PLATFORM MATERIALDIGITAL · DILEMA-K · NUMBERLAND

A Semantic Pipeline for Digital Twins of Ceramic Materials

From methodology paper to operative ontology — one end-to-end knowledge pipeline.
Reference: lead-free piezoelectric & ferrite ceramics (BNT-BT · NiCuZn ferrite)

ontocrafter.eu/introduction
Project details & poster PDF

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THE RESEARCHER'S QUESTIONS

EXPLORATION
"I want to find the best way to make a material."
Which process route should I investigate? · Which parameters are likely to matter? · What is already known? · Which experiments first?

EXPLANATION
"I want to understand why my material behaves this way."
Why did I obtain these results? · Which process step caused this behaviour? · Which publications report similar? · What to change next?

An ELN records *what you did*. The ontology connects it to *what is known* — and makes it **answerable**.

TWO INGESTION PATHS — USED SEPARATELY OR TOGETHER

INPUT A · MATERIAL SOFTWARE STACK

Structured Data from the Existing Lab Stack

Numeric measurements, process records and sample metadata — the pipeline connects to what the lab already runs instead of replacing it.

ELN — Electronic Lab Notebook
LIMS — Lab Information Management

open source, e.g. eLabFTW · Kadi4Mat · NOMAD Oasis · openBIS · RSpace

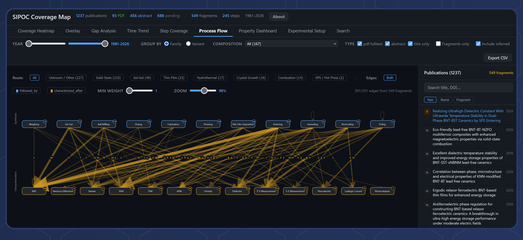
also: Spreadsheets / Excel · Measurement Data · + more

INPUT B · SIPOC EXTRACTOR — 1,237 papers

Process Fragments Mined from Publications

No single paper holds the full process. The extractor mines SIPOC fragments from full text and assembles a complete lab recipe — written straight into the OCO ABox.

Supplier → Input → Process → Output → Customer



01 · METHODOLOGY PAPER

Layered Architecture for Reusable Materials Ontologies

Pannek & Grond 2026 · arXiv 2606.14814
CC-BY 4.0 · 55 pages

v0.94

55

Formal description of a four-layer architecture — each layer independently versioned and modularly exchangeable. Methodological foundation for OCO and all future material-class extensions.

L0 — Bridges to Standards
Dozens of external vocabularies across nine domains: foundation ontologies · units & time · crystallography · LCA · industry data spaces · EU regulation · governance · international frameworks · identifiers.

L1 — Material-agnostic Skeleton
Specimen · Equipment · Measurement · Identifier · Provenance. Shared across all material classes and consortium projects.

L2 — Material & Compliance Detail
Material- and regulation-specific detail — exchanged when the material class or regulation changes, leaving the layers below untouched.

L3 — Categorical Reasoning
The ontology's competency questions are encoded as SHACL — checked against exactly what it must deliver — while its categorical axioms stay ready for an opt-in OWL 2 DL reasoner.

02 · ONTOLOGY

OntoCrafter Ceramics Ontology (OCO)

5,196 classes · 44 modules
167,348 OWL axioms · 1,172 SHACL rules
5,920 Neumann constraints (tensor × point group)

v0.94 · ontocrafter.eu

5K

Three industrial views on one shared ontology — same four-layer chassis, different consumers. Competency questions across all three views are tagged to one of ten reasoning areas (symmetry, phase, route, lifecycle, multi-axis, interoperability, quality, structure, BNT-BT, NCZF) — auditable per area.

Materials Research
Mechanistic Depth
Seven explanatory layers from symmetry to bonding — defect chemistry, connectivity, coupled effects. "Why does BNT-BT reach d_{33} ≈ 580 pC/N?" becomes a SPARQL query.

Manufacturing & DPP
Value Chain & Digital Product Passport
Material-DPP and Sector-DPP via multiple inheritance. AAS IEC 63278, Catena-X CX-0010/CX-0146, Manufacturing-X. One BNT-BT actuator in a battery is simultaneously a Material-DPP and a Battery-DPP.

EU Compliance
Regulatory Integration
11 EU regulation modules structurally integrated: CSRD/ESRS, LCA, CSDDD, CBAM, AI Act, SSbD, PPWR, R2R, Regulated Substances, Recycling, Manufacturing-X. Architecture, not appendix.

03 · ONTOCRAFTER

OntoCrafter — Making OCO Usable and Buildable

Class definition · SHACL validation
ABox population from full text and/or own experiments

v0.82 · Under development

4

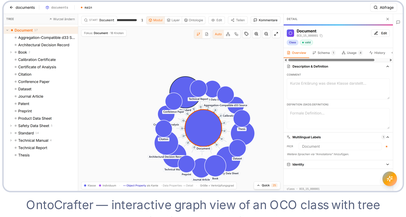
Four core functions make OCO operational in daily consortium work.

FUNCTION 1 — Project Management
Projects, versions & module assignments managed centrally.

FUNCTION 2 — Graph Visualization
Classes, relations & instances as an interactive graph.

FUNCTION 3 — Horizontal Scalability
Distribution across nodes; partners share one common TBox.

FUNCTION 4 — Plain-Language SHACL
Natural-language constraints → SHACL; plain-text validation.



OntoCrafter — interactive graph view of an OCO class with tree navigation and detail panel

PIPELINE OUTPUT

Digital Twin for Ceramic Materials

A fully structured, queryable, and validatable knowledge representation of ceramic material systems — from raw process parameters to regulatory compliance, traversable via SPARQL, verifiable via SHACL.

PROJECT
DILEMA-K
Digital Lifecycle of Lead-Free Piezoelectric and Ferrite High-Performance Ceramics
MaterialDigital 3
BMFTR 03 2025 – 02 2029
Grant Number 13XP5228C

CONSORTIUM
CeramTec GmbH (Lead)
Aixacct Systems GmbH
Ernst-Abbe-Hochschule Jena
Fraunhofer IKTS
HappyOps GmbH
KMS Technology Center GmbH
Numberland
SONOTEC GmbH
TRIDELTA Weichferrite GmbH
TU Berlin
VIA Electronic GmbH

Semantic Data Pipeline & Ontology

RESOURCES
arXiv 2606.14814
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