Digital Transformation in Materials Science

PMD Core Ontology (PMDco) 3.0 – Patterns & Applications

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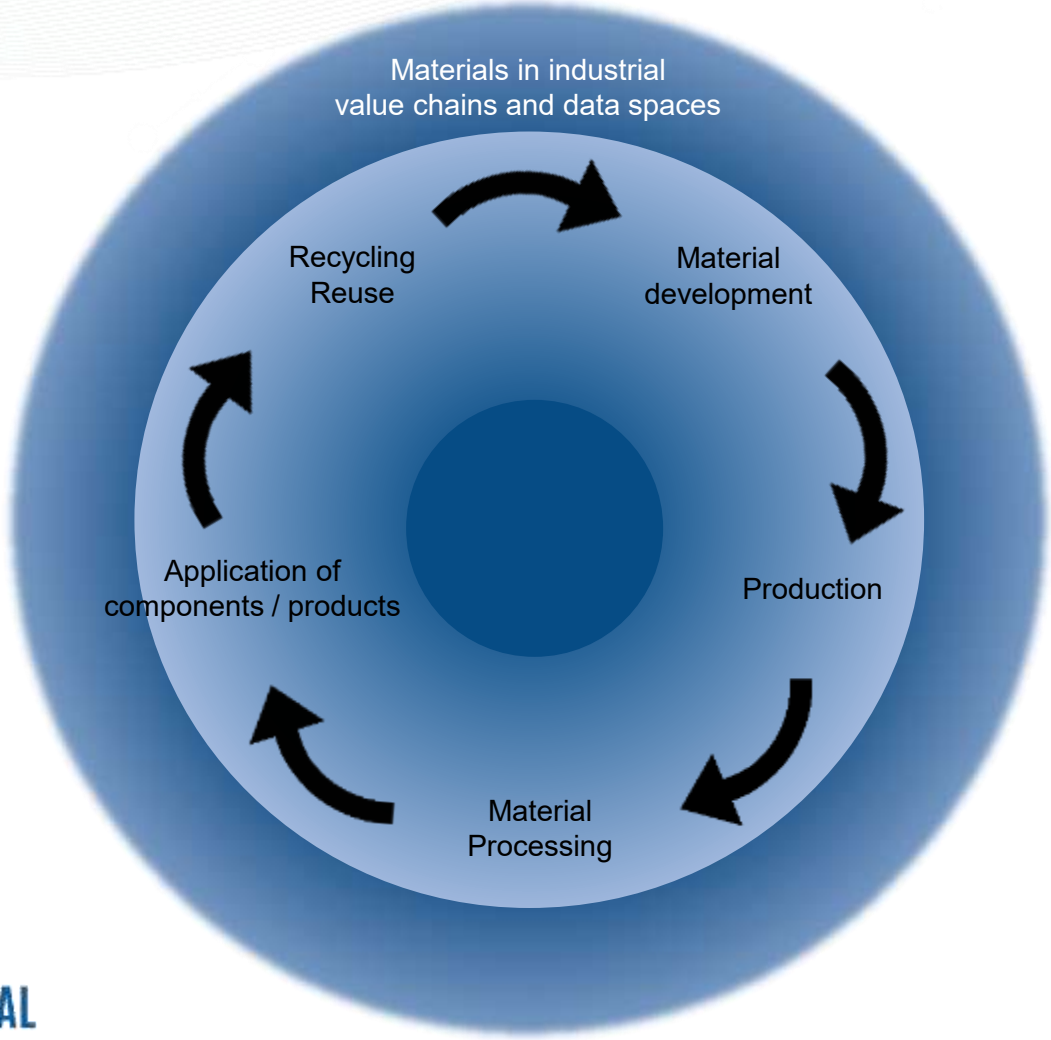
Material data | Value creation in the 21st century

- Materials are **fundamental components** of all (industrial) products.
- Development of "**advanced materials**" aims to improve control over material behavior.
- Key basis for **innovation** (e.g., in energy transition and circular economy).
- Material **properties change** during the manufacture and use of products.
- **Efficient application** is only possible with digital material images/models.



→ **Initiative & Platform MaterialDigital (PMD)**

- PMD Core Team + Partner Projects
- Third funding period (2019 - 2028)

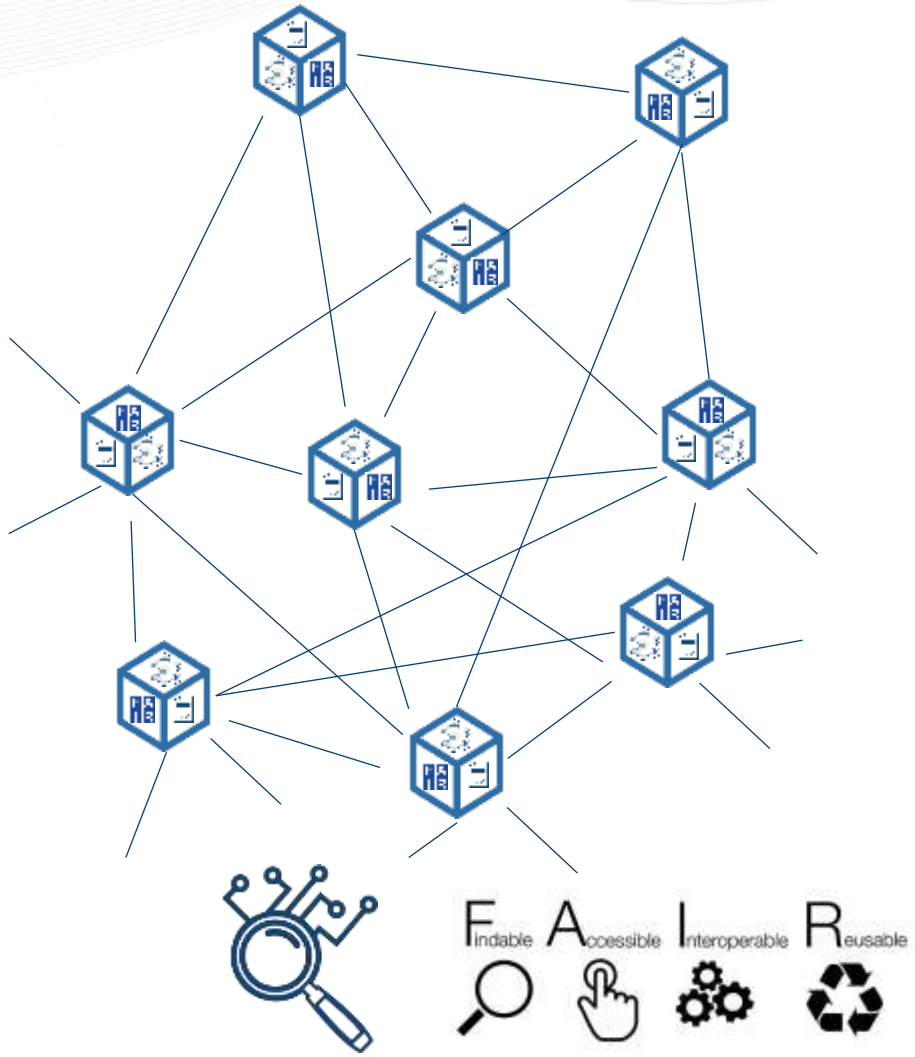
Initiative MaterialDigital | Vision

Goal

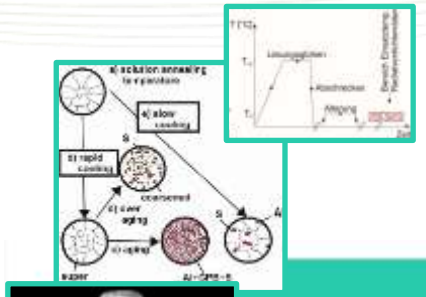
A virtual **material data space** that contains all available **material data** in FAIR format and can consolidate information from various sources and sub-areas.

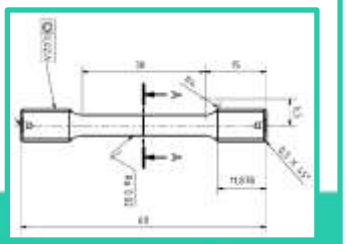
Approach

- Consensus on (de-facto) **standards for structured data** and interfaces for a uniform approach
- Provision of **software tools** for easy access
- **Decentralized data storage** – data sovereignty is retained (copyright protected)

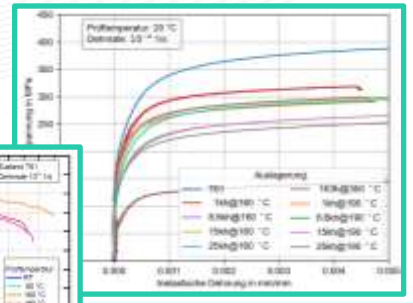


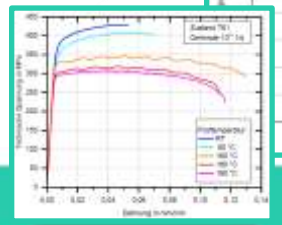
Experiments Data Pipelines

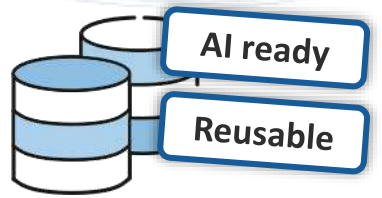




T (°C)	t (h)
None	0
190	24
190	100
190	250
190	1,000
190	2,500
190	5,000
190	8,760
190	25,000







Manufacturing Process

Test Pieces

Defined Aging Process

Tensile Testing

Time Series

Data Processing

HT Component

Material States

Results

Publications

Manufacturing Process

Defined Aging Process

Mechancial Analysis

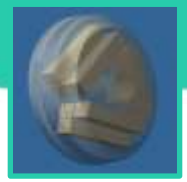
Microstructural Analysis

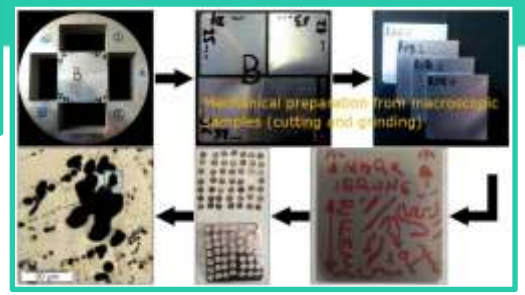
Image Data Processing

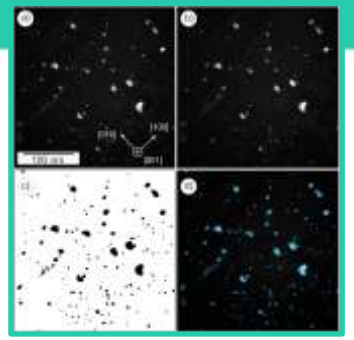
Samples

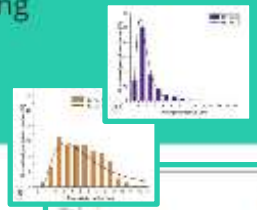
TEM Process

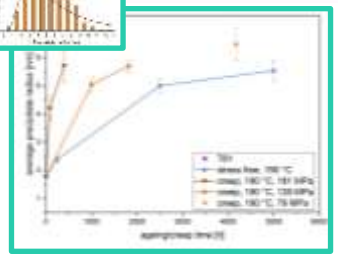
Image Data









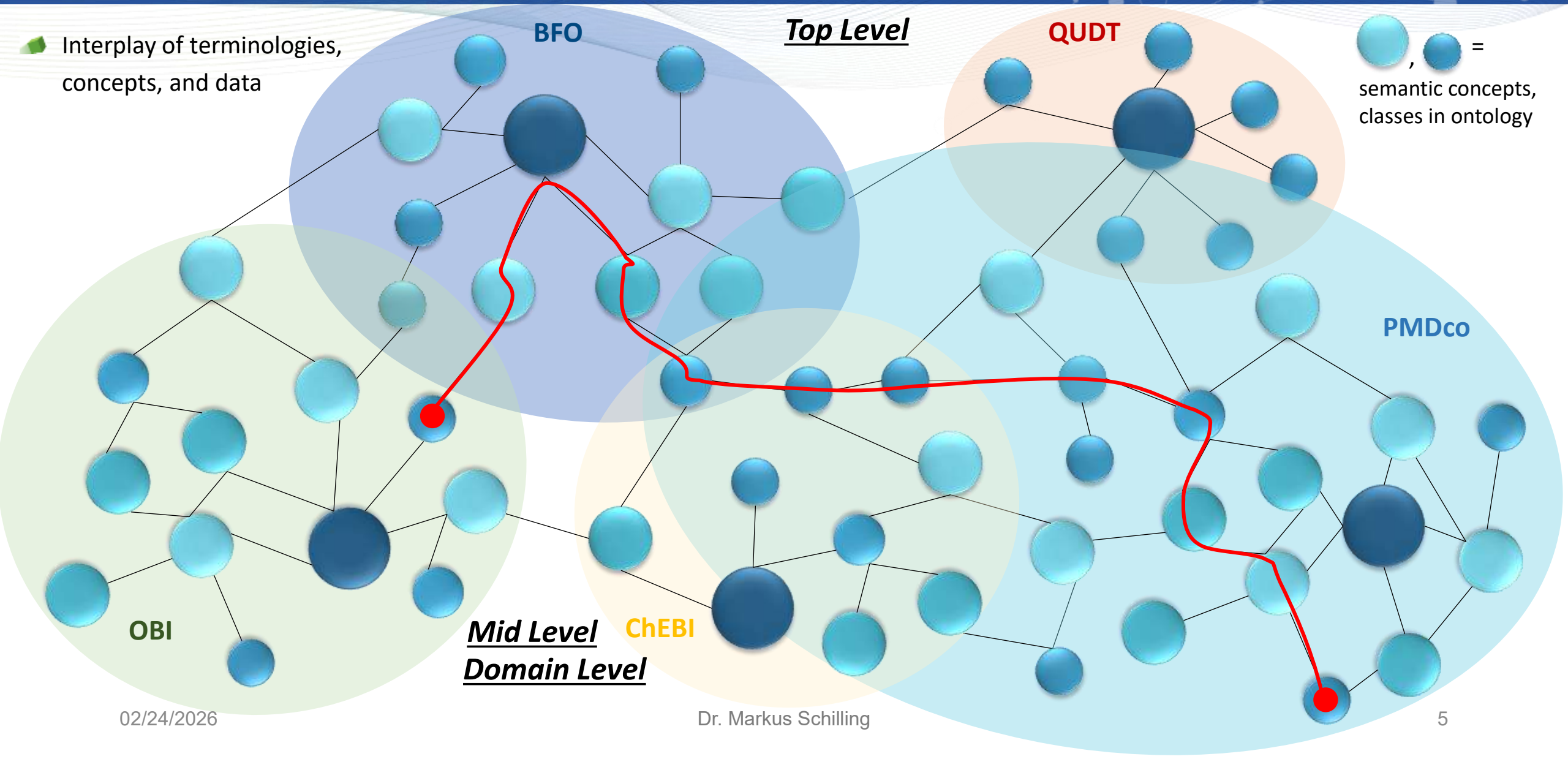


AI ready

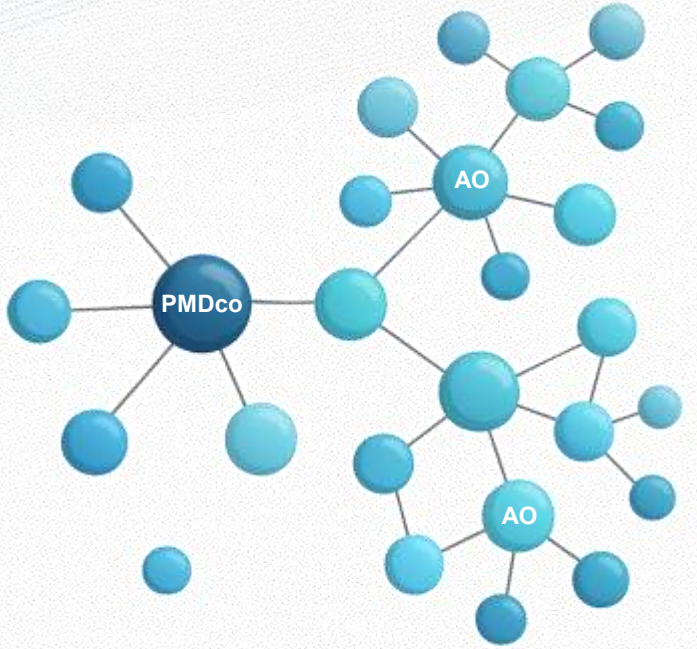
Reusable

Semantic Technologies | Ontology Layers

- Interplay of terminologies, concepts, and data



PMD Core Ontology (PMDco) 3.0



GitHub

PMDco

- Semantic framework for materials science
- Machine-processable, interoperable material and process data
- Support FAIR principles and promote reproducibility
- Facilitate traceability of (meta)data along entire value chains
- Aligned with standardized BFO (ISO 21838)
- Homogeneous (re)use of concepts
- Unified SPARQL querying
- Guide in Design and Curation Decisions

Evolution of PMDco

GitHub

PMDco 1.0 (0.1) 07/2021 → **PMDco 2.0.8** 09/2024 → **PMDco 3.0** 02/2026

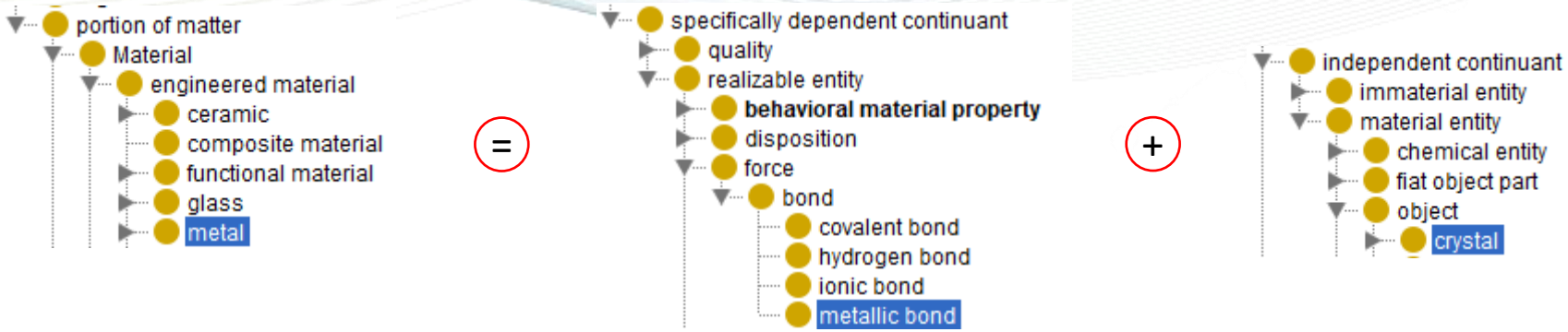
- Vision of ontology for MSE
- Creation of ‘semantic data’

- PROV-O aligned
- Low entry barrier
- Education and Training
- Demonstration
  - NLP approach
  - Harmonization of datatypes
  - Data Acquisition Pipeline (DAP)
  - ELN Data Acquisition

- BFO2020 aligned
- Fundamental conceptualization
- Long-term improvement
- Broad Semantic Interoperability
- Homogeneous (re)use of object properties
- Unified SPARQL Querying
- Guide in Design and Curation Decisions
- Reasoning capabilities
- Relevant for usage in industry

PMD Core Ontology (PMDco) | Patterns

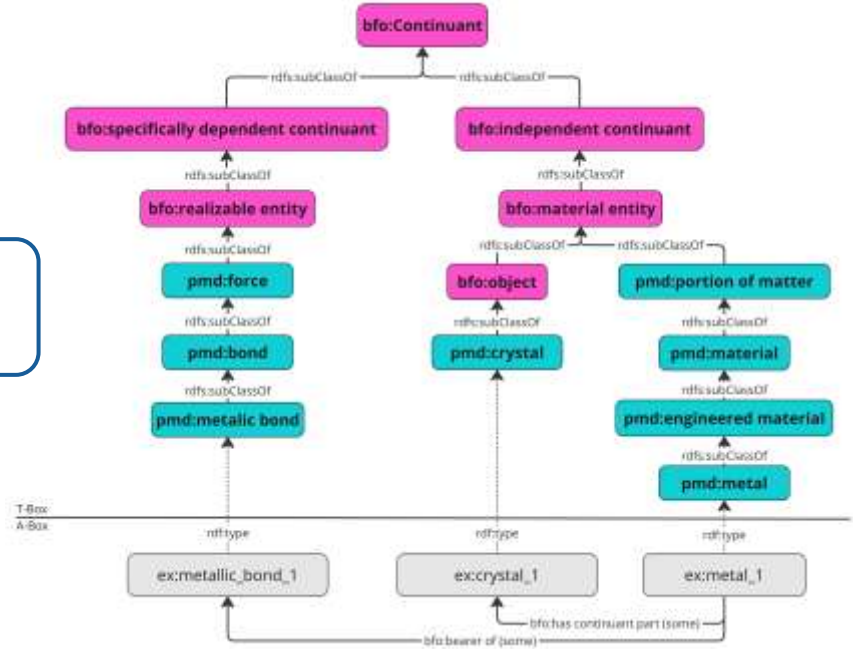
Concepts (Classes)



Axiom

```
'engineered material'
  and ('has continuant part' some
    (crystal
     and ('bearer of' some 'metallic bond')))
```

Pattern

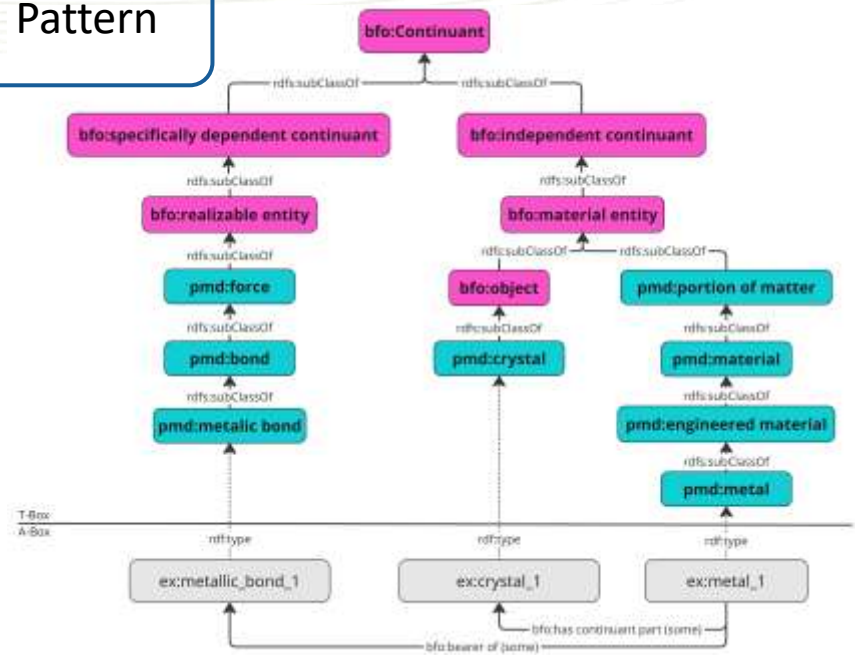


Textual Expression

A metal is an engineered material, that has a crystal as a (continuant) part that itself bears a metallic bond.

PMD Core Ontology (PMDco) | Patterns, SHACL

Pattern



Textual Expression

„A metal is an engineered material, that has a crystal as a (continuant) part that itself bears a metallic bond.“

SHACL Shape

```
@prefix sh: <http://www.w3.org/ns/shacl#> .
@prefix ex: <http://example.org/> .
@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix bfo: <http://purl.obolibrary.org/obo/> .
@prefix pmd: <https://w3id.org/pmd/co/>.

ex:materialShape
   a sh:NodeShape ;
   sh:targetClass ex:engineeredMaterial ;
   sh:property [
      sh:path bfo:hasContinuantPart ;
      sh:node [
         sh:class ex:crystal ;
         sh:property [
            sh:path ex:bearerOf ;
            sh:class ex:metallicBond ;
            sh:minCount 1 ;
         ] ;
      ] ;
      sh:minCount 1 ;
   ] .
```

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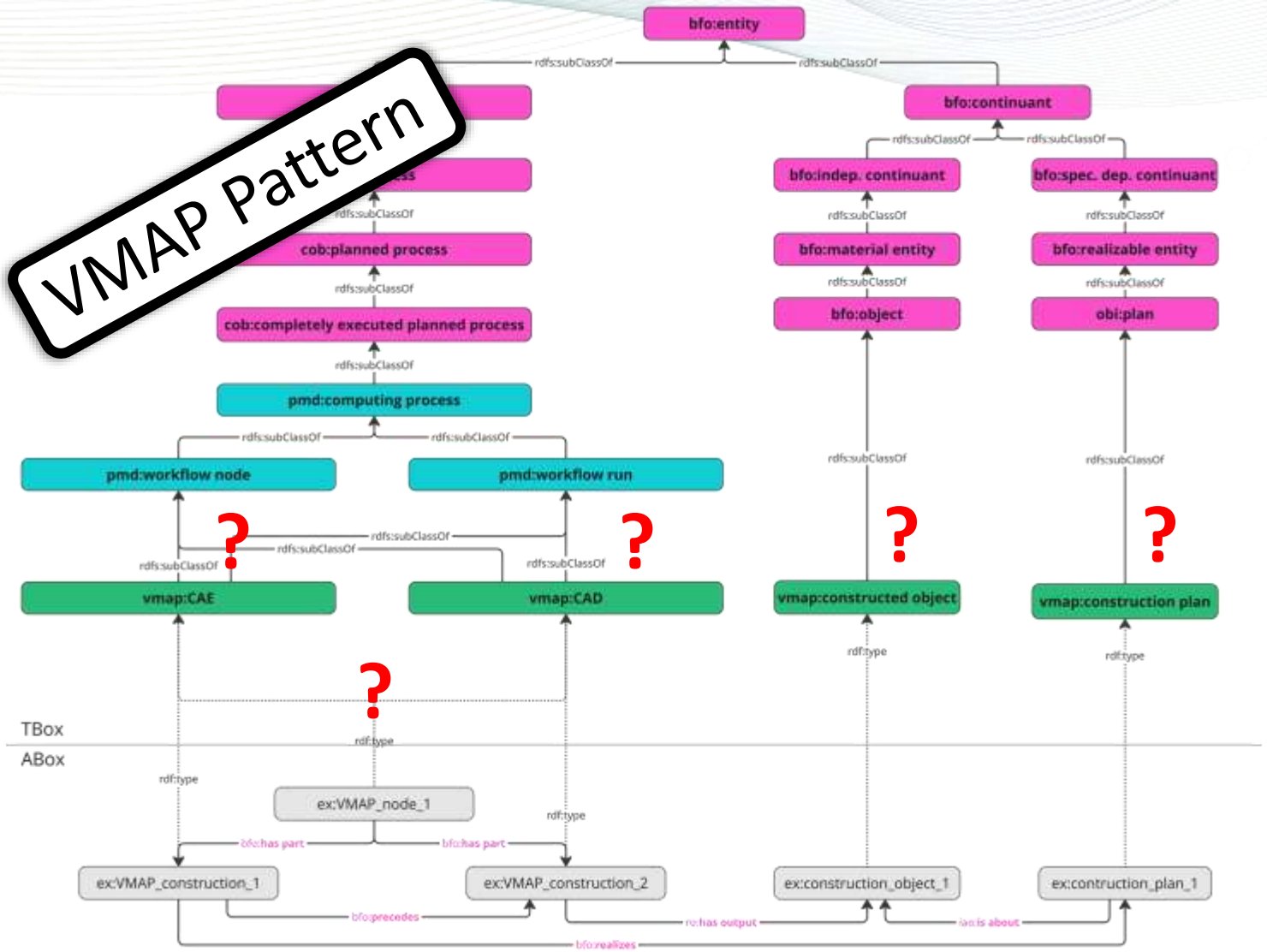
PMD Core Ontology (PMDco) | Patterns, VMAP

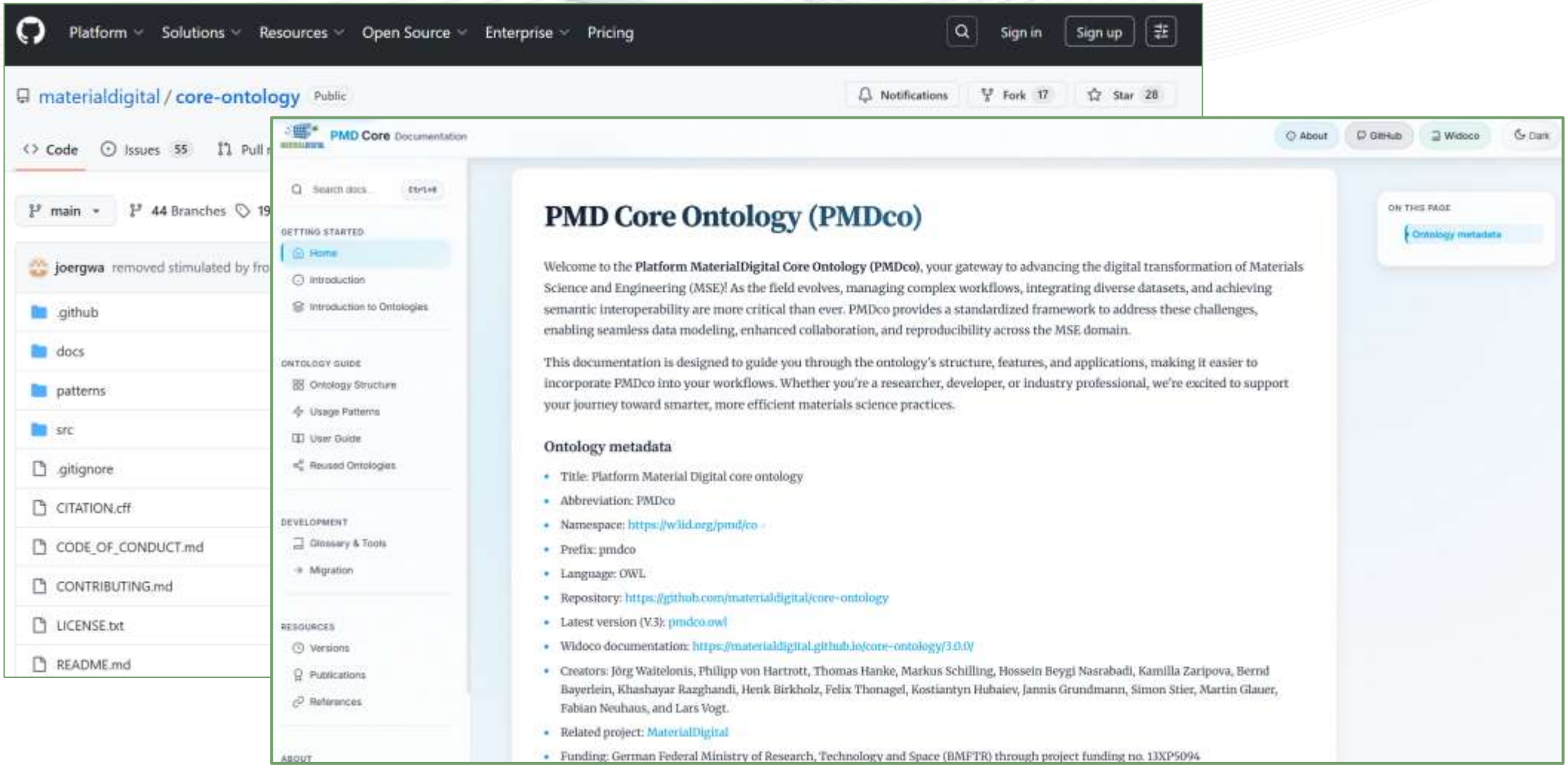


Thomas Hanke

(02/24/2026 | 15:00)

VMAP as Enabler:
Expanding PMDco's Computational Scope and Shaping AAS Standards for Engineering Simulations

PMD Core Ontology (PMDco) | Repository

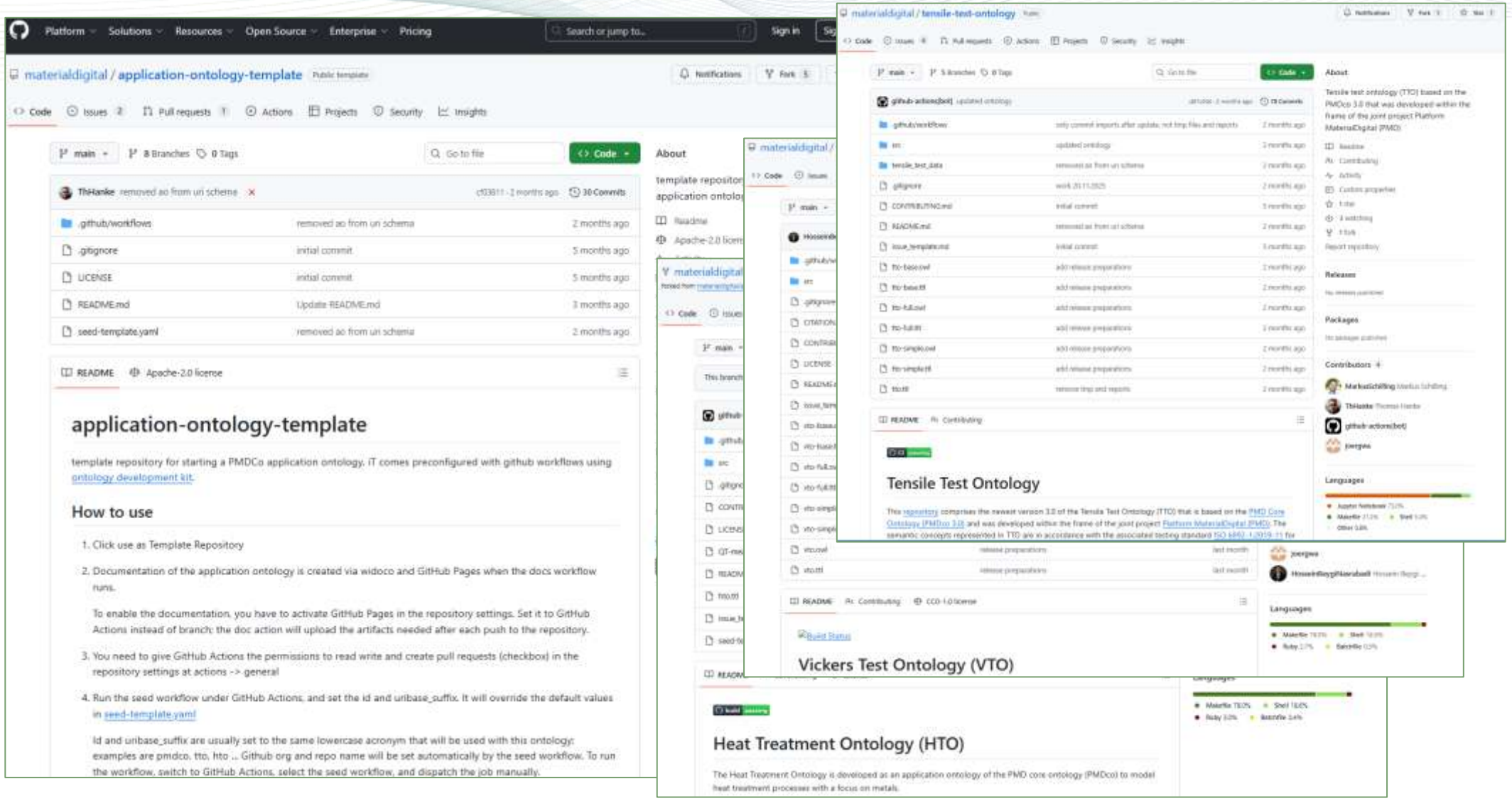


GitHub

PMDco

materialdigital.github.io/core-ontology/docs

Application Ontologies



GitHub

PMDco

Contact us!

info@material-digital.de

www.materialdigital.de

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