Platform MaterialDigital Core Ontology

an Ontological Framework for Materials Science & Engineering

Agenda

09:00 – 10:30 **Block 1 - Semantic Interoperability & PMDco Basics**

Brief Introduction to Ontologies

Break (15min)

Intented for

- 1st contact with Ontology
- MSE Actors

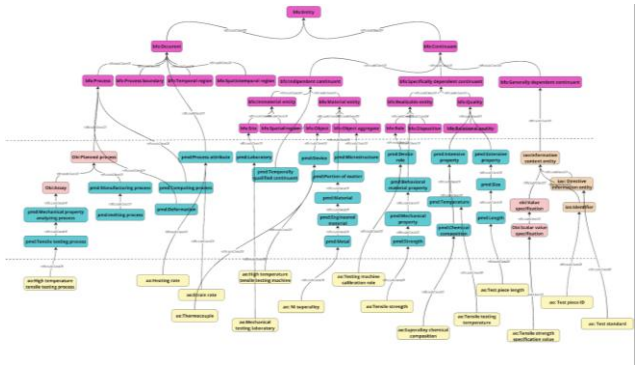
10:45 – 11:45 **Intro. to Platform Material Digital Core Ontology (PMDco)**

11:45 – 12:15 **Q&A**

Lunch Break (45min)

13:00 – 14:30 **Block 2 - Hands-on PMDco Workshop**

Hands-on Session



14:30 – 15:00 **Wrap-up & Feedback**

- Q&A

Intented for

- MSE Actors
- Potential PMDco User

Who I am?

2001 – 2006: B.Sc. MSE - Industrial **Metallurgy** @Sharif Uni.Tech.

2007 – 2009: M.Sc. MSE - Applied **Polymer** Science @Martin Luther Uni.

2010 – 2014: Dr.-Ing. MSE - **Biomaterials** @MPIKG @TU Berlin @ ETH

2014 – 2023: R&E **Interdisciplinary Materials-X** @Exc.Cluster MoA @HU Berlin @MPIKG)

Materials **Philosophy** - Materials **Design** - Materials **Sustainability**

2025 – now : R&D MSE - Materials **Ontology** @Platform Material Digital @BAM

Dr.-Ing. Khashayar Razghandi

PMDco - walkthrough

PMDco Intro.

20 min

- **PMDco** as an “anchor” mid-level Ontology, supporting Semantic Interoperability in MSE
- PMDco structure; modules; classes; properties etc.

PMDco Tools-scape

15 min

- **GitHub** – as a Collaboration tool; PMDco Repositories
- **Protégé** – open-source Ontology Editor
- **ODK** – Ontology Developement Kit

PMDco Potentials

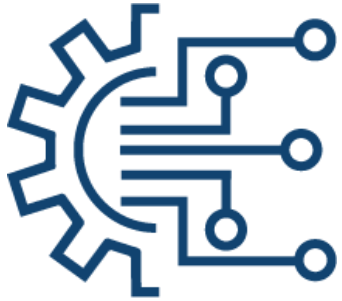
10 min

- **Reuse**: PMDco-anchored Application/Domain ontologies
- **Integration**: PMDco uptake in Industry & Academia

PMDco Processes

10 min

- **Development Process** - How we work as a community
- **Community Channels** - How to engage with the community



Our **ongoing goal** is to **establish data structuring standards** & **agreements** that **facilitate technological semantic interoperability** of (meta)data and services among all stakeholders in **Material Science & Engineering**, in alignment with **FAIR data principles**.

To achieve this, prototype **ontologies** are **created**, **continuously enhanced**, and **shared in repositories**, with **ongoing engagement** & **collaboration** within the **community**.

an **Ontology**

interpretable by machines

consensus

is an **explicit**, **formal** **specification** of **shared** **conceptualisation** and **their relationships** that describe a domain in a consistent, machine-interpretable way.

meaning of all terms is clearly & unambiguously defined

abstract model (domain, relevant terms, relations)

Platform MaterialDigital Core Ontology (PMDco)

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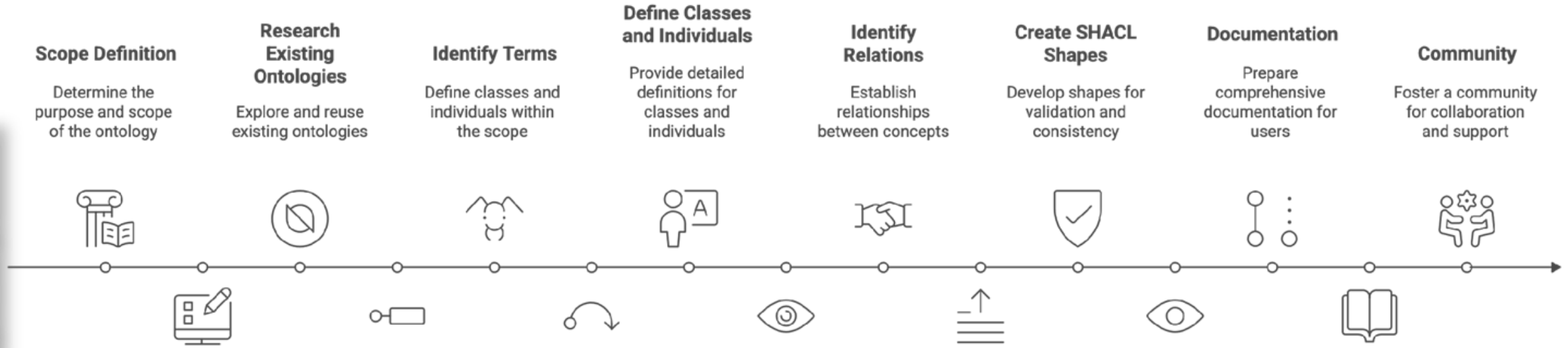

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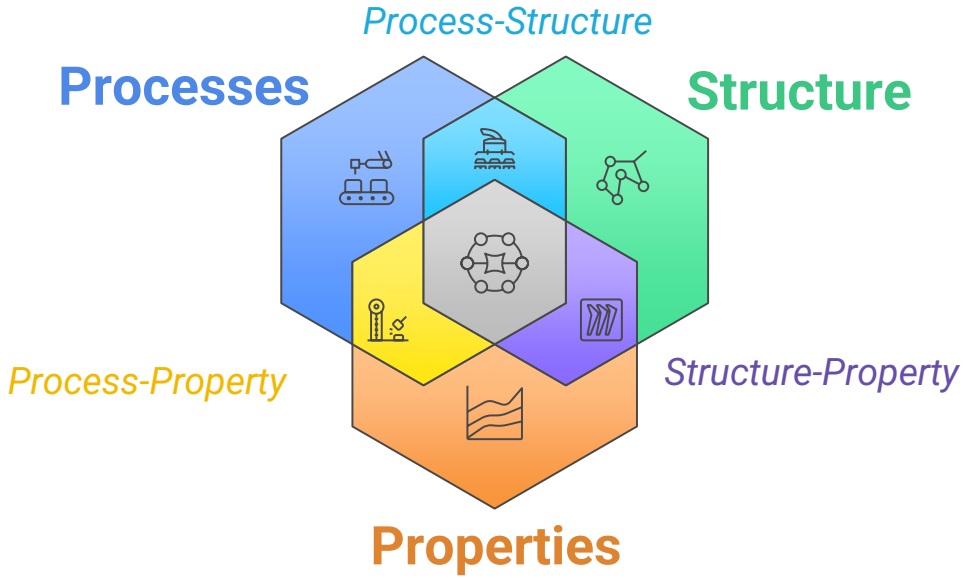
Material Science & Engineering

ontologies provide a common framework for materials, processes, structures, properties, and data, enabling information to be organized, linked, and reused across tools, experiments, workflows & actors.



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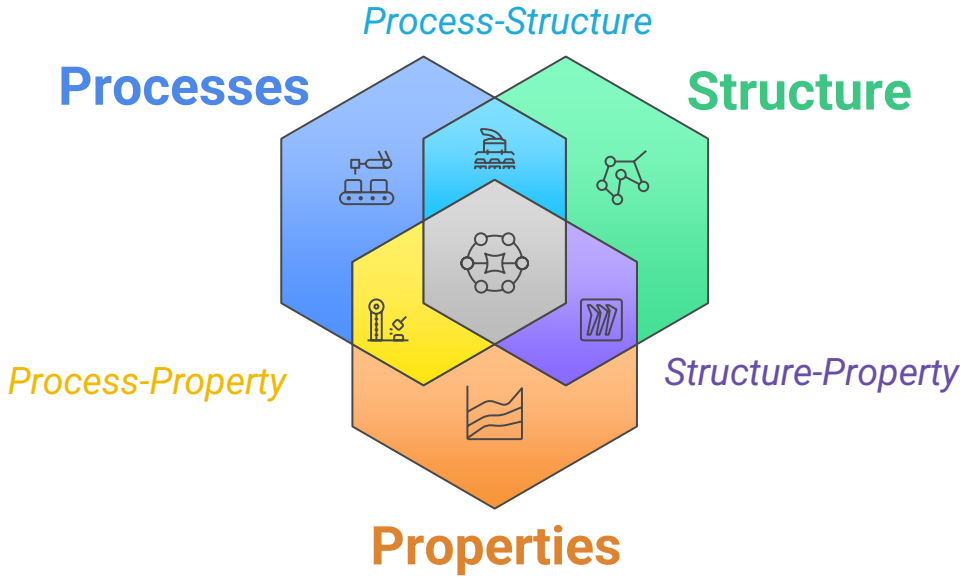
Material Science & Engineering

- Achieve **interoperable** materials and processes data
- Traceability of (meta-)data **across the value chain**
- Support **FAIR** data principles for reproducibility & reliable **reuse**

Findability
Accessibility
Interoperability
Reusability



Semantic Interoperability

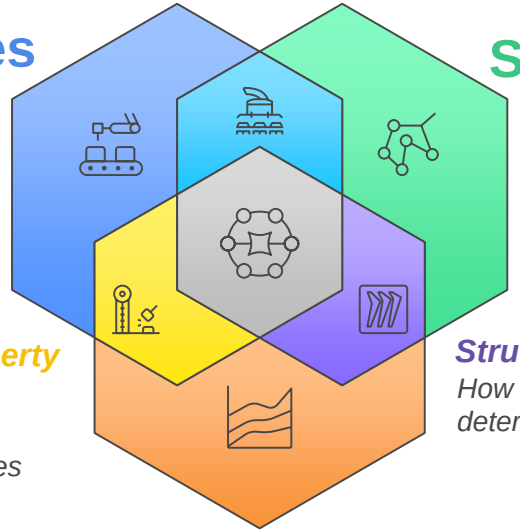
Materials Science & Engineering

across the value chain

Process-Structure
How processes influence material structure

Processes
Materials Manufacturing and simulation

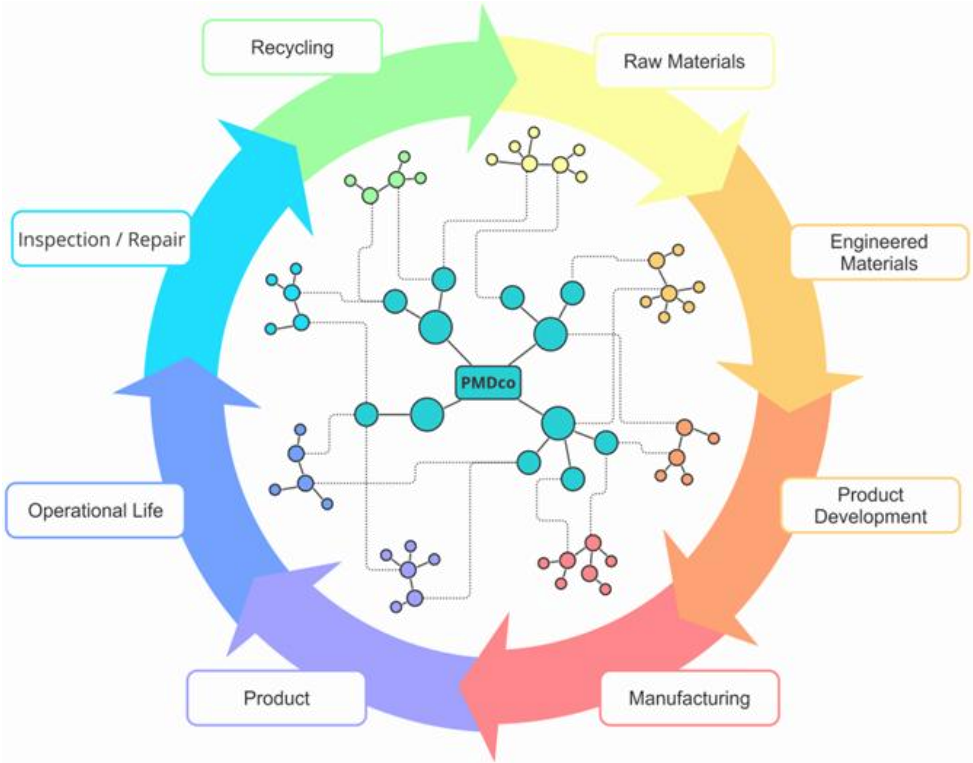
Structure
Material composition and features



Process-Property
How processes influence material properties

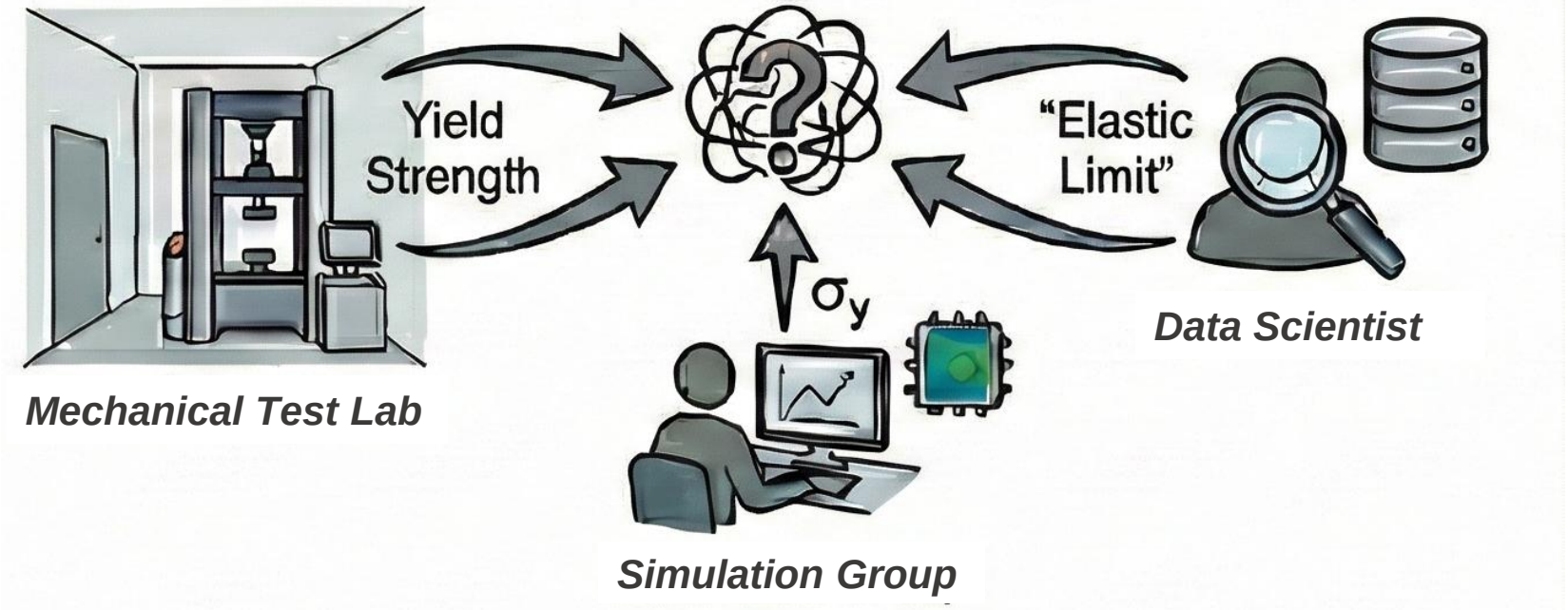
Structure-Property
How material structure determines behavior

Properties
Material qualities and behaviors



Semantic Ambiguity

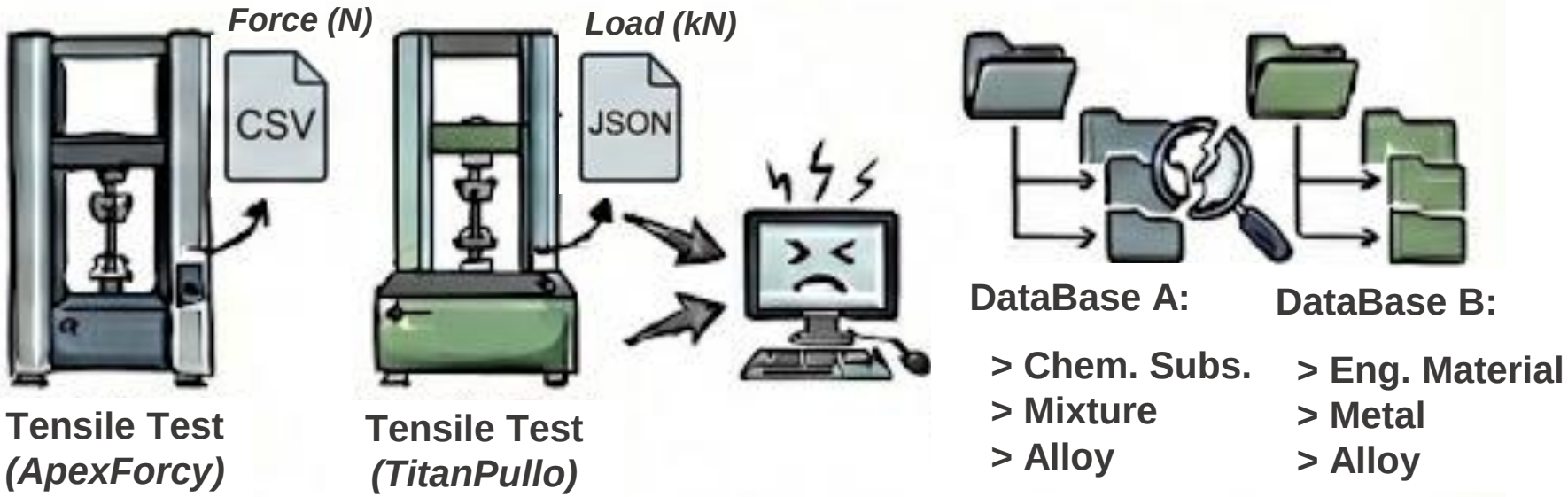
Semantic Interoperability



- Ambiguity in the **diverse nomenclature of concepts** in Materials Science & Engineering

Semantic Ambiguity

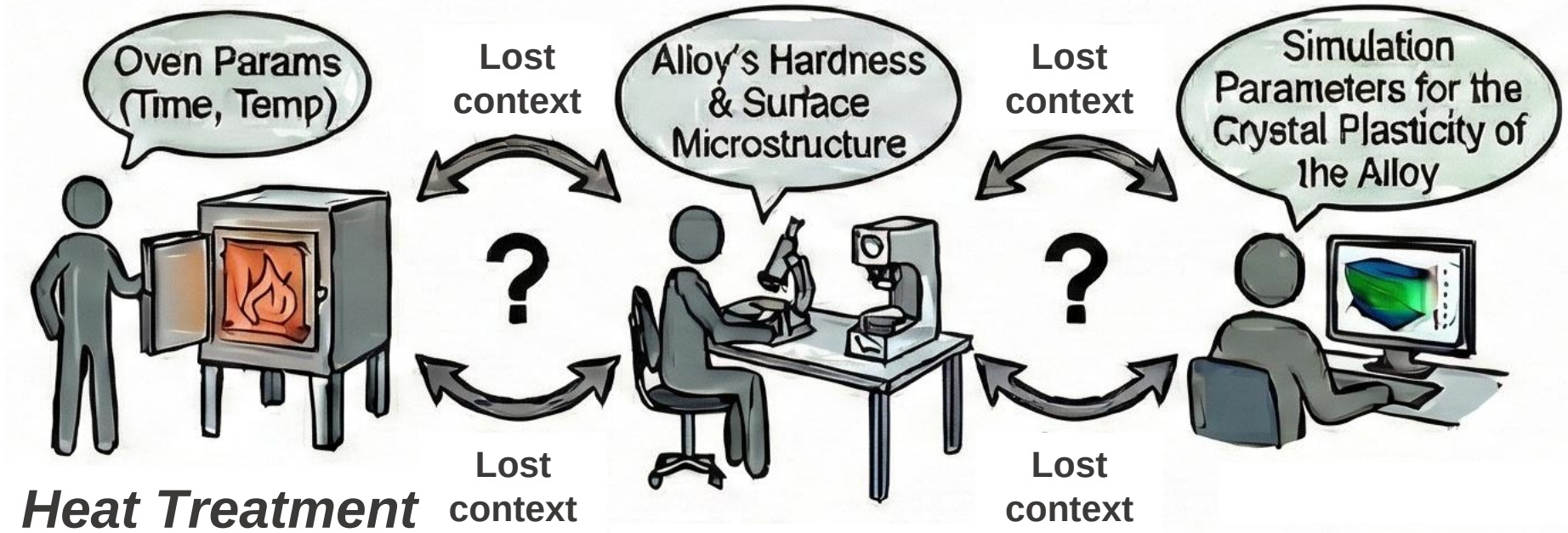
Semantic Interoperability



- Ambiguity from inconsistent **outputs, labeling, units, database categorization etc.**

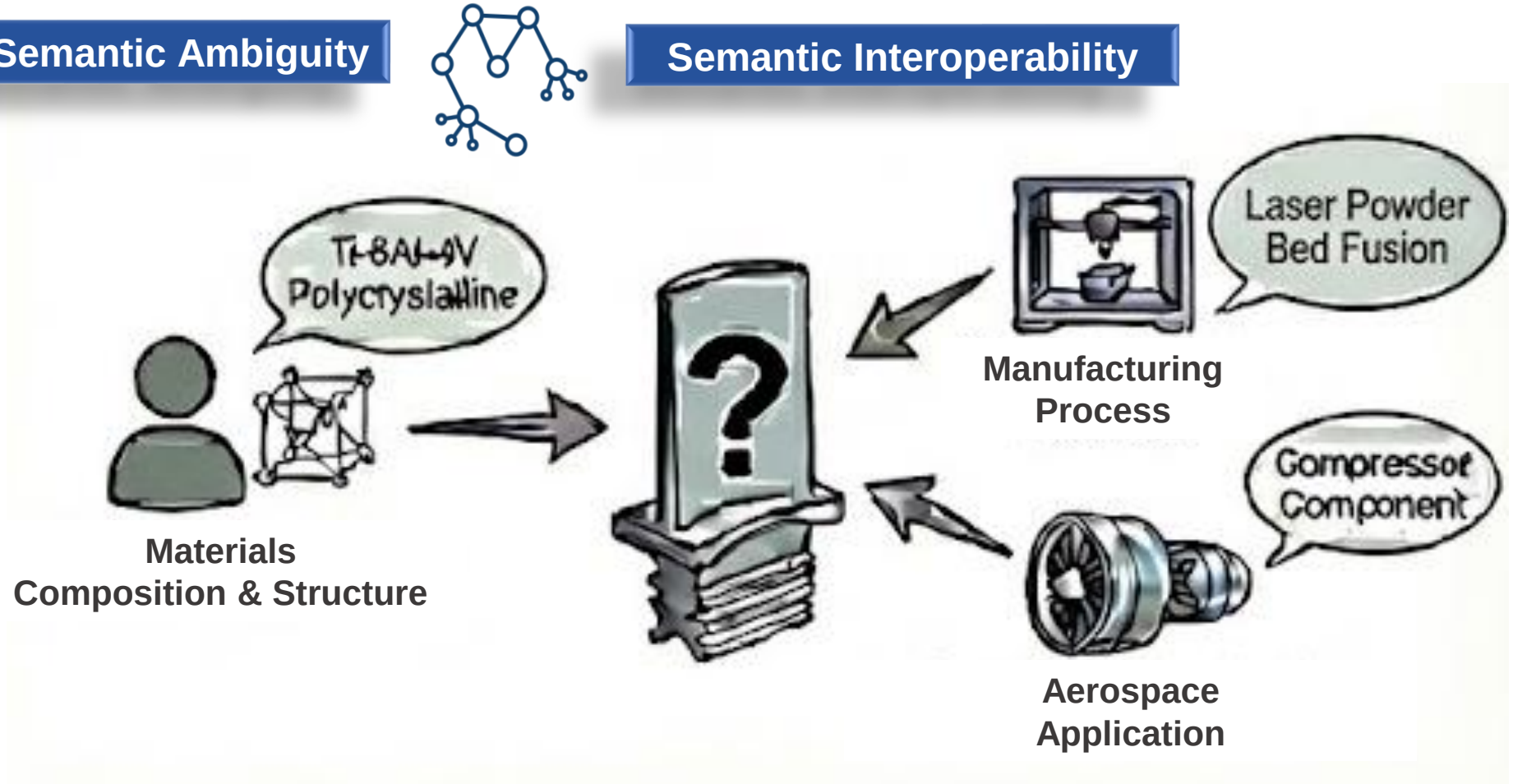
Semantic Ambiguity

Semantic Interoperability



- Ambiguity from the **diversity of interests & focus of different Actors** around the same process.

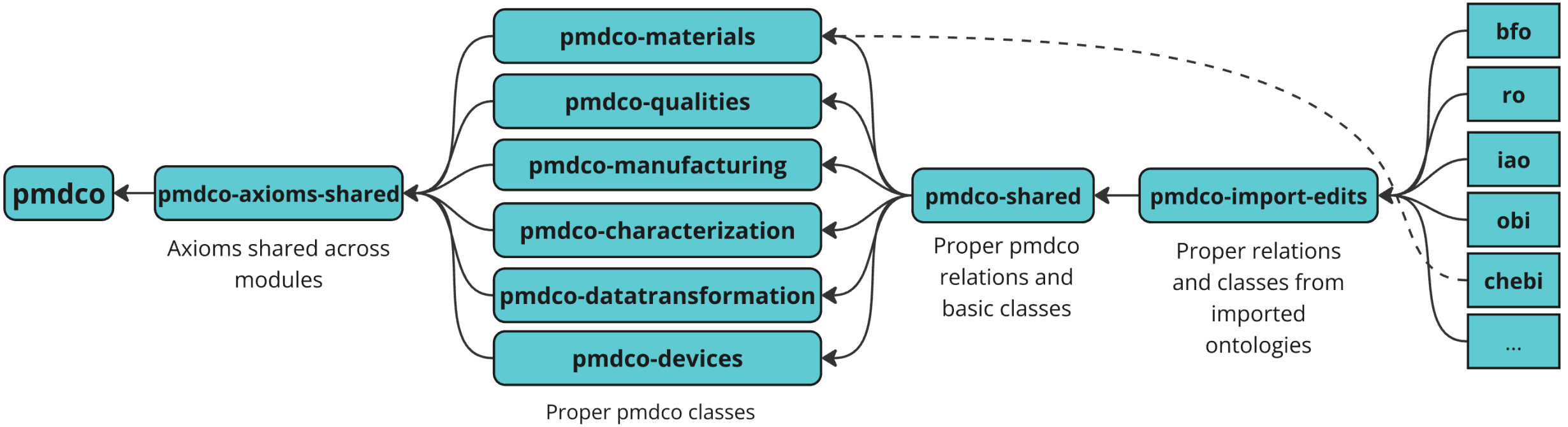
Semantic Ambiguity **Semantic Interoperability**



- Ambiguity from the **diversity of perspectives throughout the Value Chain**

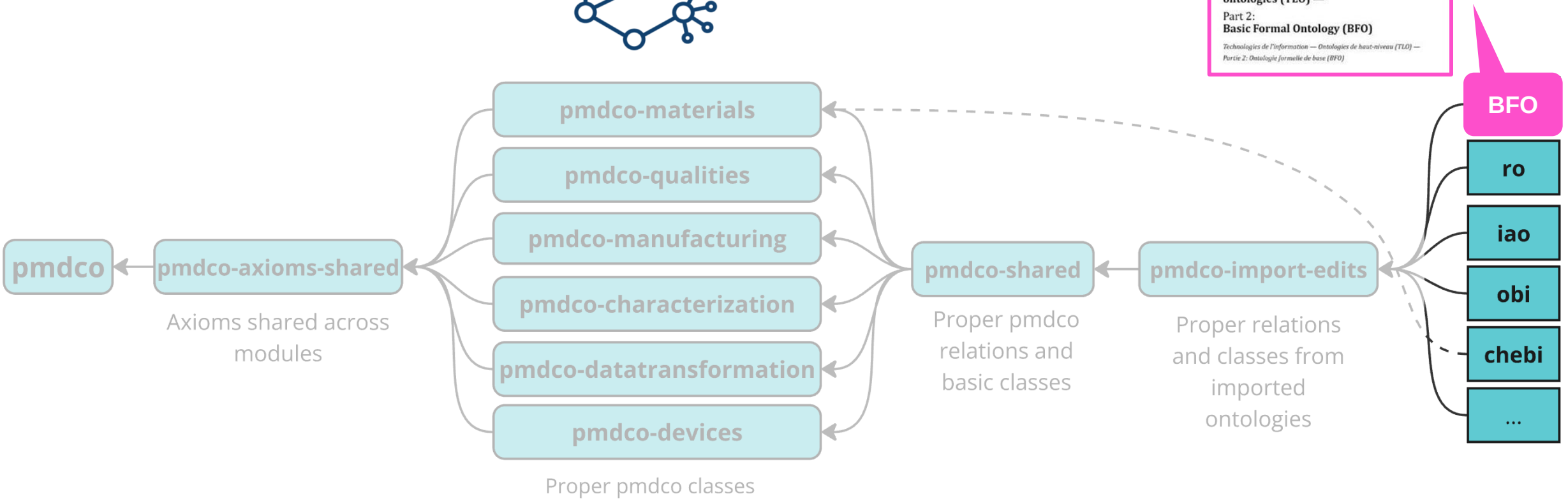
*"… in the **Platform MaterialDigital**, **MSE ontologies** are created, continuously enhanced, and shared in public repositories, with ongoing engagement within the community… "*

How… !?

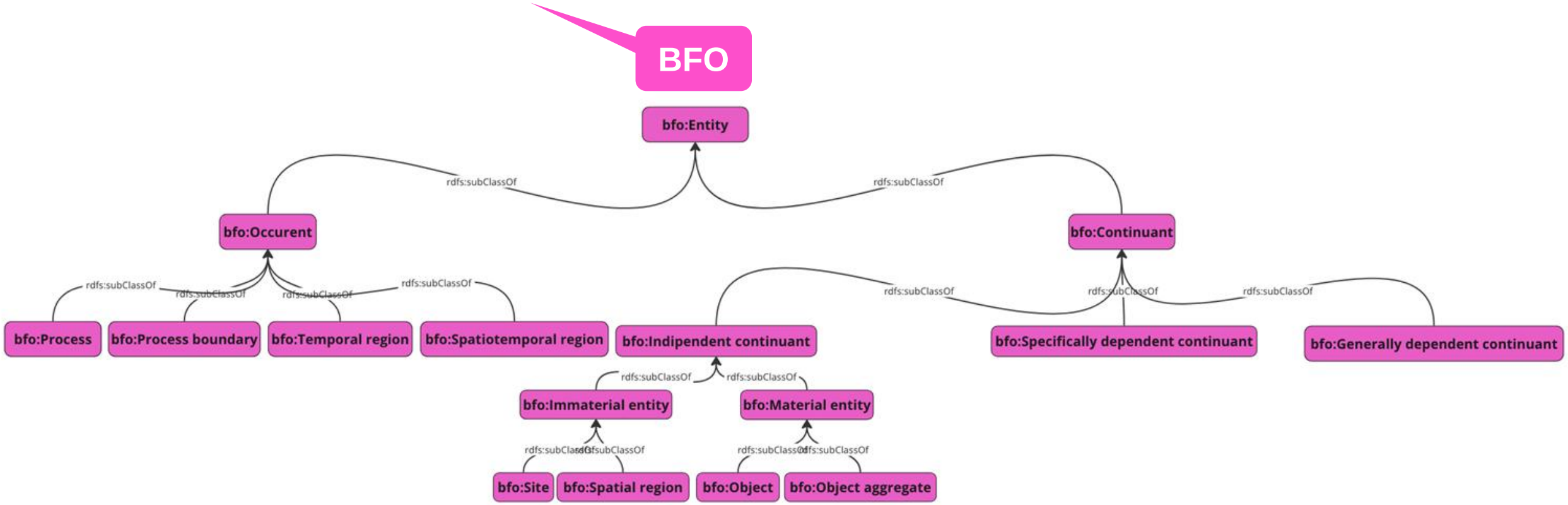


PMDco v3.0 mid-level core ontology anchored to the **Basic Fromal Ontology (BFO 2020 Standards)**


INTERNATIONAL STANDARD
ISO/IEC 21838-2
First edition 2021-11
ISO IEC
Information technology — Top-level ontologies (TLO) —
Part 2:
Basic Formal Ontology (BFO)
Technologies de l'information — Ontologies de haut-niveau (TLO) —
Partie 2: Ontologie formelle de base (BFO)



Basic Fromal Ontology at the Top as a domain-neutral upper ontology



Basic Fromal Ontology at the Top as a domain-neutral upper ontology

Top-Level
Ontology

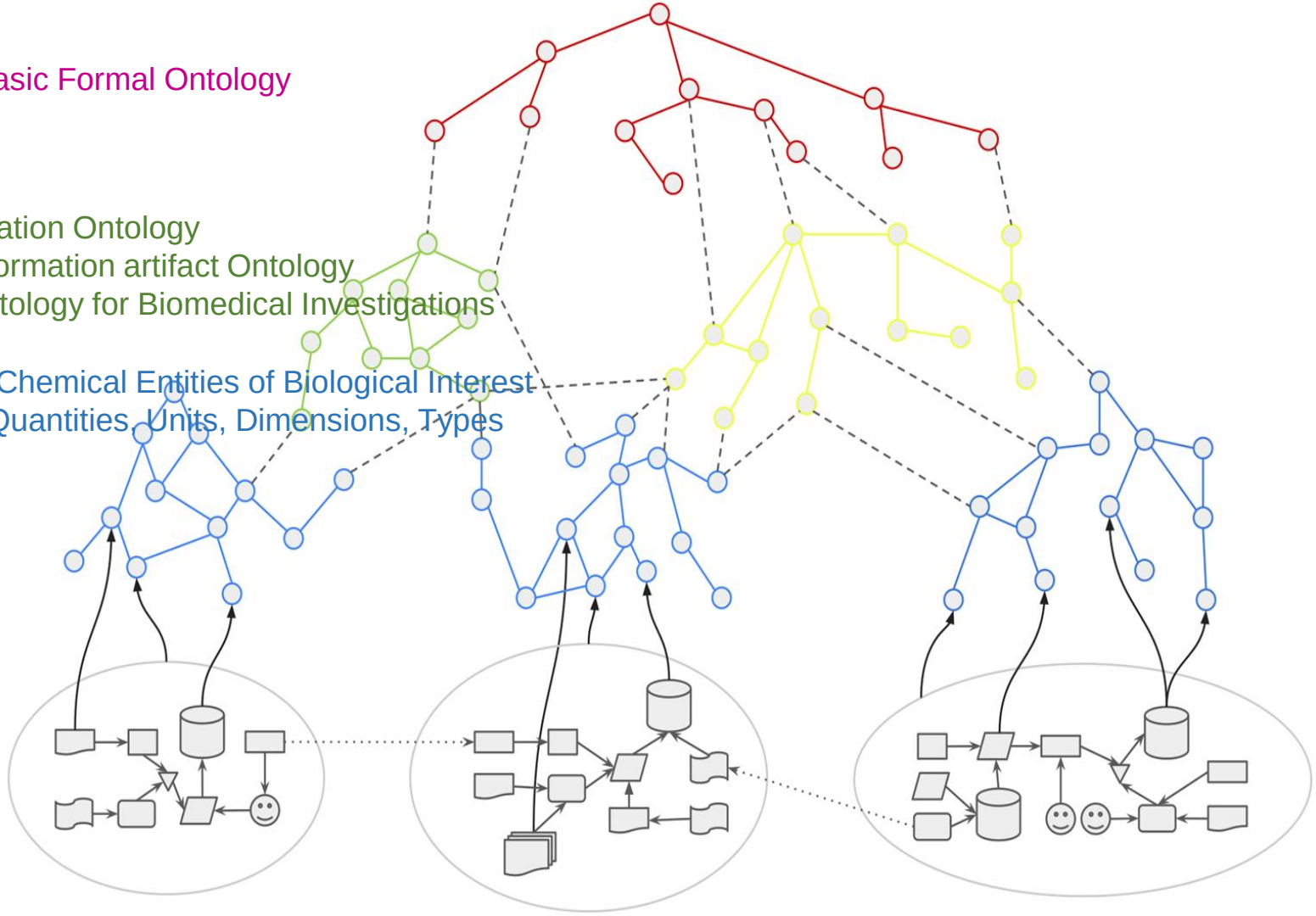
BFO - Basic Formal Ontology

Mid-Level
Ontology

RO - Relation Ontology
IAO - Information artifact Ontology
OBI - Ontology for Biomedical Investigations

Domain / Application
Ontology

CHEBI - Chemical Entities of Biological Interest
QUDT - Quantities, Units, Dimensions, Types



Domains:
Raw-Data, Processes, Processed Data

PMDco v3.0 mid-level Core Ontology

Top-Level
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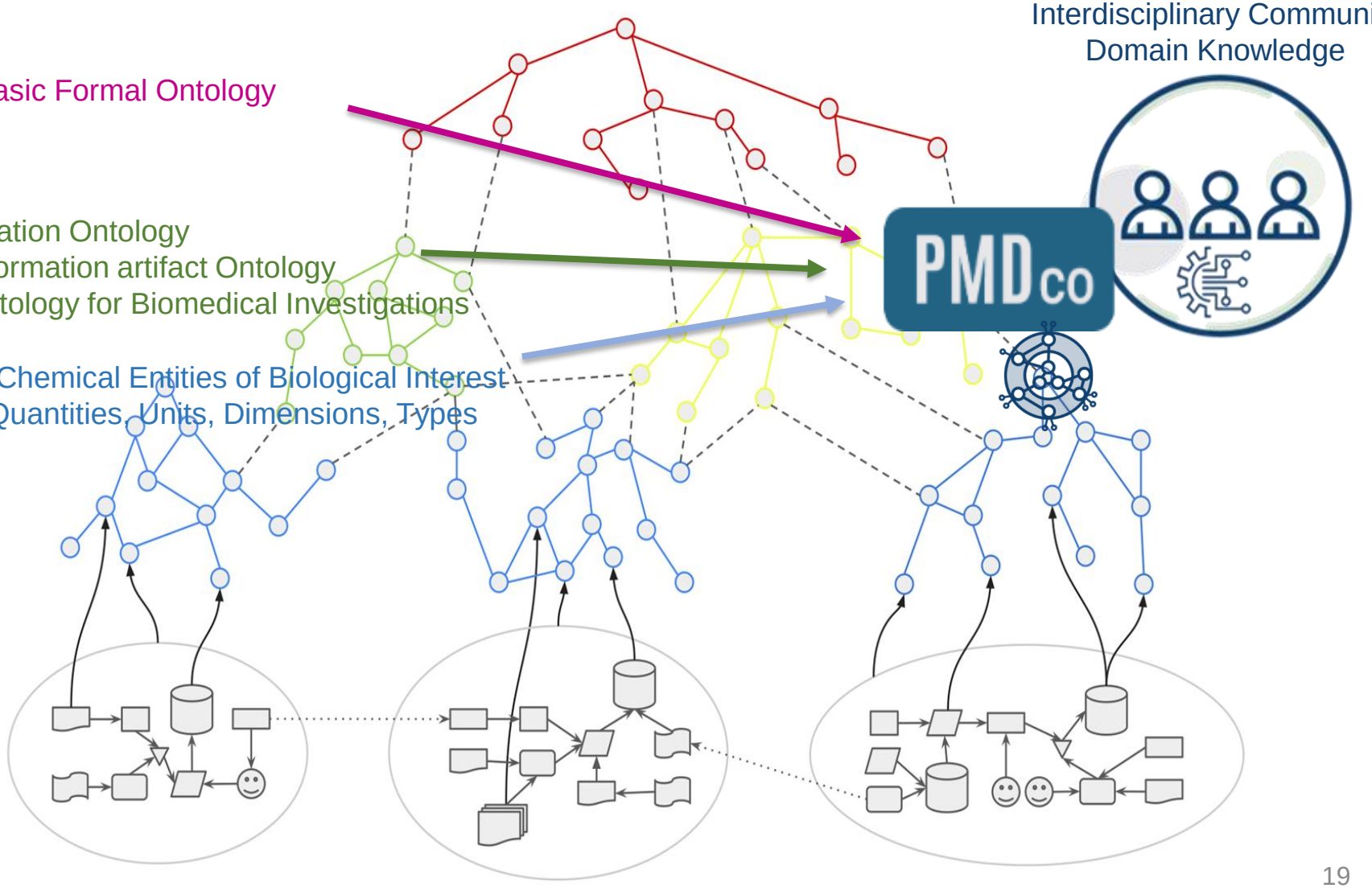

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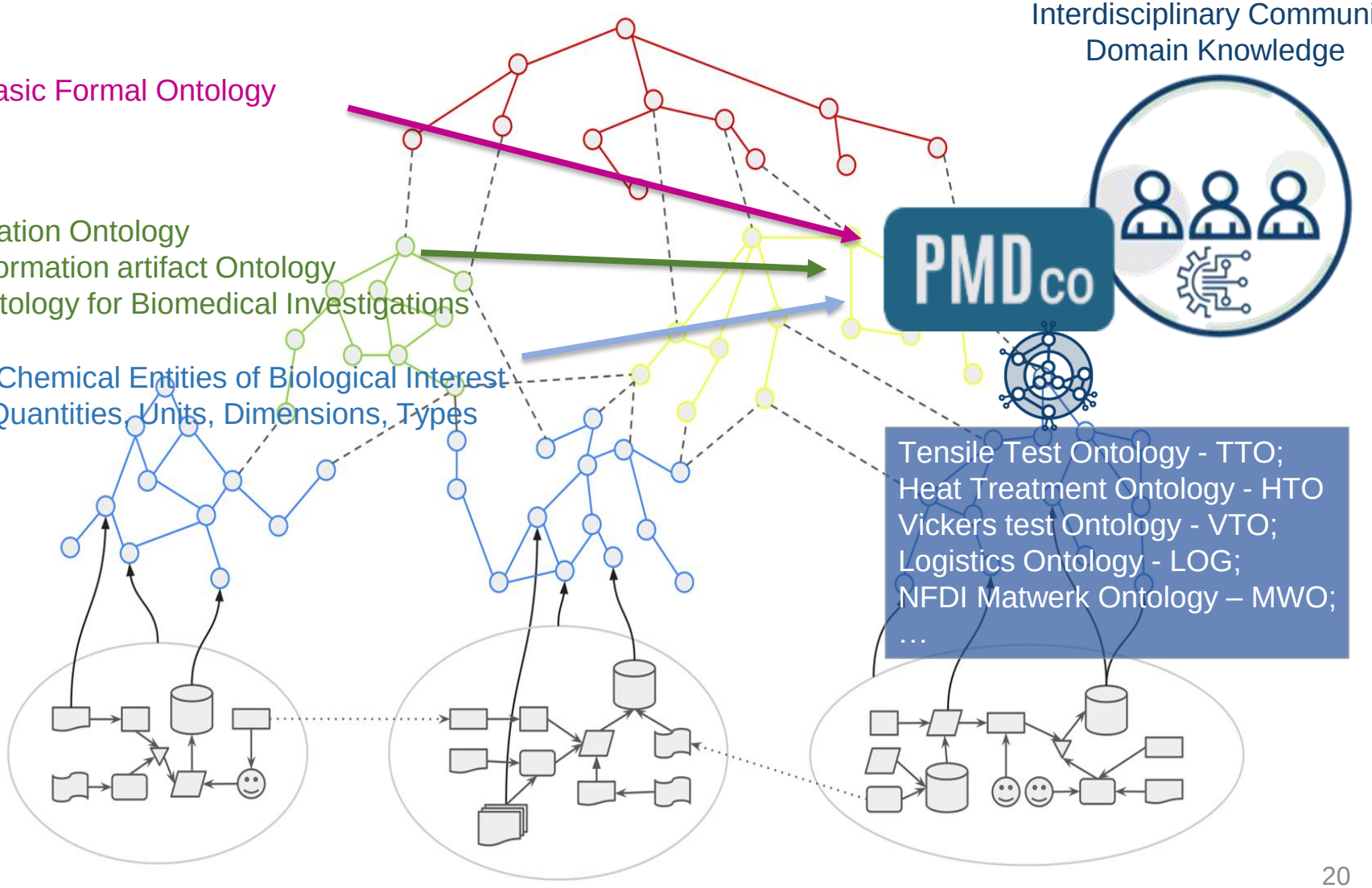

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Top-Level Ontology

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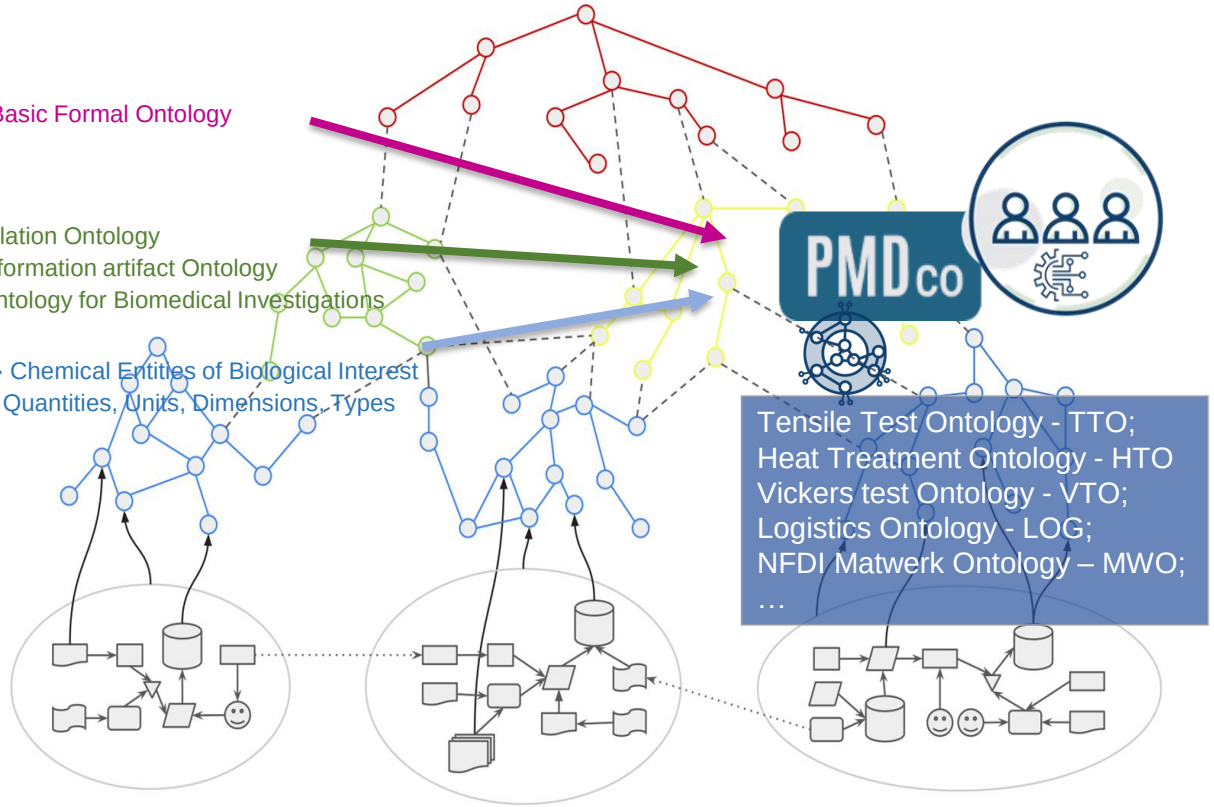
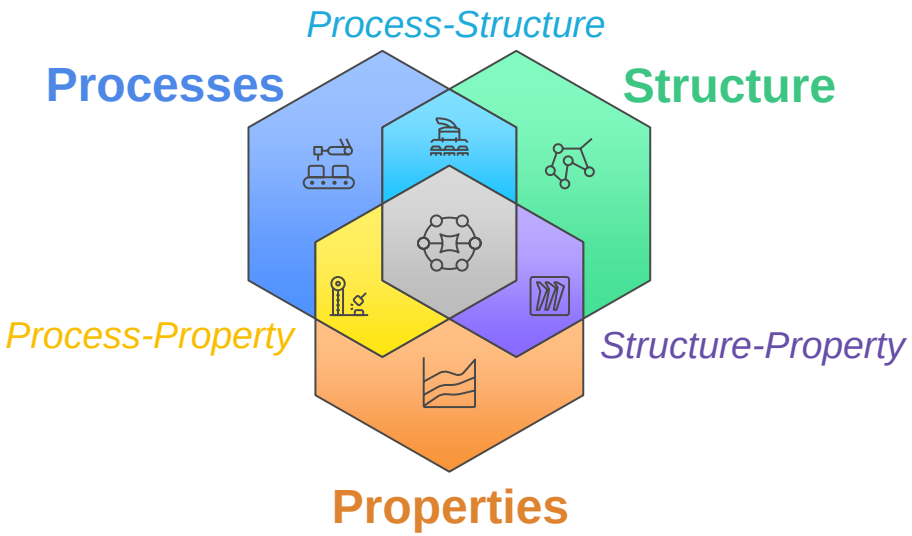
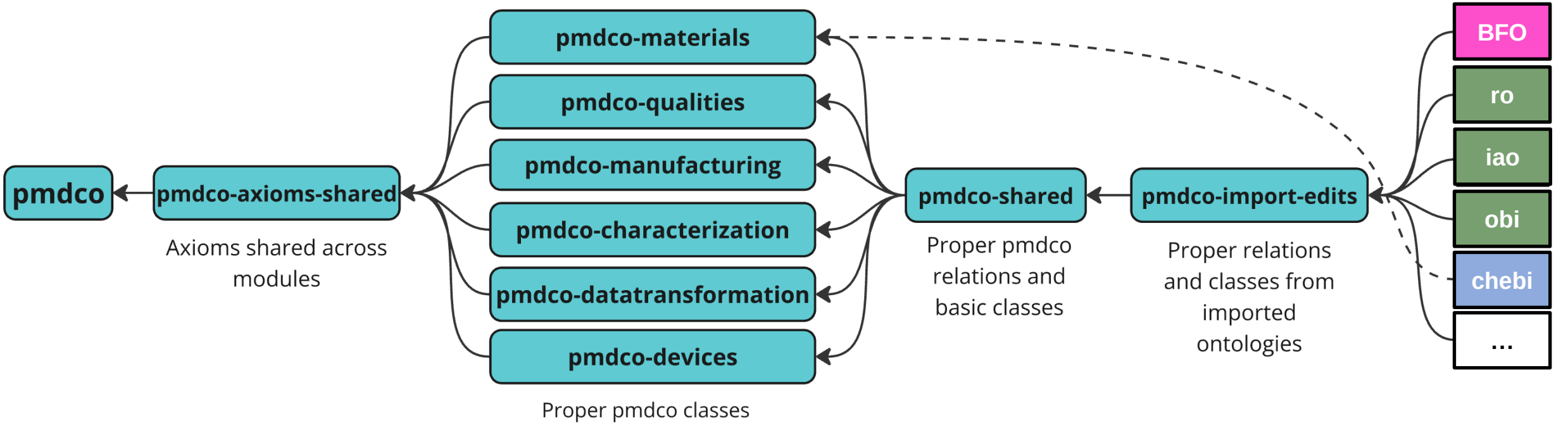




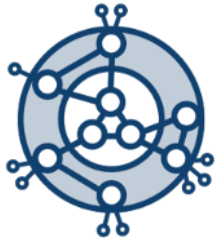
PMDco as an "Anchor" mid-level Ontology… **… supporting Semantic Interoperability in MSE**

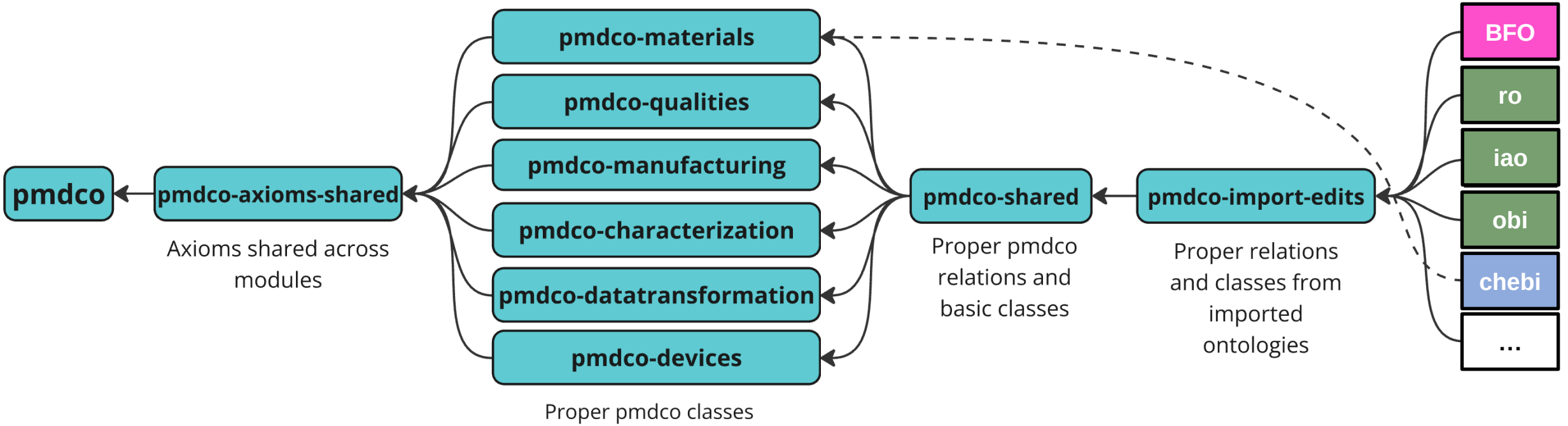
PMDco v3.0 mid-level core ontology



PMDco v3.0 mid-level core ontology

Modularized… facilitates scalable expansion of the ontology

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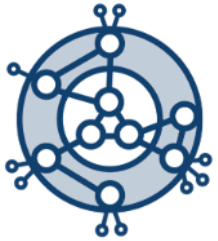

- **Self-Contained Subdomains:** PMDco is divided into **six core modules** for Materials Science and Engineering.
- **Distributed Engineering:** Modularization allows different parts of the ontology to be developed, maintained & evolved independently without affecting the rest.
- **Efficient Reasoning & Querying:** breaking the ontology into coherent fragments, allows faster logic-based reasoning & more tractable data query.
- **Automated Maintenance via ODK (Ontology Development Kit):** Specialized modules handle external terms and logical rules automatically, ensuring consistency.
- **Interoperable Building Blocks:** They serve as reusable "fragments," allowing PMDco to easily integrate with other digital materials tools and global standards.

- pmdco-materials
- pmdco-qualities
- pmdco-manufacturing
- pmdco-characterization
- pmdco-datatransformation
- pmdco-devices

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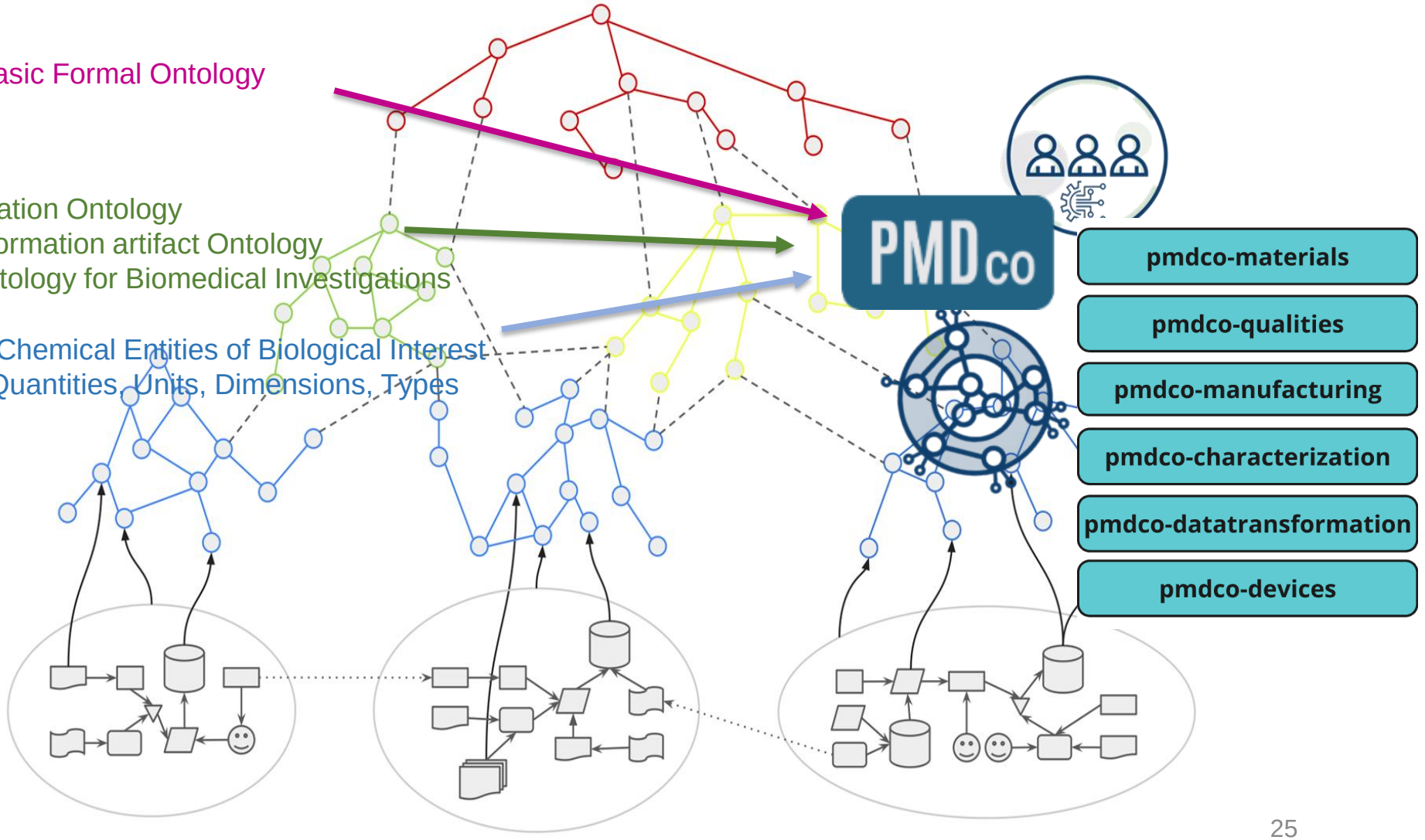

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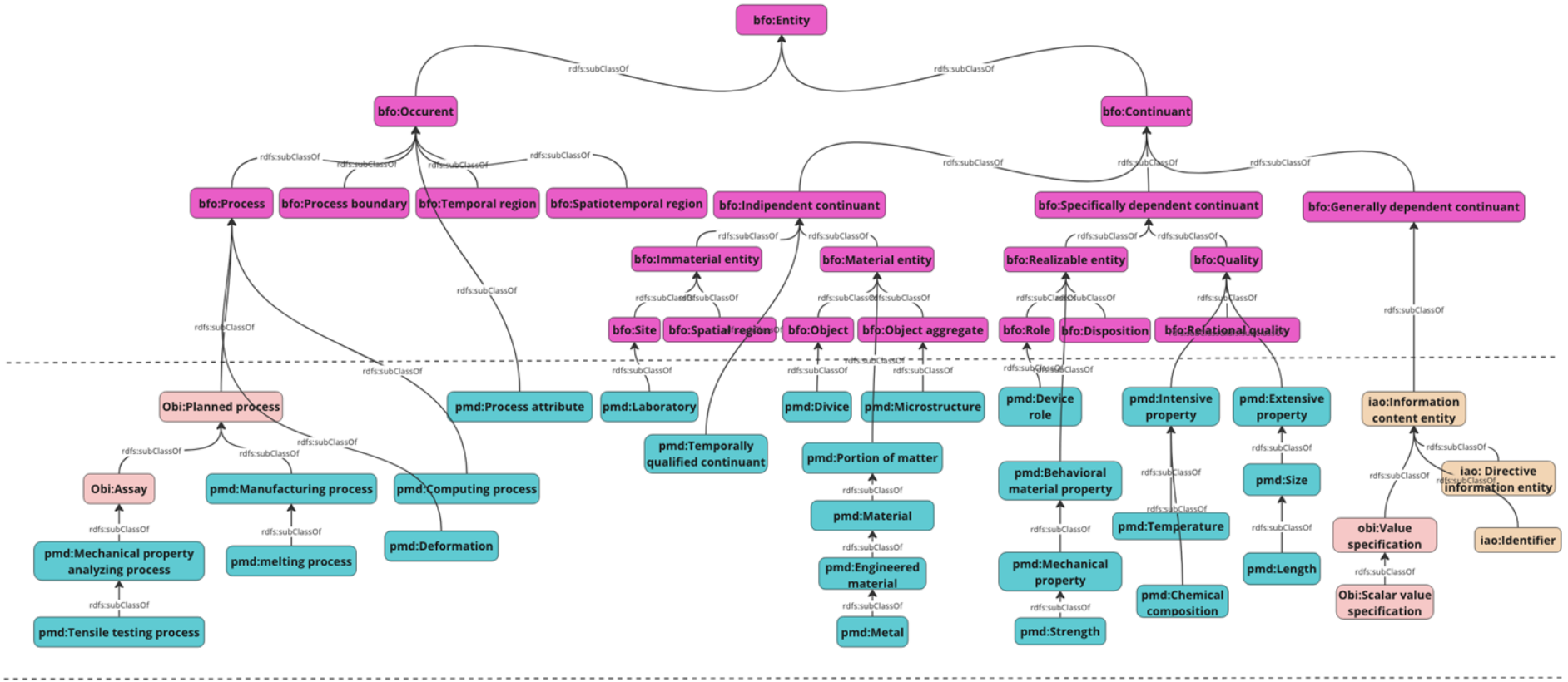
PMDco v3.0 mid-level core ontology

Top-Level BFO

Mid-Level PMD



- pmdco-materials
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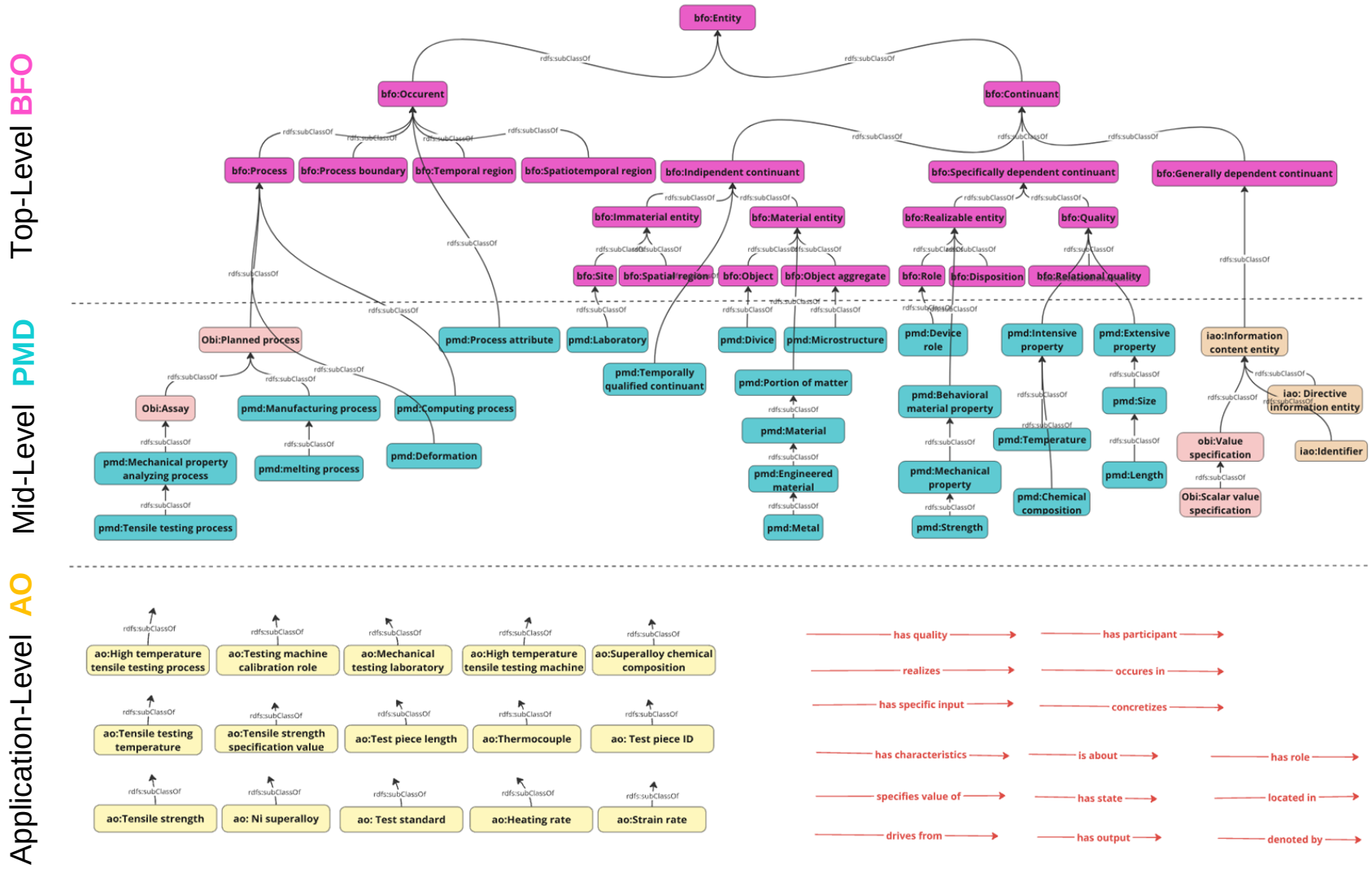
PMDco – Hands-on Tutorial

Hands-on workshop

this fternoon 1-2 pm

Dr. Hossein Beygi Nasrabadi

Walk through how **PMDco** fits into this..
&
develop your **Application Ontology**
& Model Processes



PMDco – Tools Space

PMDco Intro.

- PMDco as an “anchor” mid-level Ontology, supporting Semantic Interoperability in MSE
- PMDco structure; modules; classes; properties etc.

PMDco Tools-scape

- **GitHub** – as a Collaboration tool; PMDco Repositories
- **Protégé** – open-source Ontology Editor
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PMDco Potentials

- Reuse: PMDco-anchored Application/Domain ontologies
- Integration: PMDco uptake in Industry & Academia

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- Development Process - How we work as a community
- Community Channels - How to engage with the community

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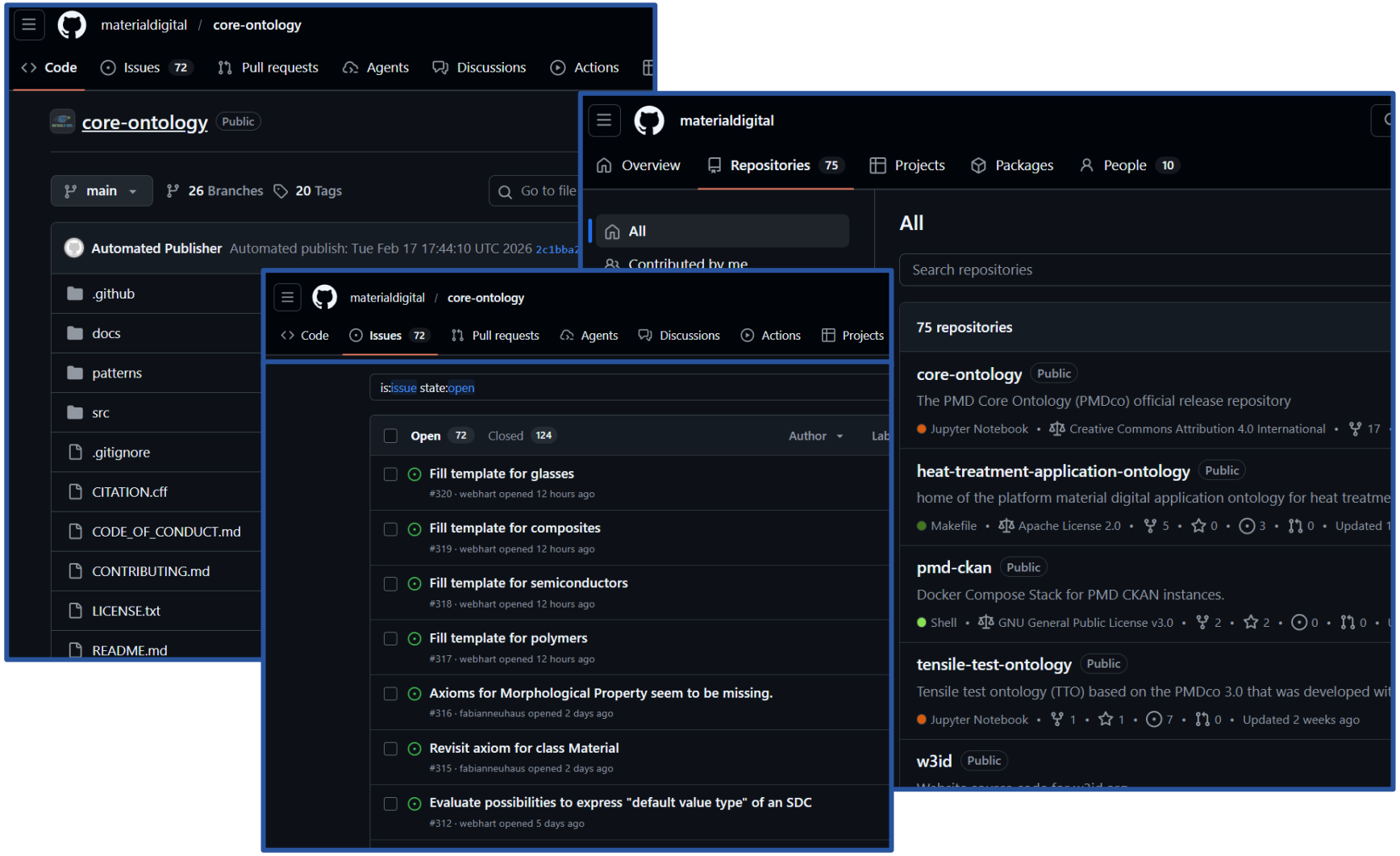

GitHub

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Protégé is a free, open-source platform developed by Stanford University. It provides a suite of tools to construct domain models and knowledge-based applications using ontologies. It is widely considered the "de facto" standard for Semantic Web development.

Why Protégé?

- **Standardization:** Fully compliant with **W3C standards** (OWL 2, RDF, SPARQL), ensuring your data is interoperable across the Semantic Web.
- **Extensibility:** Features a highly **pluggable architecture,** with community-contributed plugins exist for visualization, matrix editing, & querying.
- **Zero Coding Required:** Provides a graphical user interface to build complex logical expressions without needing to write raw XML or Turtle syntax manually.

What Protégé Provides

- **Editing -** Hierarchical class browsers, property editors, and wizard-based creation of complex axioms.
- **Reasoning -** Direct interface to automated reasoners to find contradictions and hidden relationships.
- **Querying** - Support for DL Query (Description Logic) and SPARQL to extract specific data from the ontology.
- **Interoperability** - Export and import support for various formats including RDF/XML, Turtle, and OBO.
- **Visualization** - Graphs and trees (e.g., OntoGraf) to see how concepts are interconnected visually.

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odk
ONTOLOGY DEVELOPMENT KIT

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PMDco – Tools Space

ODK is an open-source lifecycle management system that acts as the automated "packaging and delivery" layer, using tools like **ROBOT** and **Docker** to transform your manual edits in **Protégé** into a standardized, error-free, publicly releasable version.

odk
ONTOLOGY DEVELOPMENT KIT

Why ODK?

- **Reuse** terms from existing ontologies without bloating or losing axioms.
- Keep **imports** up to date and OWL-profile compliant.
- Avoid breaking anything during **edits**
- Provide standardized user **access** & Support **multi-developer** editing.
- Manage releases **transparently**.
- **Automate** QC, reasoning, imports, releases.

What ODK Provides

- Open-source toolkit + ontology lifecycle management.
- Automates imports, releases, consistency checks, reasoning, QA.
- Enforces ontology best practices.
- Modular architecture (main, extension, edit, imports).
- Uses ROBOT, Docker, GitHub Actions.
- Built-in documentation via MkDocs.

- a **toolbox** of various ontology related tools such as **ROBOT, owltools, dosdp-tools** and many more, **bundled as a docker image**
- a set of **executable workflows** for managing your **ontology's continuous integration, quality control, releases and dynamic imports**.

PMDco - Potentials

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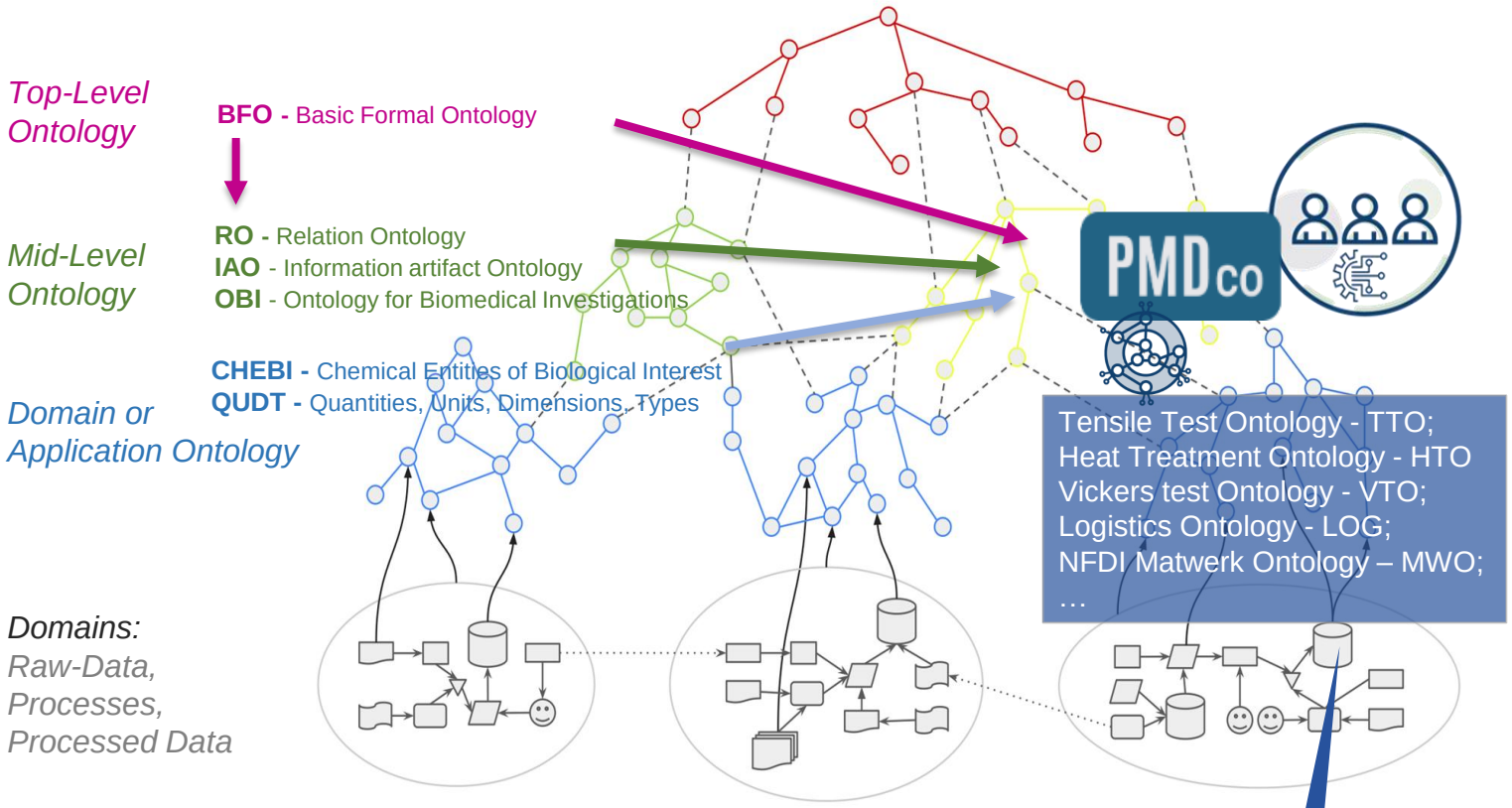
PMDco – Reuse & Integration



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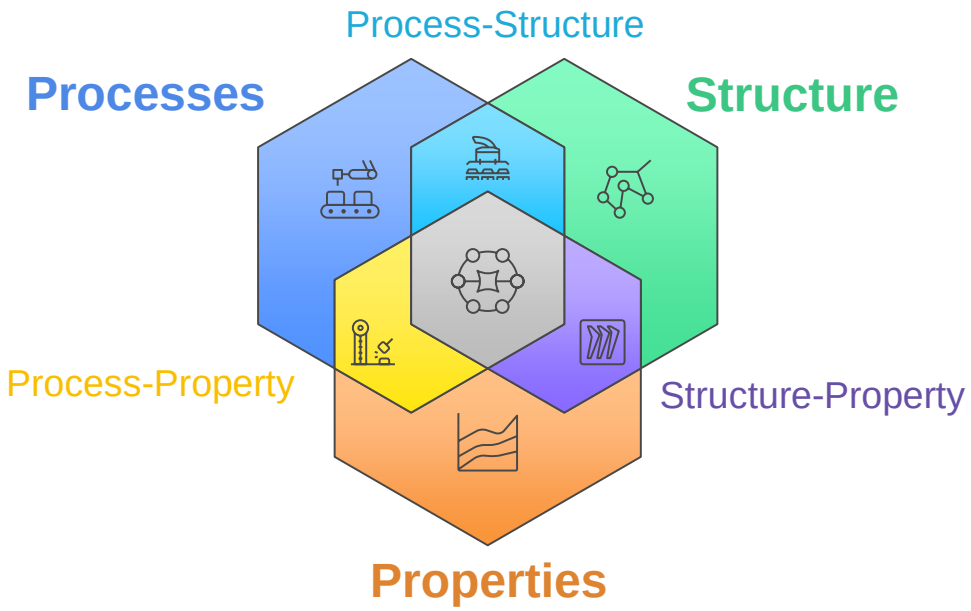
Findability
Accessibility
Interoperability
Reusability

PMDco – Reuse & Integration



- Achieve **interoperable** materials and processes data
- Traceability of (meta-)data **across the value chain**
- Support **FAIR** principles for reproducibility & reliable **reuse**.

Findability
Accessibility
Interoperability
Reusability

Logistic Application Ontology (LOG)

Vickers Testing Ontology (VTO)

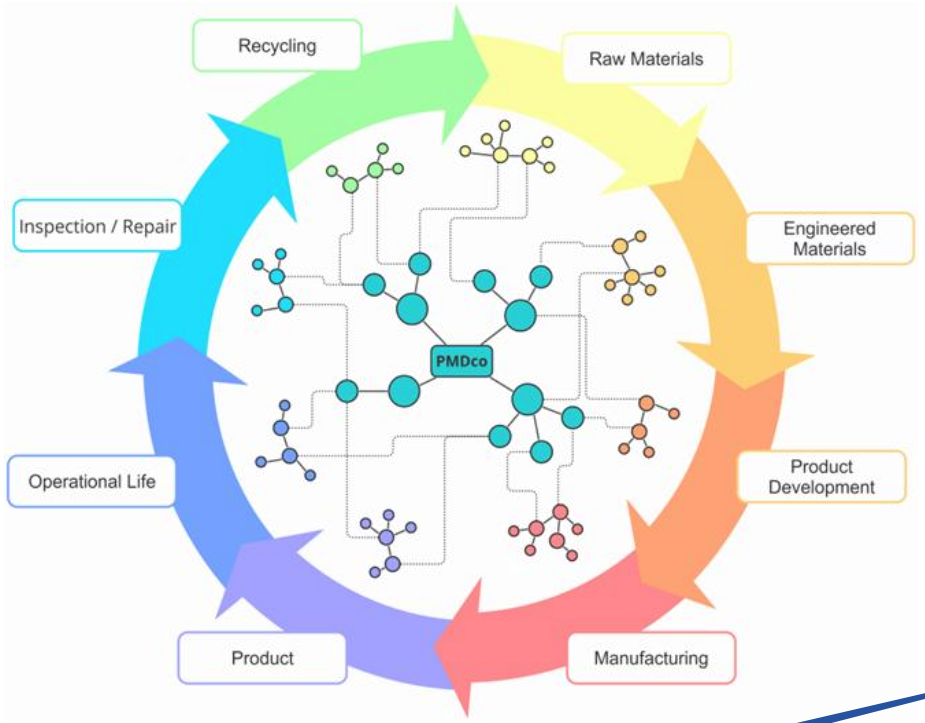
Tensile Testing Ontology (TTO)

Heat Treatment Ontology (HTO)

NFDI MatWerk Ontology (MWO)

Bio-inspired Meta-Materials Ontology (BiMMO)

PMDco – Reuse & Integration



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ELSEVIER

Materials & Design
Volume 237, January 2024, 112603

PMD Core Ontology: Achieving semantic interoperability in materials science

Bernd Bayerlein [a], Markus Schilling [a], Henk Birkholz [b], Matthias Jung [c], Jörg Waitelonis [d], Lutz Mädler [b e], Harald Sack [d]

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https://doi.org/10.1016/j.matdes.2023.112603

Highlights

- The PMD Core Ontology (PMDco) bridges semantic gaps in Materials Science and Engineering, enabling data interoperability.
- The PMDco supports the FAIR principles and enables materials and process data conversion into machine-processable format.
- Community-driven curation ensures PMDco's usability and evolution, with applications in domain-specific ontology development.
- The PMDco serves as a valuable resource, fostering scientific discovery, innovation, and sustainable research practices.

PMDco – Reuse & Integration

Materials Commons 4EU

PMD-X EDcar

PMd-X MAPRO

NFDI MatWerk

Industrial Ontologies Foundry

Catena-X Automotive Network

MANUFACTURING-X

nfdi Nationale Forschungsdaten Infrastruktur

- Achieve **interoperable** materials and processes data
- Traceability of (meta-)data **across the value chain**
- Support **FAIR** principles for reproducibility & reliable **reuse.**
- **academic & industrial integration** enabled by cross-domain interoperability

PMDco – Community Processes

PMDco Intro.

- PMDco as an “anchor” mid-level Ontology, supporting Semantic Interoperability in MSE
- PMDco structure; modules; classes; properties etc.

PMDco tools-space

- GitHub – as a Collaboration tool; PMDco Repositories
- Protégé – open-source Ontology Editor
- ODK – Ontology Developement Kit

PMDco Potentials

- Reuse: PMDco-anchored Application/Domain ontologies
- Integration: PMDco uptake in Industry & Academia

PMDco Processes

- **Development Process** - How we work as a community
- **Community Channels** - How to engage with the community

PMDco – Core Team

… meeting **twice a week**
Interactive Development of PMDco…

… with ongoing **engagement** & collaboration within the **community**

IWM *Fraunhofer Institut für Werkstoffmechanik*
Dr. Philipp v. Hartrott
Dr. Thomas Hanke
Kamilla Zaripova

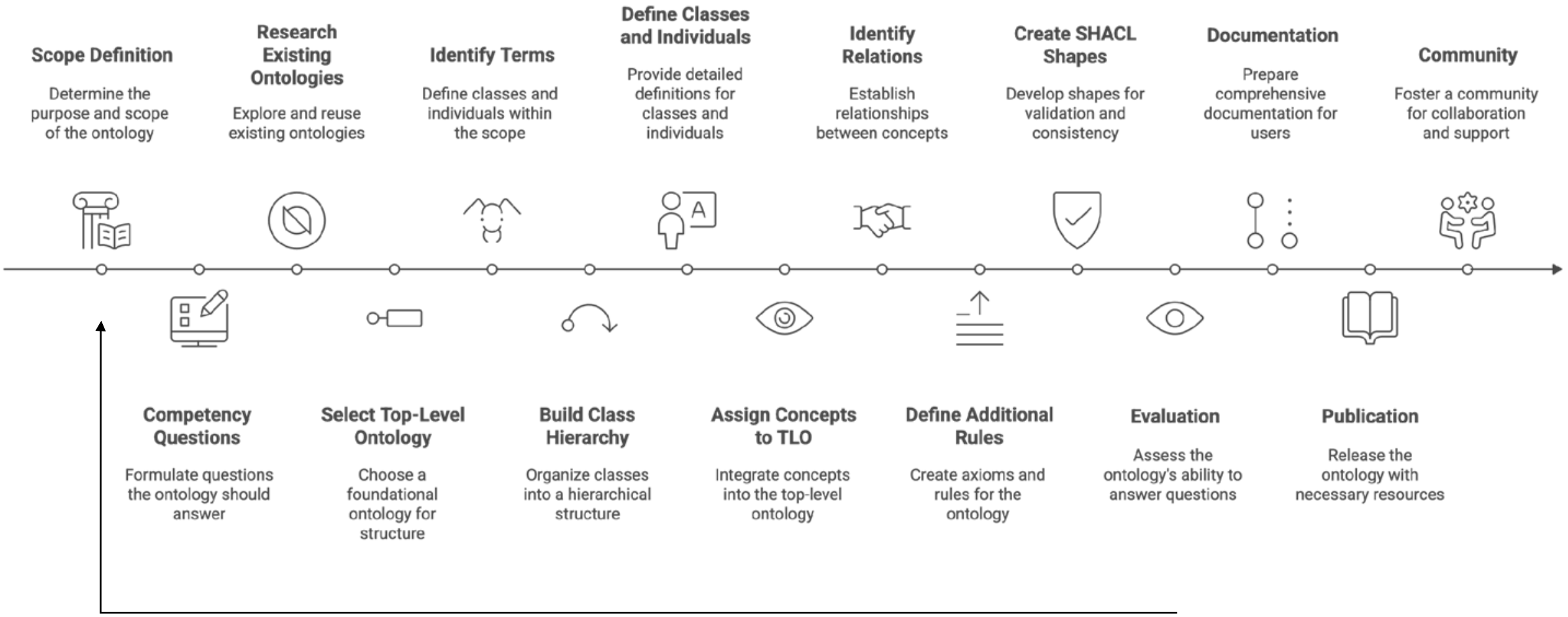
BAM *Bundesanstalt* für Materialforschung und -prüfung
Dr. Markus Schilling
Dr. Bernd Bayerlein
Dr. Khashayar Razghandi

FIZ *Leibniz-Institut für Informationsinfrastruktur*
Dr. Jörg Waitelonis
Dr. Hossein Beygi Nasrabadi
Dr. Gunjan Singh

IWT *Leibniz Institut für Werkstofforientierte Technologien*
Dr. Henk Birkholz
Felix Thonagel
Divya Gosula

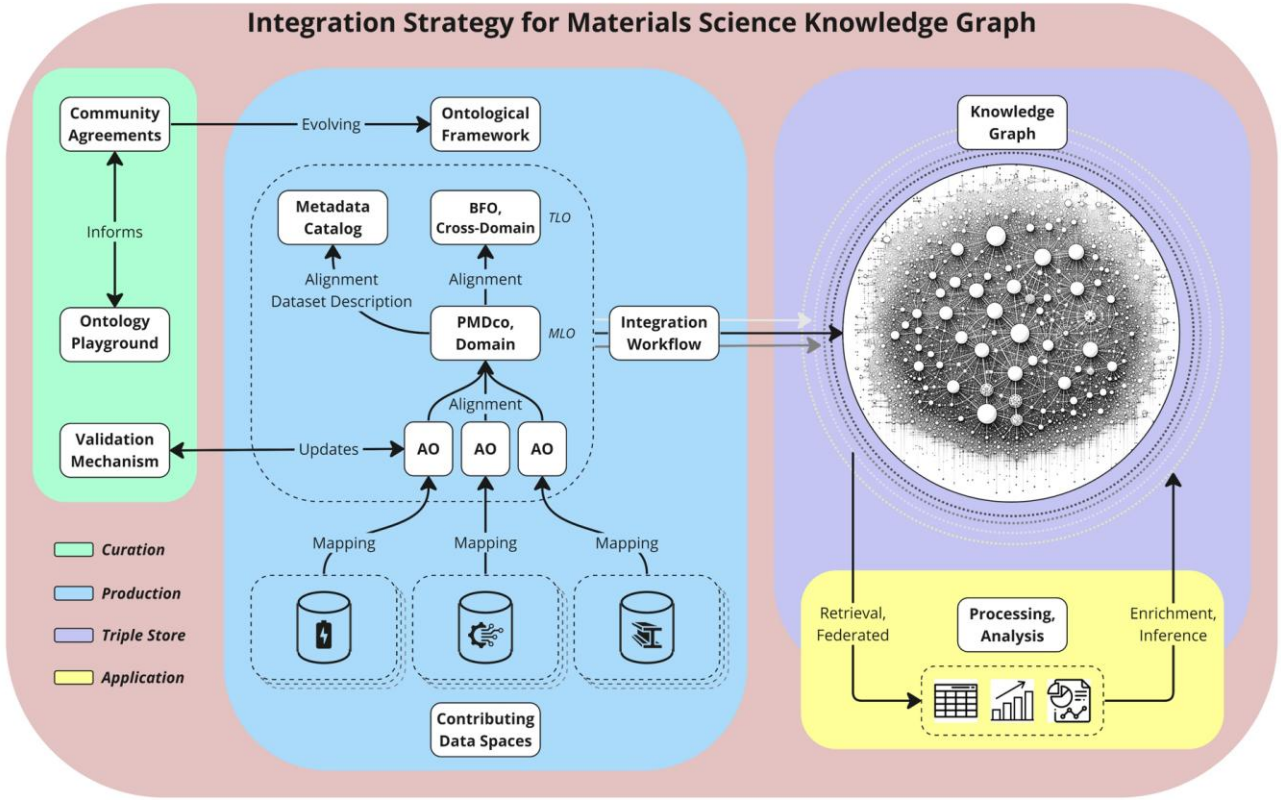
PMD Hackathon
October 2025 @ BAM

PMDco - Development Process



PMDco - Integration Strategy

- **Consensus**-building (Core Team, Playground, Hackathon)
- **BFO** & **PMDco**: **Cross-domain interoperability**
- Data space-specific **Application Ontologies**
- **Standardized metadata catalog**
  for consistent **dataset descriptions**
- Workflow for **knowledge graph** integration
- SPARQL queries for efficient **multi-scale**
  information retrieval & **enrichment**



A Unified Concept for a Materials Data Space – Insights from the MaterialDigital Initiative

Bernd Bayerlein Jörg Waitelonis Henk Birkholz Matthias Jung Markus Schilling Philipp v. Hartrott Marian Bruns Osamu Waseda Jörg Schaarschmidt Kristian Beilke Marcel Mutz Vincent Nebel Veit Königer Lisa Beran Tobias Kraus Akhilesh Vyas Lars Vogt Moritz Blum Basil Ell Ya-Fan Chen Tina Waurischk Akhil Thomas Ali Riza Durmaz Sahar Ben Hassine Carina Fresemann Hossein Beygi Nasrabadi Gordian Dziwis Thomas Hanke Melissa Telong Stephan Pirskawetz Mohamed Kamal Thomas Bjarsch Ursula Pähler Peter Hofmann Mena Leemhuis Özgür L. Özçep Lars-Peter Meyer Birgit Skrotzki Jörg Neugebauer Wolfgang Wenzel Harald Sack Chris Eberl Pedro D. Portella Tilmann Hickel Lutz Mädler Peter Gumbsch*

Advanced Engineering Materials / Volume 27, Issue 8 / 2500484

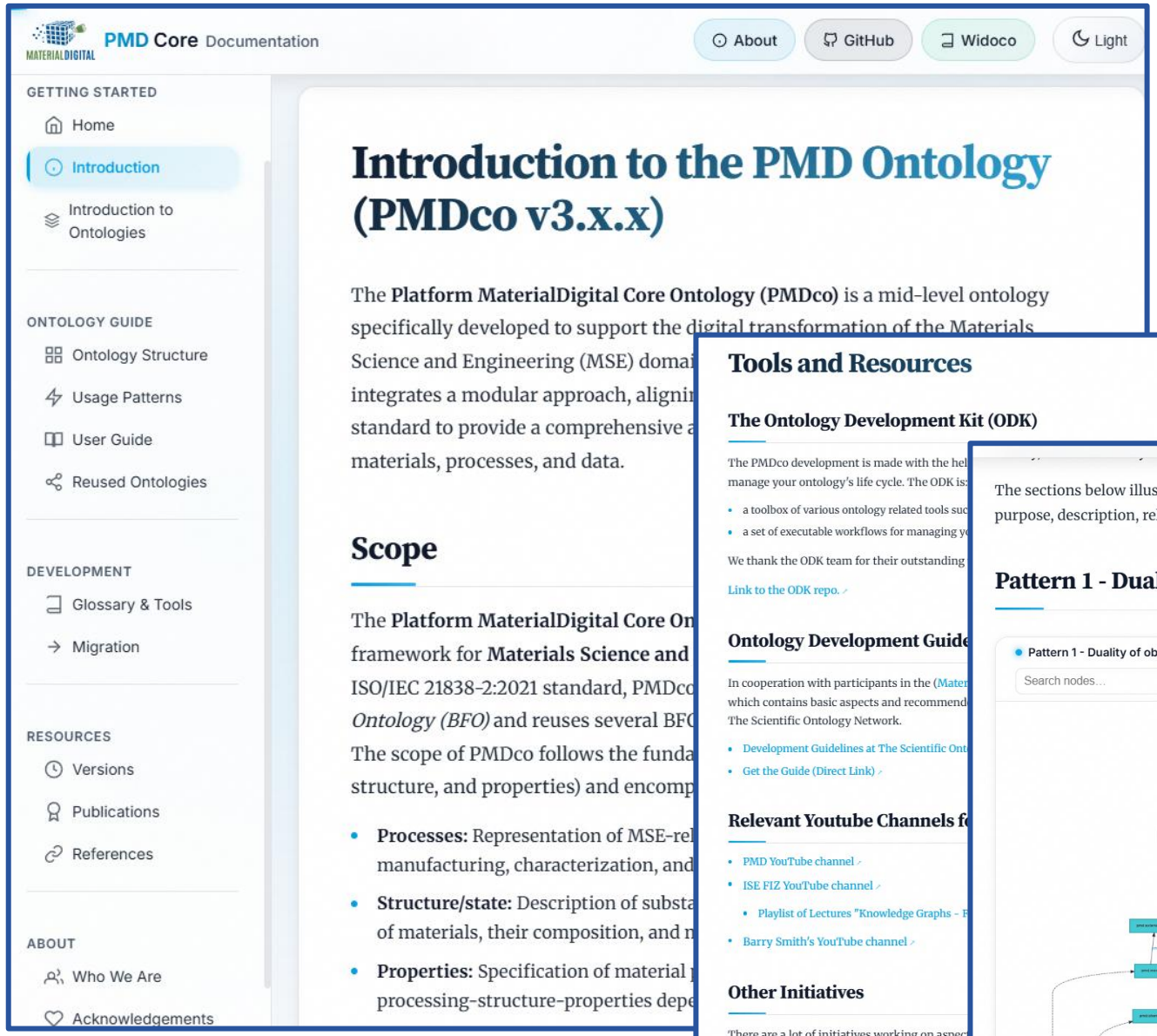
Guest Editorial | Free Access

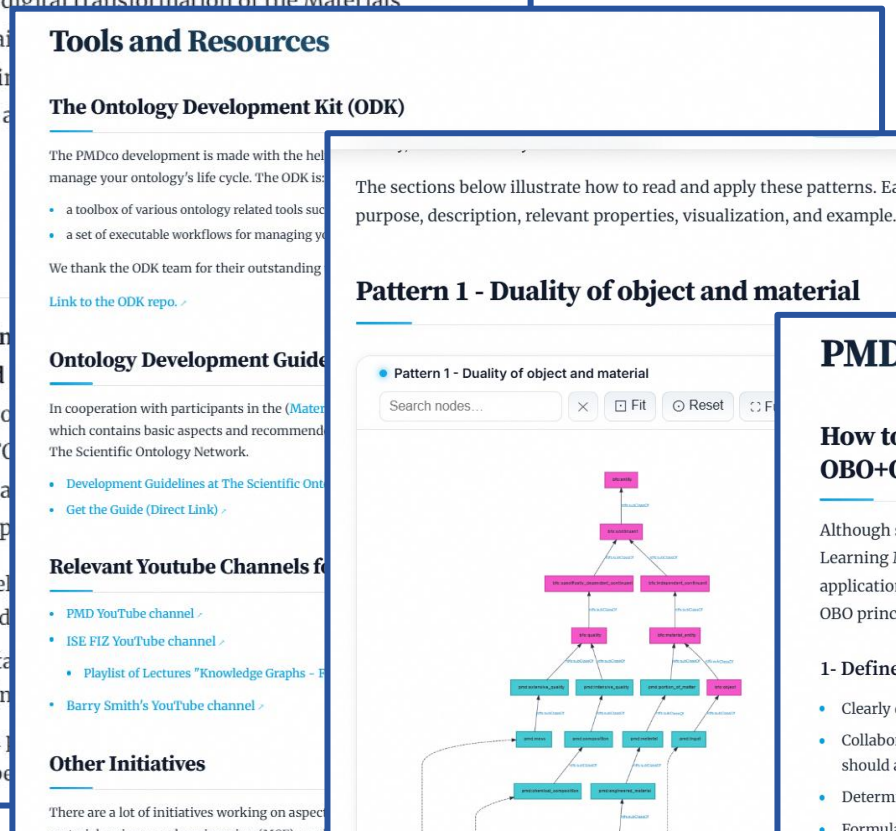
Special Issue on “Digitalization in Materials Science and Engineering”

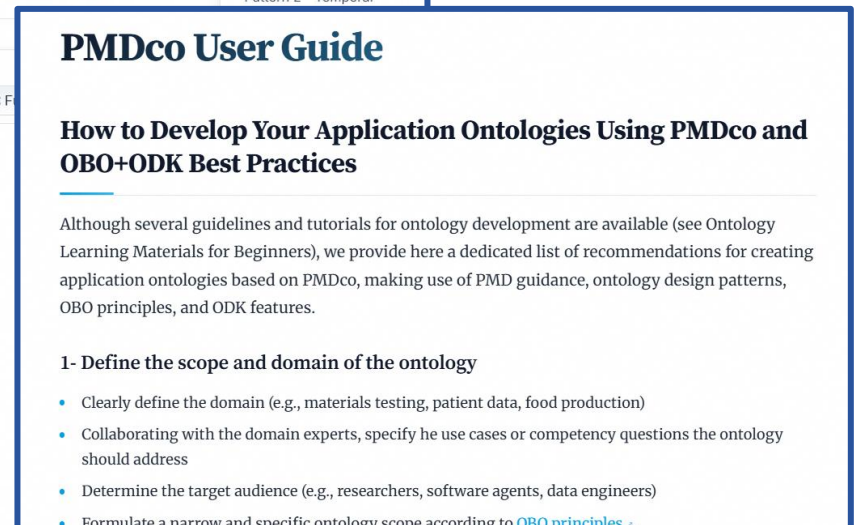
Peter Gumbsch ✉, Pedro Dolabella Portella

First published: 22 April 2025
https://doi.org/10.1002/adem.202500484

PMDco - Documentation

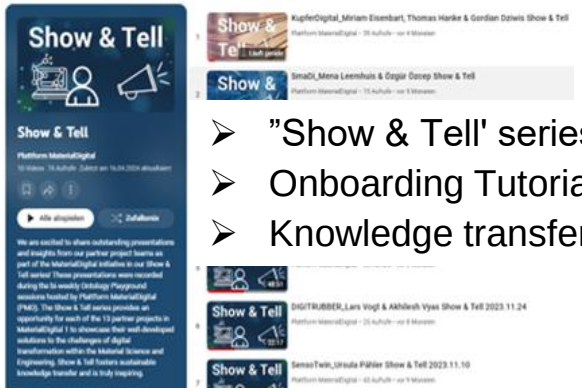






PMDco - Collaborate / Contribute / Engage …

Check out our **Channel**



- ”Show & Tell' series
- Onboarding Tutorials
- Knowledge transfer

Check & Engage with our **PMDco GitHub Repositories**

- Explore the latest developments…
- join **discussion forum** …
- create an **issue** …
- report a Bug… suggest Improvements…
- request Features …
- raise specific Modeling concerns …

Join our bi-weekly **online Ontology Playgrounds**

- connecting the proactive community
  - Knowledge transfer
  - Experience exchange
  - tackling Modeling challenges
  - User insights
- all driven by community consensus.

Next Hackathon

MATERIALDIGITAL

Thank You!

The Material Digitalization Platform - a joint project by:

KIT Karlsruher Institut für Technologie

BAM Bundesanstalt für Materialforschung und -prüfung

MAX-PLANCK-INSTITUT FÜR NACHHALTIGE MATERIALIEN GMBH

Fraunhofer IWM

IWT Leibniz-Institut für Werkstofforientierte Technologien

FIZ Karlsruhe Leibniz-Institut für Informationsinfrastruktur

Bundesministerium für Forschung, Technologie und Raumfahrt