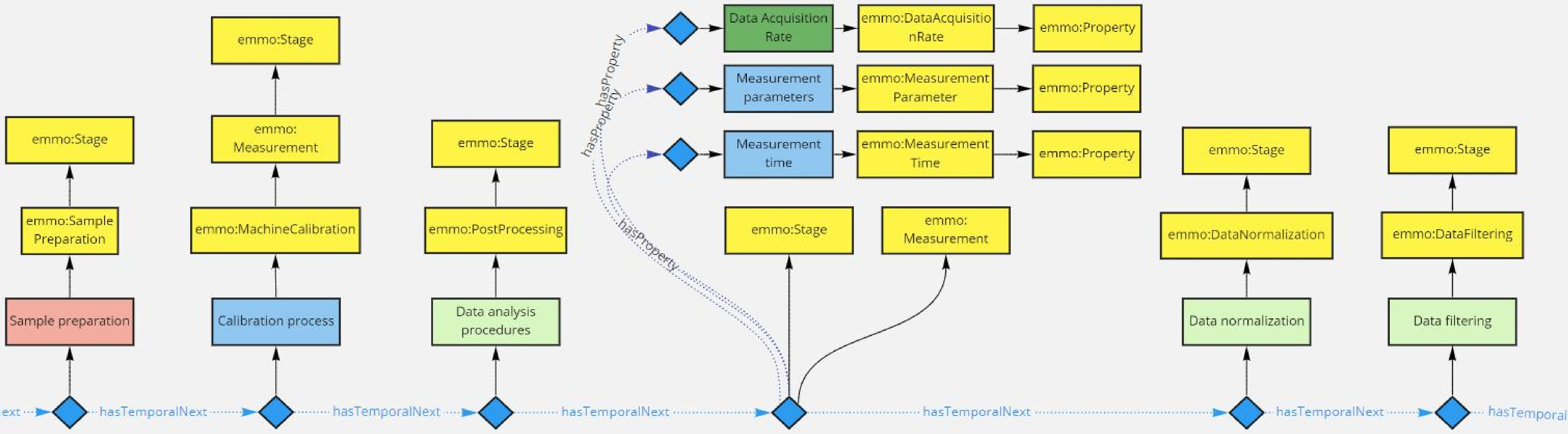
Typically **multi-perspective**

- Sample is Object and Material
- Sample holder is an Object and has a Role
- etc

This project is supported by the European Union under the HORIZON2020 Framework Programme Grant Agreement no. 952869.

CHAMEO ontology

(Some) stages of the characterisation



https://github.com/emmo-repo/domain-characterisation-methodology

This project is supported by the European Union under the HORIZON2020 Framework Programme Grant Agreement no. 952869.

Conclusions

EMMO is about **Pluralistic Parallelism** (represent things in many different and coexisting ways) instead of **Serial Stratification** (things are represented in a one and one only way).

The focus for EMMO development is on **capturing the multiple** ways in which a real world object is expressed by communities.

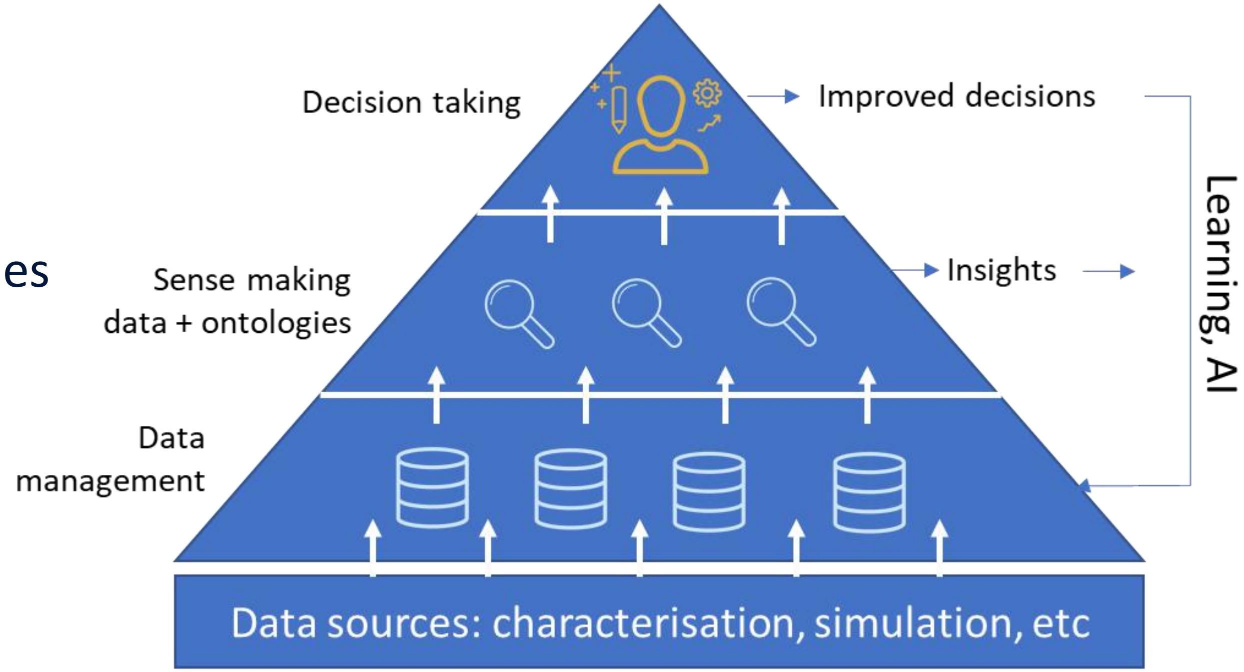
Conclusion: Embrace complexity

The **importance** of a **semantic approach to knowledge** is that is provides **a new language**, **digitally and machine friendly**, that can **push for the transition towards Industry 5.0**.

- Bottleneck: **compartmentalized human approach to knowledge**.
- **Need to embrace and manage complexity, and not to fight it**
- **Ontologies** are a field in which **multidisciplinary is acting at its best**: can be **catalyst toward multidisciplinarity**.

Towards accelerated materials design and development

- **Data/knowledge generators**
  - Materials models (physics and data-based)
  - Characterisation, sensing
- **Data management and Knowledge capture**
  - Eco-system of interconnected, managed ontologies
  - FAIR data supported by ontologies
- **Multiply knowledge generation**
  - AI boosted by ontologies
    (AI with a 'helping hand' is much more powerful)
- **Knowledge interrogators**
  - Multi-perspective, multi-role views on complex information:
  - Support complex assessment of materials options regarding the ever increasing range of criteria



Materials 2030 Roadmap Draft

https://materialsmodelling.com/materials-2030-roadmap-draft-published/

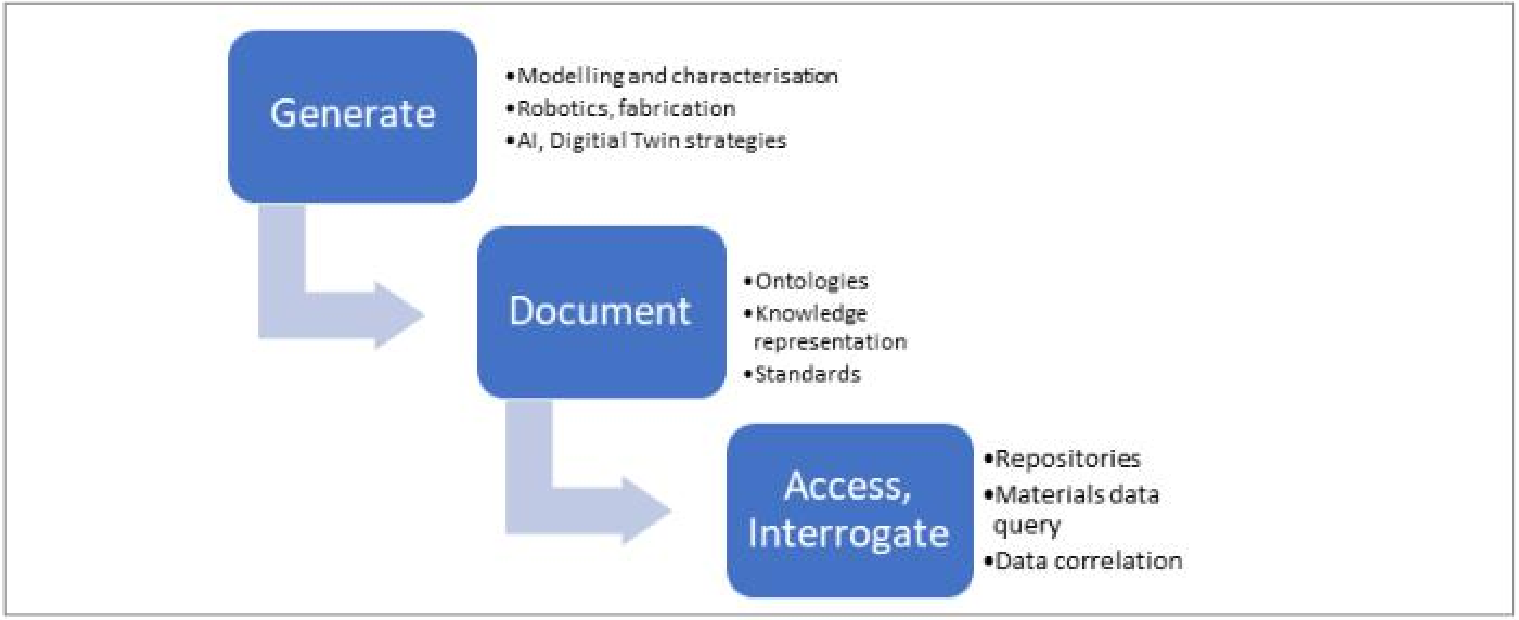


Figure 3: *Three priorities to achieve the data-driven development of advanced materials*

Generating new data and knowledge to process and scale up materials solutions

ONTO COMMONS
ONTOLOGY-DRIVEN DATA DOCUMENTATION FOR INDUSTRY COMMONS

Join OntoCommons

Cooperation

Top Reference Ontology

Industrial Domain Ontologies

Ontology Commons Ecosystem Toolkit

Demonstration

Standardisation

Infrastructures

Please register and fill in the expert survey on

ontocommons.eu

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OntoCommons “Ontology-driven data documentation for Industry Commons” has received funding from the European Union’s Horizon Programme call H2020 -NMBP-TO-IND-2020-singlestage, Grant Agreement number 862136

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