Joint Webinar
Ontologies in Science and Technology

19 January 2021, 3 pm

https://nfdi4chem.de
https://twitter.com/nfdi4chem
contact@nfdi4chem.de
https://lists.nfdi.de/postorius/lists/
https://www.youtube.com/channel/UCQlKQDjyYFzlUFrDfR9vVJg

https://nfdi4ing.de
https://twitter.com/nfdi4ing
contact@nfdi4ing.de

http://nfdi4cat.org
https://twitter.com/nfdi4cat
info@nfdi4cat.org
https://www.linkedin.com/company/nfdi4cat

Agenda

Moderation Dr. Dorothea Iglezakis, NFDI4Ing, University of Stuttgart, FoKUS	 Questions in the chat  Event is recorded  Slides are provided
Introduction to the NFDI Dr. Oliver Koepler, NFDI4Chem, TIB Leibniz Information Centre for Science and Technology	
Introduction to Ontologies – What is it all about? Dr. Iryna Mozgova, NFDI4Ing, LUH – Leibniz University Hannover, Dr. Oliver Koepler, NFDI4Chem	
Ontologies in CRCs from the engineering sciences Tatyana Sheveleva, TIB Leibniz Information Centre for Science and Technology	
Introduction to OntoCape Prof. Norbert Kockmann, NFDI4Cat, TU Dortmund	
Ontology Management, Knowledge Systems, Digitalization in R&D Dr. Alexander Garcia Castro, BASF	
Discussion	

Introduction to the NFDI

Dr. Oliver Koepler, Leibniz Information Centre for Science and Technology TIB

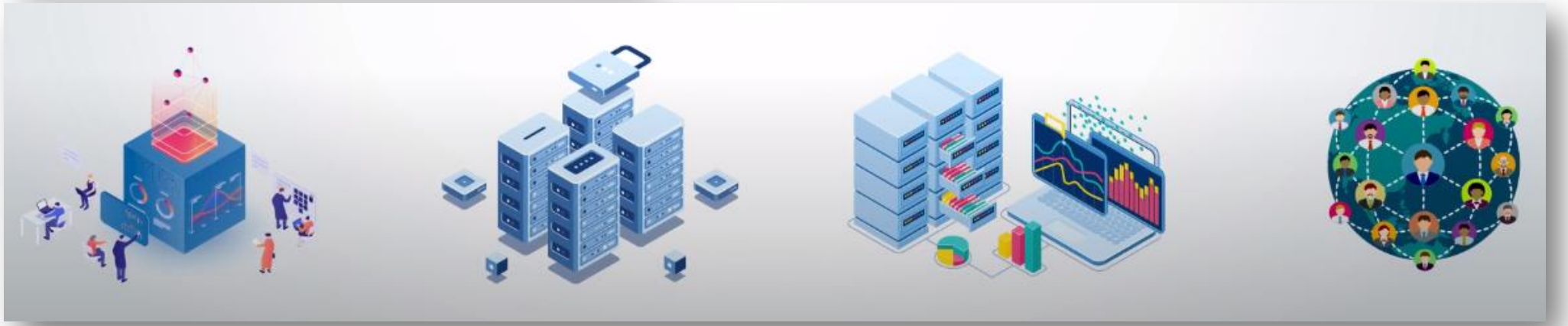
What is the NFDI?

Introduction videos by DFG

- https://www.youtube.com/watch?v=x3Cvn1vNQ98
- https://www.youtube.com/watch?v=XTzwPwMAqHM

FAIR Data Principles

Findable, **A**ccessible, **I**nteroperable and **R**e-usable

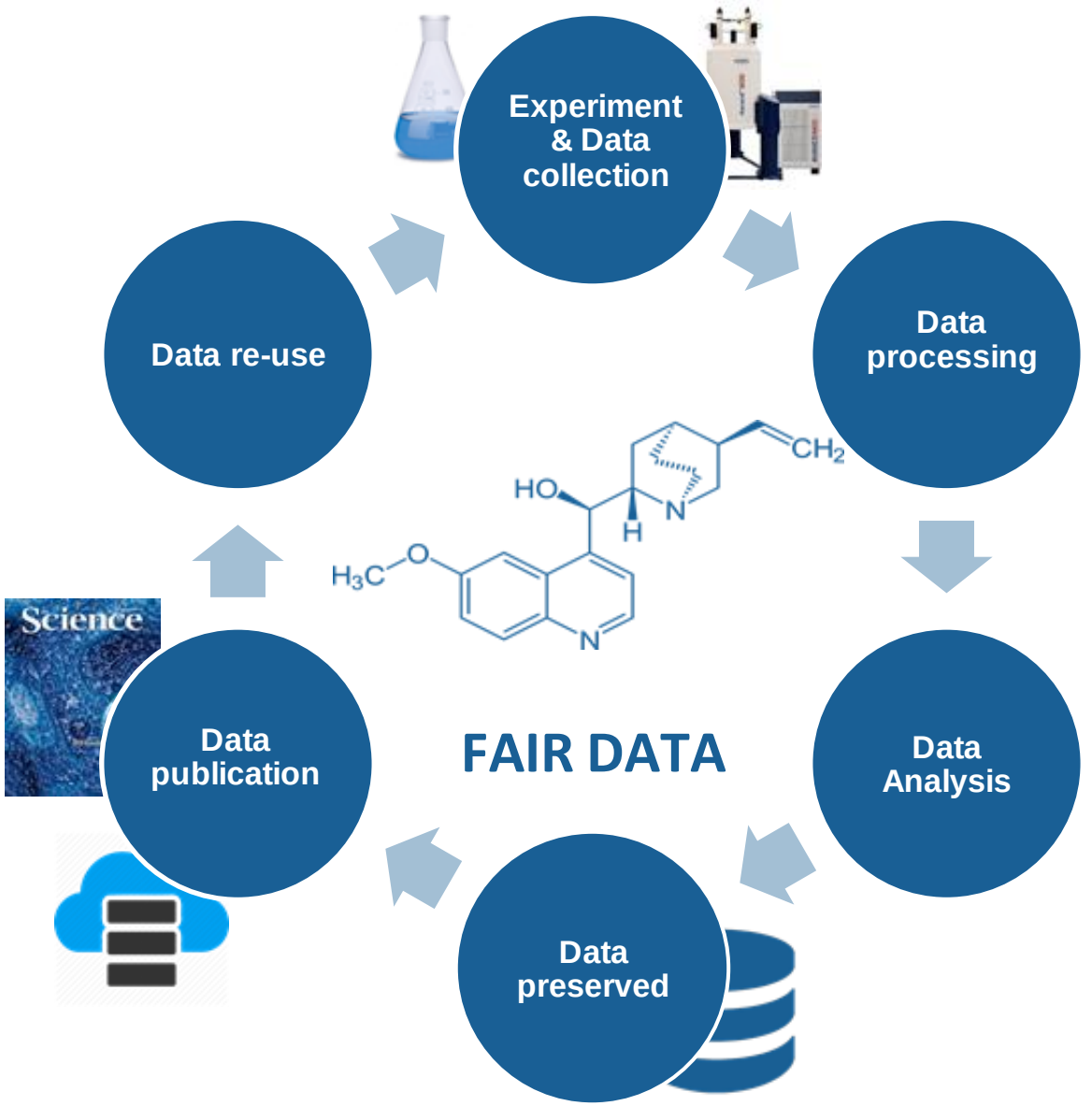


Source: What is the National Research Data Infrastructure (NFDI)?, DFG, https://www.youtube.com/watch?v=x3Cvn1vNQ98

Our Vision

1927

- Digitalisation
- Standards
- Community



NATIONALE FORSCHUNGS-
DATENINFRASTRUKTUR FÜR DIE
INGENIEURWISSENSCHAFTEN

NFDI4Ing

National research data infrastructure for the engineering sciences

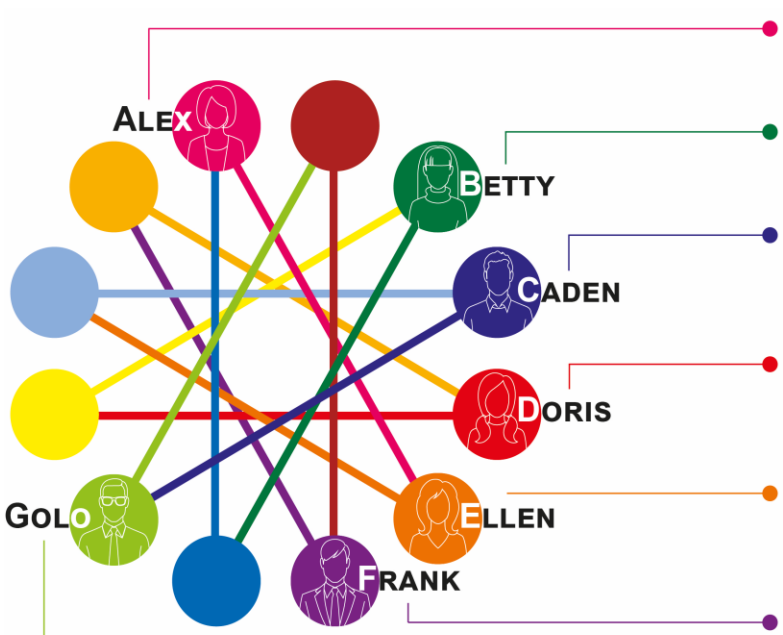
www.nfdi4ing.de

7 Archetypes

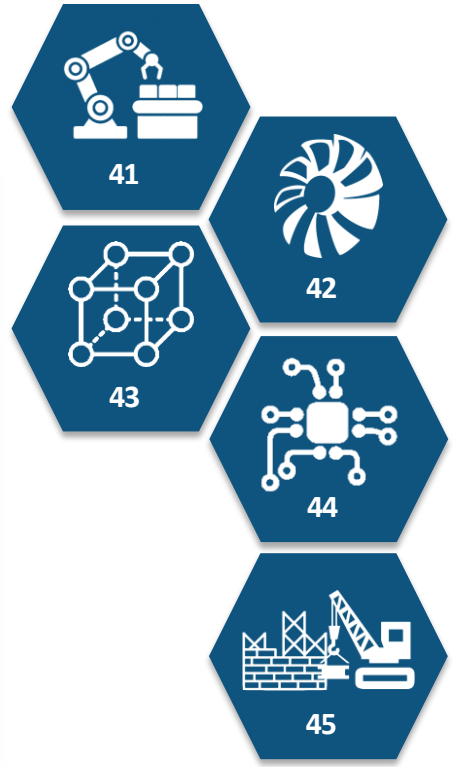
Management

Base Services

Community Clusters

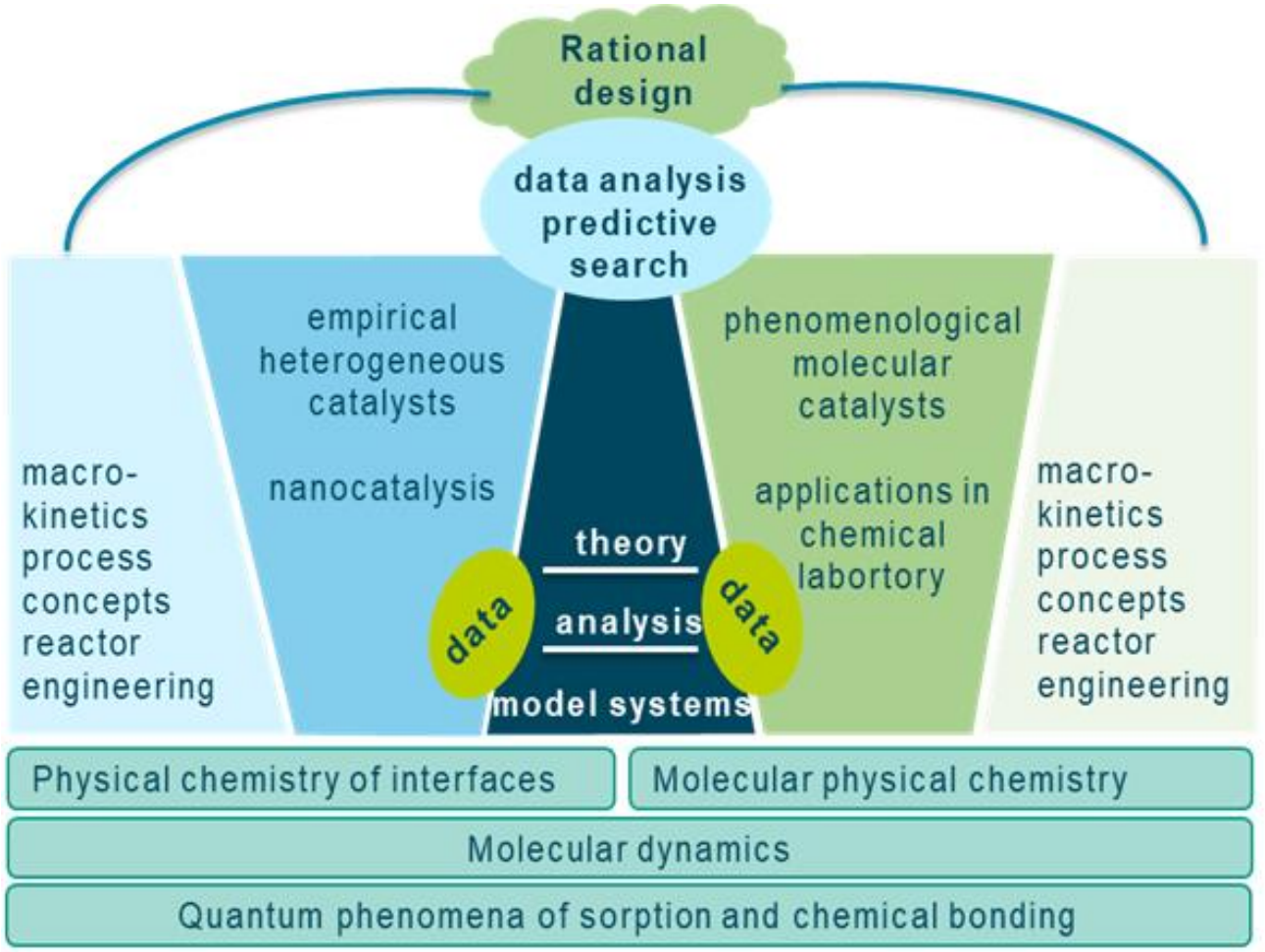


- Bespoke experiments
- Engineering research software
- Provenance tracking of physical samples and data samples
- High performance measurement and computation with very large data
- Extensive and heterogeneous data requirements
- Many participants and simultaneous devices
- Field data and distributed systems



Our Ambition: Digital Catalysis

- Bringing “digital catalysis” into action.
- Cross-disciplinary research in fundamental and applied catalysis.
- Improve digital and RDM skills in the community.
- Use of open well-defined data structures and metadata standards.
- Facilitate collaboration on data level.
- Provide education and training.



Introduction to Ontologies

–

What is it all about?

Dr. Oliver Koepler, Leibniz Information Centre for Science and Technology TIB
Cord Wiljes, Bielefeld Center for Data Science, Bielefeld University
Dr. Iryna Mozgova, Leibniz University Hannover

„Wouldn‘t it be great if we would be able to combine any dataset with any other dataset we would want to?“

EOSC Strategic Implementation Plan, p.4

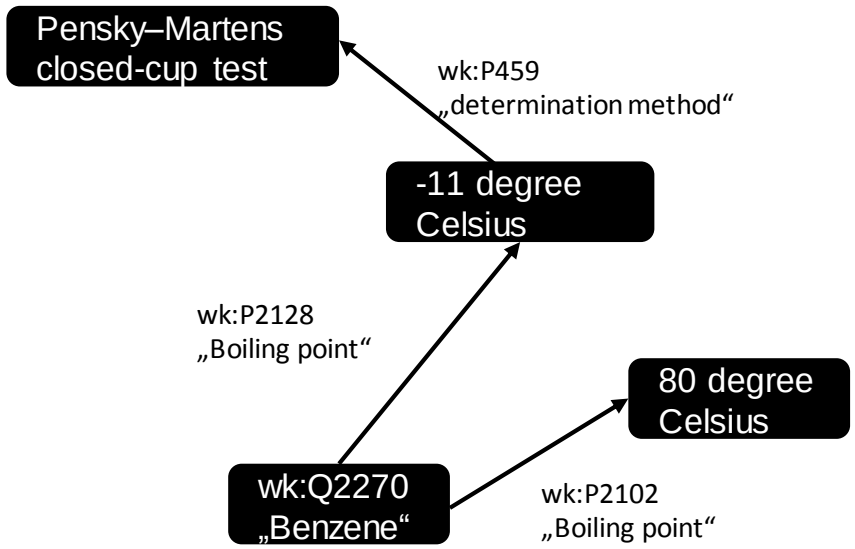
Research Data and Ontologies

Why are Ontologies important for Research Data Management?

	T	T	T
Ethanol	78	14	369
Methanol	65	11	455
n-Octane	126	12	210
Isooctane	99	-12	410
Benzene	80	-11	555

Research Data and Ontologies

Why are Ontologies important for Research Data Management?



	Boiling temperature T [°C]	Flash temperature T [°C]	Autoignition temperature T [°C]
Ethanol	78	14	369
Methanol	65	11	455
n-Octane	126	12	210
Isooctane	99	-12	410
Benzene	80	-11	555

Simplified RDF-like statements for Benzene: https://www.wikidata.org/wiki/Q2270

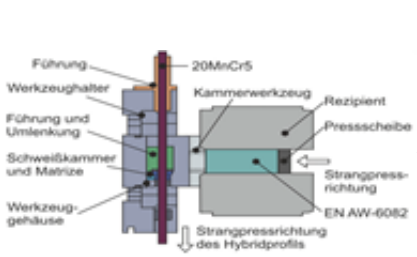
How ?

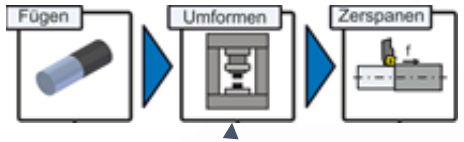
What is the most efficient and affordable catalyst for my hydroformylation?

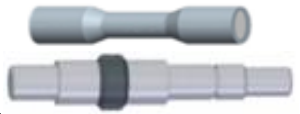
I would like to retrieve the data on all samples forged on 09/28/2020.

Show me all molecules having a biological activity similiar to my molecule?

Describing things in engineering sciences







20MnCr5/
EN AW6082

84 mm

∅ 68 mm

?

?

?

REAL WORLD

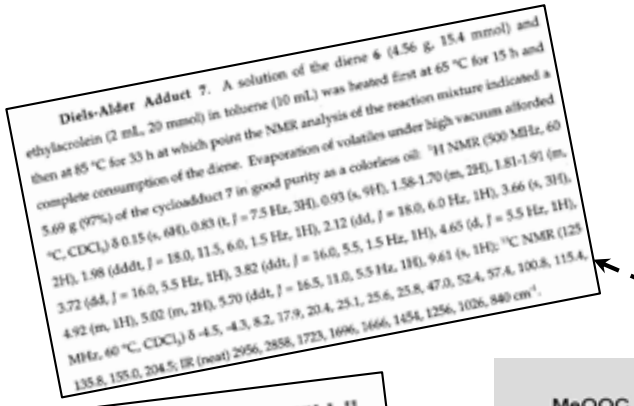
visualization/presentation understandable for people

machine-readable representation of properties and relations to other objects in the environment

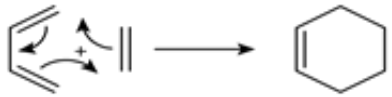
machine-readable language-independent designation

DIGITAL WORLD

Describing things in chemistry

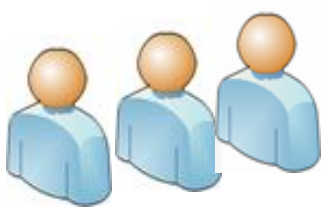


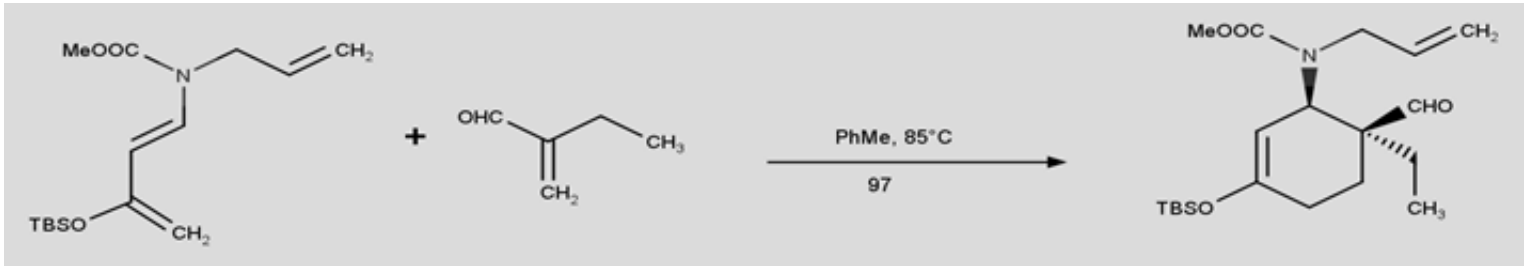
Diels-Alder Adduct 7. A solution of the diene 6 (4.56 g, 15.4 mmol) and ethylacrolein (2 mL, 20 mmol) in toluene (10 mL) was heated first at 65 °C for 15 h and then at 85 °C for 33 h at which point the NMR analysis of the reaction mixture indicated a complete consumption of the diene. Evaporation of volatiles under high vacuum afforded 5.69 g (97%) of the cycloadduct 7 in good purity as a colorless oil. ^{1}H NMR (500 MHz, 60 °C, $CDCl_3$) δ 0.15 (s, 6H), 0.83 (t, J = 7.5 Hz, 3H), 0.93 (s, 9H), 1.58-1.70 (m, 2H), 1.81-1.91 (m, 2H), 1.98 (dddt, J = 18.0, 11.5, 6.0, 1.5 Hz, 1H), 2.12 (dd, J = 18.0, 6.0 Hz, 1H), 3.66 (s, 3H), 3.72 (dd, J = 16.0, 5.5 Hz, 1H), 3.82 (ddt, J = 16.0, 5.5, 1.5 Hz, 1H), 4.65 (d, J = 5.5 Hz, 1H), 4.92 (m, 1H), 5.02 (m, 2H), 5.70 (ddt, J = 16.5, 11.0, 5.5 Hz, 1H), 9.61 (s, 1H). ^{13}C NMR (125 MHz, 60 °C, $CDCl_3$) δ -4.5, -4.3, 8.2, 17.9, 20.4, 25.1, 25.6, 25.8, 47.0, 52.4, 57.4, 100.8, 115.4, 135.8, 155.0, 204.5; IR (neat) 2956, 2858, 1723, 1696, 1666, 1454, 1256, 1026, 840 cm^{-1}.



Diels – Alder reaction

Conjugated (substituted) Diene reacts with substittued alkene to substituted cyclohexene





?

?

?

REAL WORLD

Open and machine-readable data formats for spectra

machine-readable representation of properties and relations to other objects

Open and machine-readable data formats for chemical structure and reactions

DIGITAL WORLD

https://pubs.acs.org/doi/10.1021/ja983198k

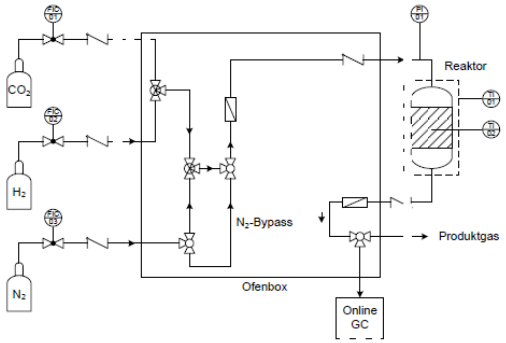
NFDi4ing

nfdi4chem

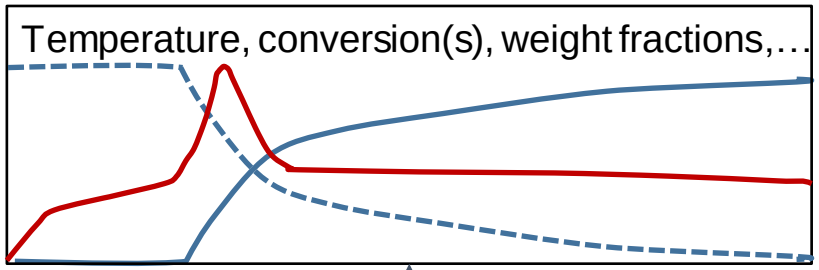
NFDI4Cat

Describing things in catalysis and chemical engineering

process and product



Overall setup



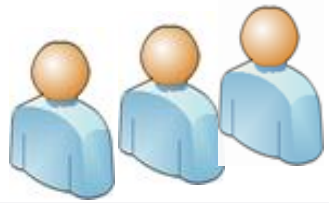
Reactor dimensions,
Massflow,
Catalyst,
Heating/Cooling,
…

Scale-Up,
Catalyst,
Reaction rate parameters,
Mass transport coefficients,
Thermokinetic parameters,
Reactor stability

Inlet stream
($T, p_i, c_i, m_{in,i}$)

packed bed reactor

Outlet stream
($T, p, c_i, m_{out,i}$)



REAL WORLD

Visualization/ presentation understandable for community

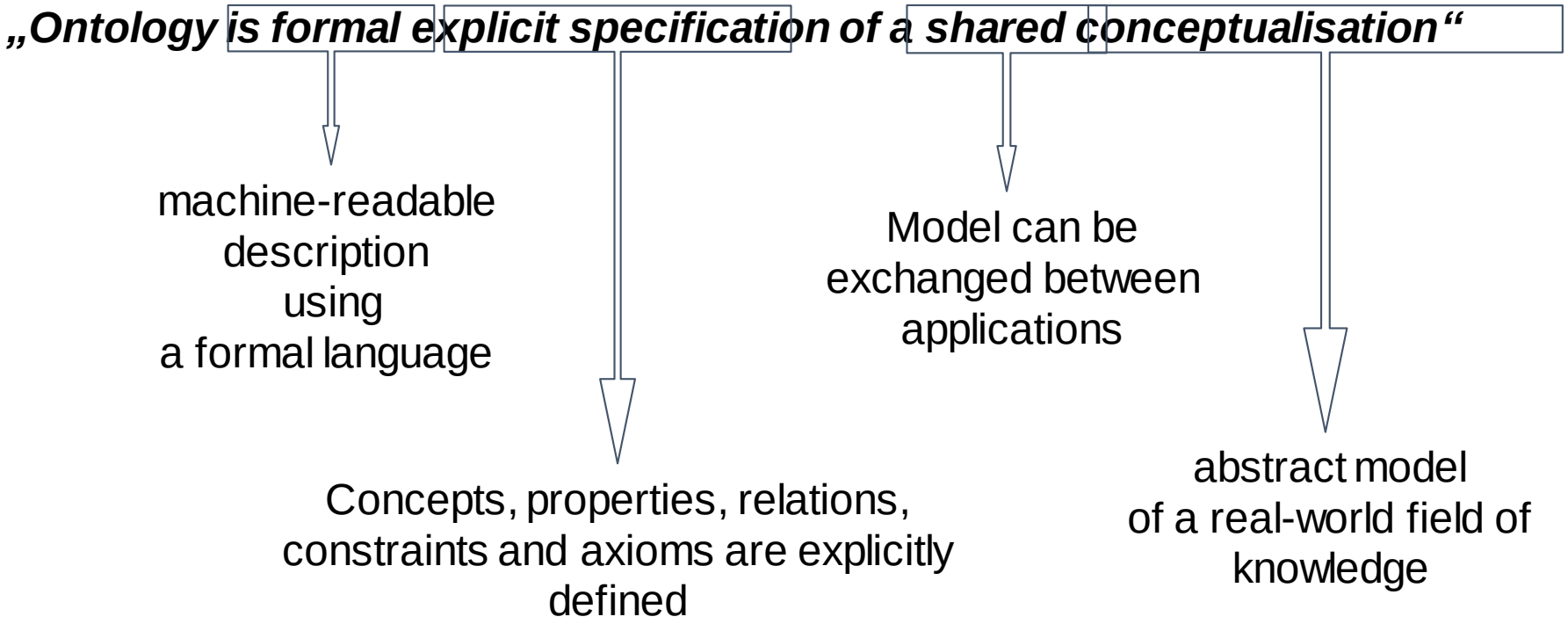
machine-readable representation of properties and relations to other objects in the environment, exchange within the user community

machine-readable language-independent designation

DIGITAL WORLD

Alexander Behr, **2020**

Ontology



R. Studer, R. Benjamins, and D. Fensel. Knowledge engineering: Principles and methods. Data & Knowledge Engineering, 25(1–2):161–198, 1998

Semiotic Triangle

… Ethanol

„organic compound with at least one hydroxyl group bound to a satured carbon atom ….“

shared concept

Ethanol

Wodka

Methanol

Concept

awakens

refers to

Symbol

“Alcohol”

stands for

Object

Syntax

Semantics

Pragmatics

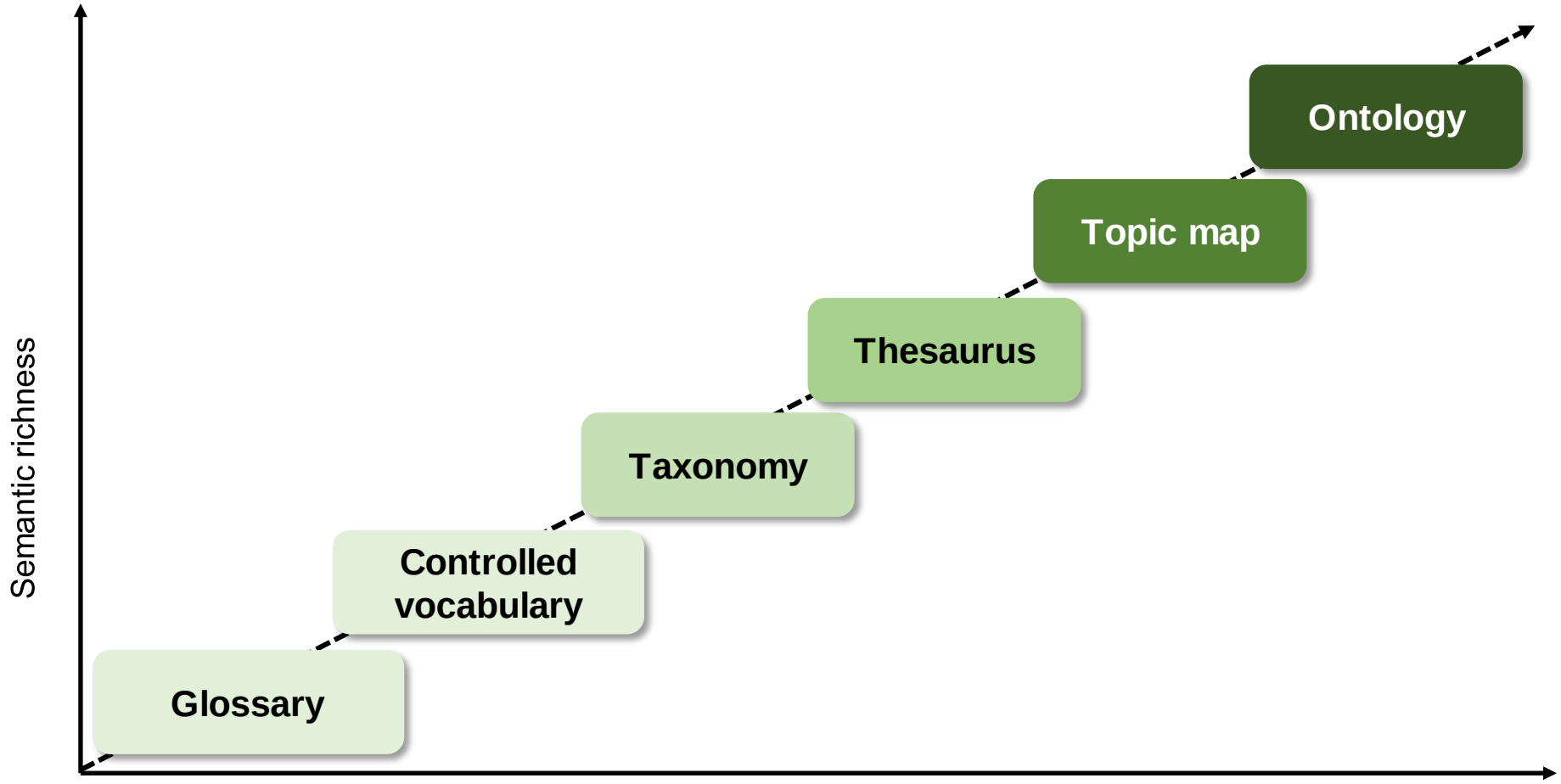
Experience

Context

Kamil_Śliwiński,_Pernod_Ricard_Poland,_CC_BY-SA_3.0

https://www.analytics-shop.com/

Formalization - Semantic staircase



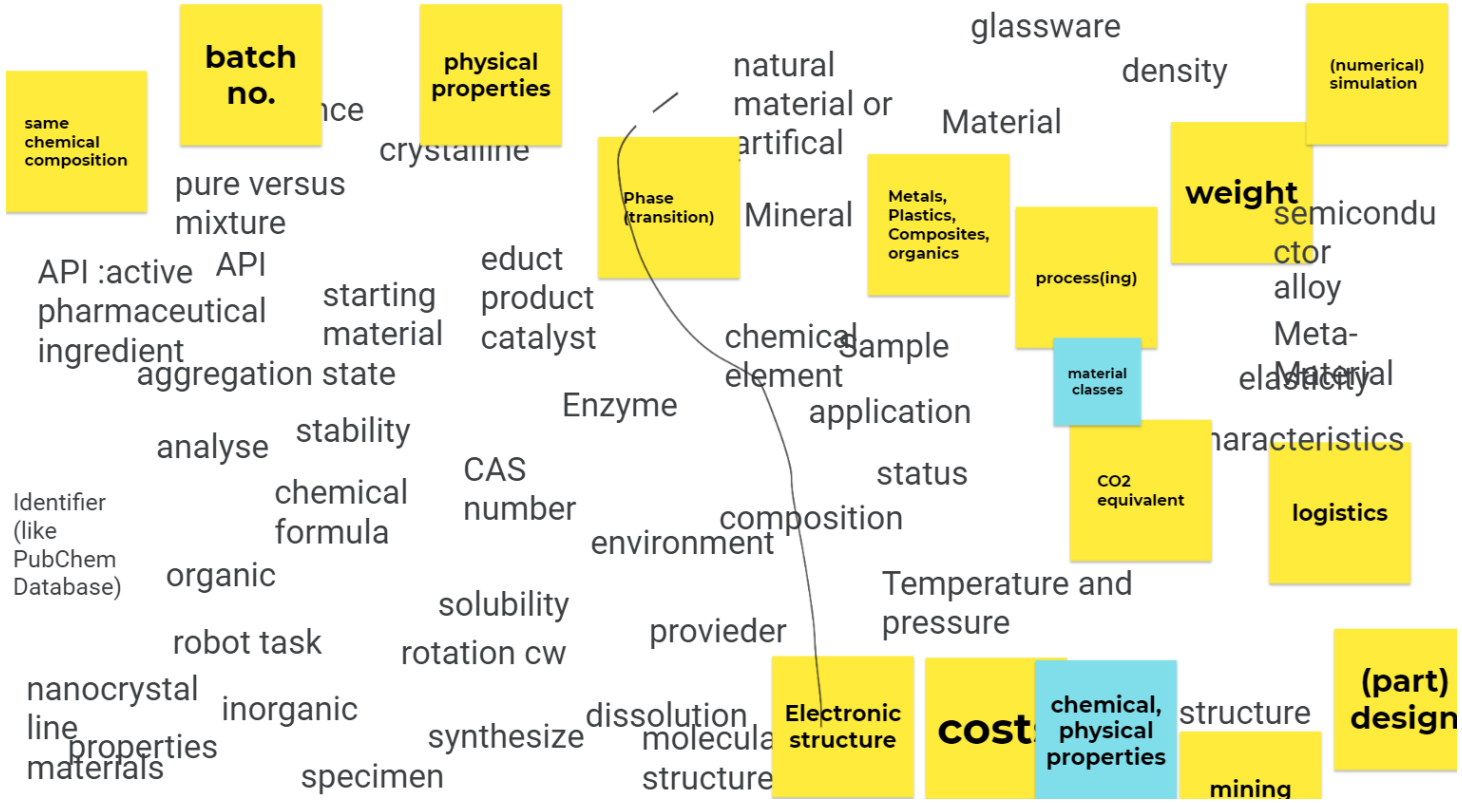
Source: According Dengel, A.: Semantic technologies : foundations - concepts - applications. Heidelberg: Spektrum Akademischer Verlag, 2012

Practical exercise

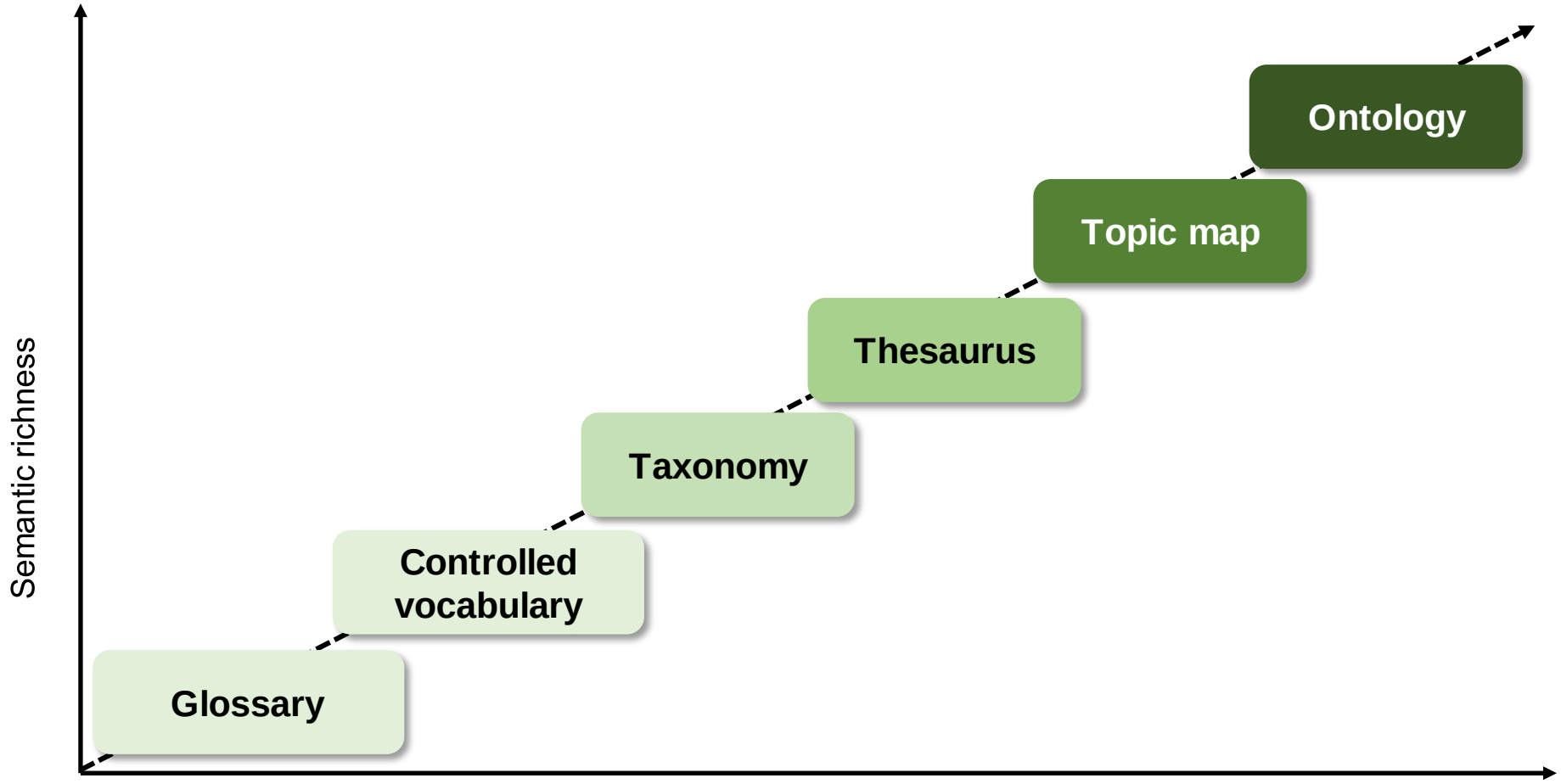
Describe your world

Which terms are relevant to the topic of "substance" or "material" in your research work?

Result:



Formalization - Semantic staircase



Source: According Dengel, A.: Semantic technologies : foundations - concepts - applications. Heidelberg: Spektrum Akademischer Verlag, 2012

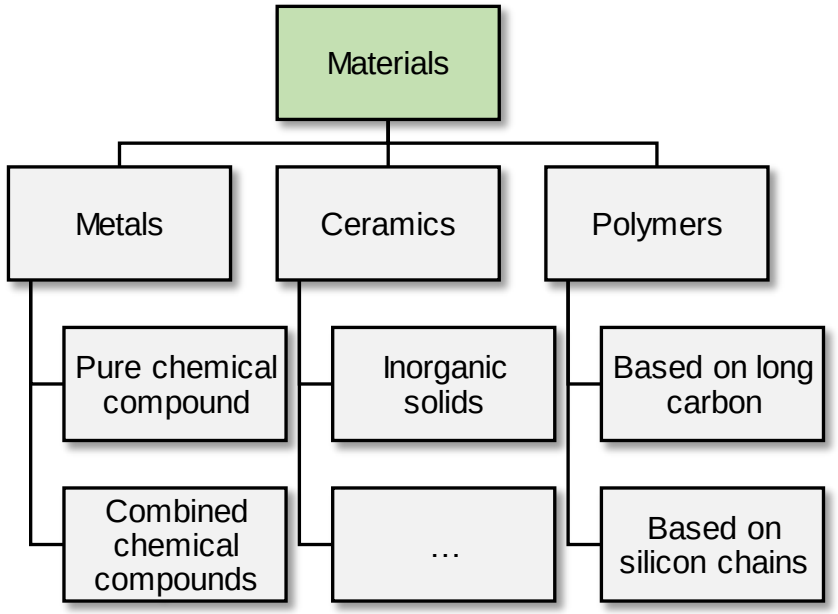
Controlled vocabulary and taxonomy

Controlled vocabulary

- **Set of terms** (vocabulary) of a knowledge domain
- Designations are **clearly** assigned to terms for example in the form of glossaries or reference works

Taxonomy

- **Hierarchical class division of** terms of a knowledge domain
- Describes superordinate and subordinate relationships
- The basis is a closed and specific vocabulary



Example of a material taxonomy

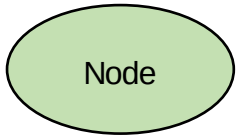
Topical map

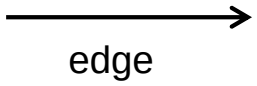
Formal models consist of

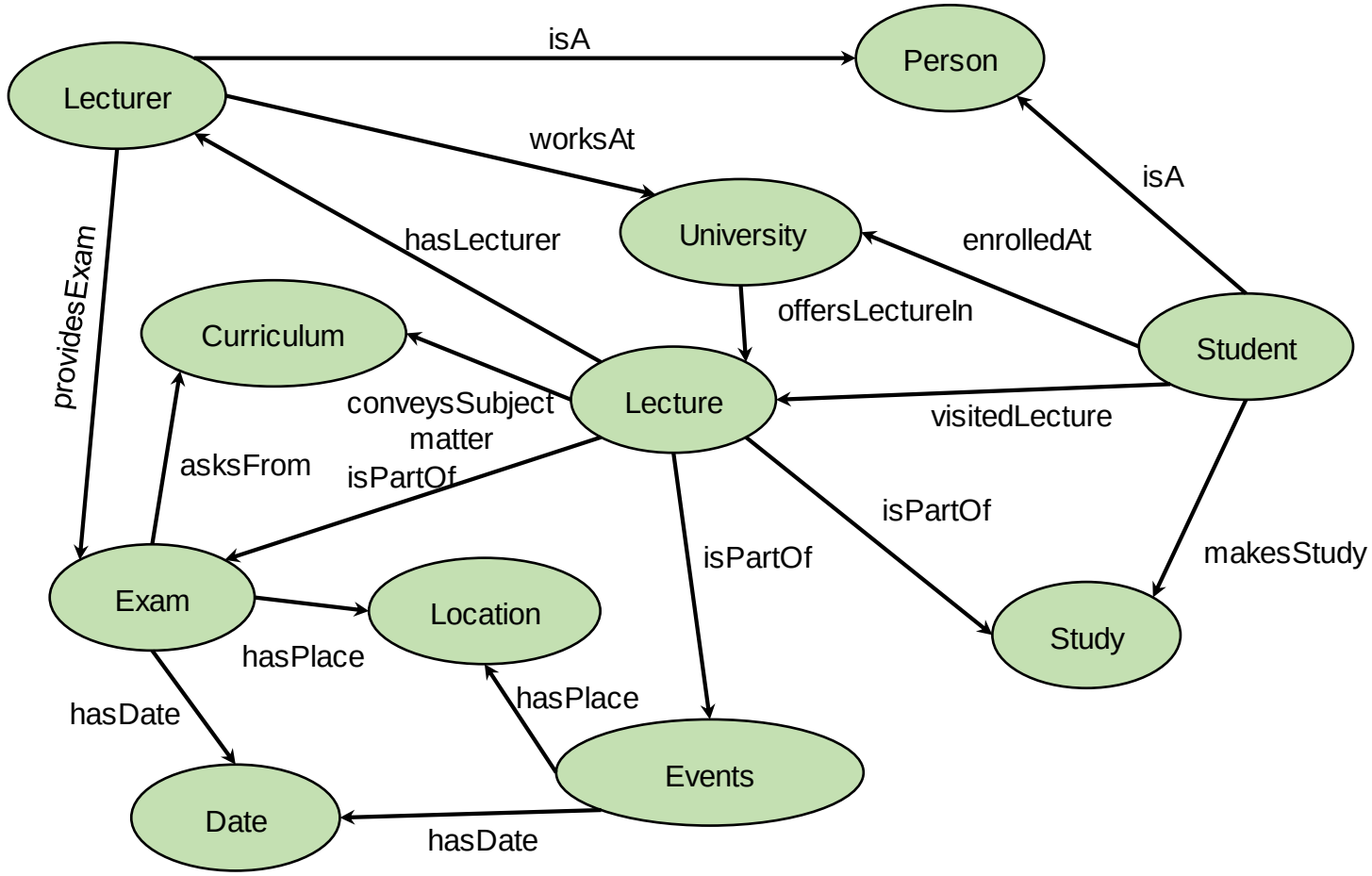
- Concepts: concrete objects or a class of objects
- Relations: conceptual relationships

Allows description of complicated relationships between concepts

Representation in graph form

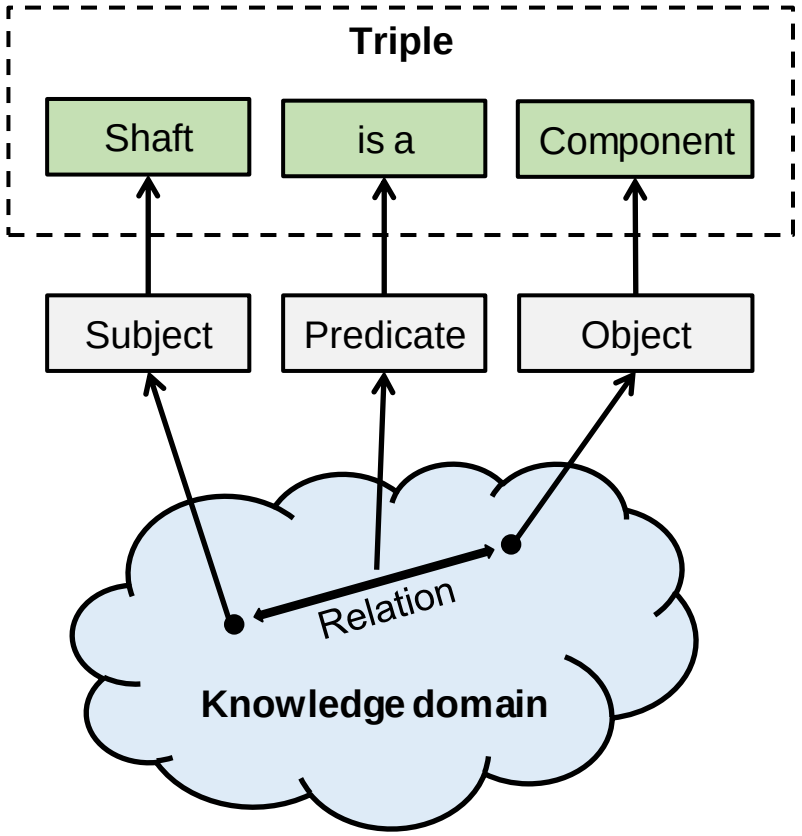
- Concept 

- Relation 



Formalization of statements

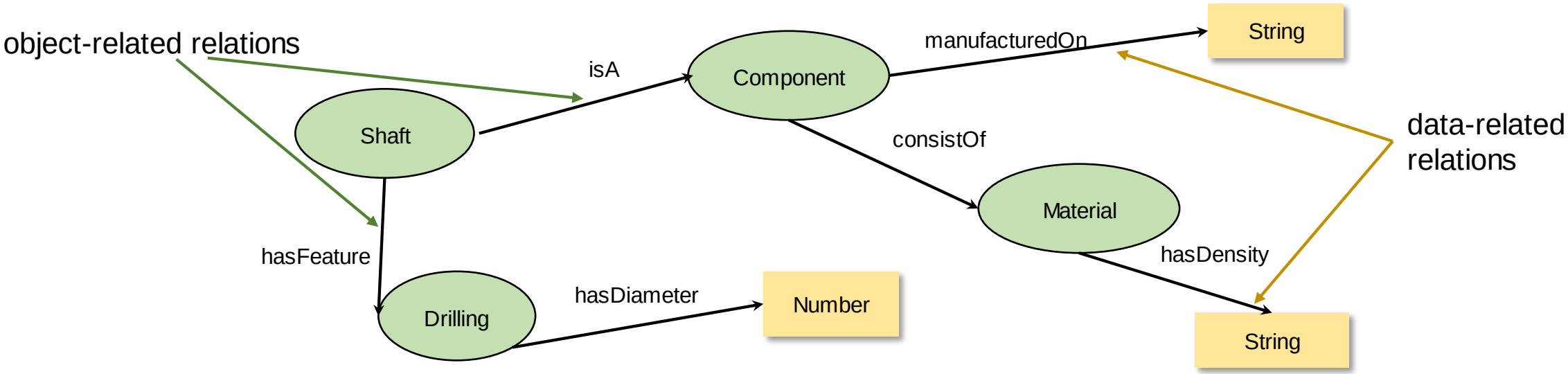
- Formalization is done via triples based on natural language
- Consist of a **subject**, a **predicate** and an **object**
- Subject and object are objects of a domain of knowledge
- Predicate represents the **relationship** between subject and object
- Triples are a formal requirement and can be processed by machines



Construction of an Ontology: logical connection of several triples

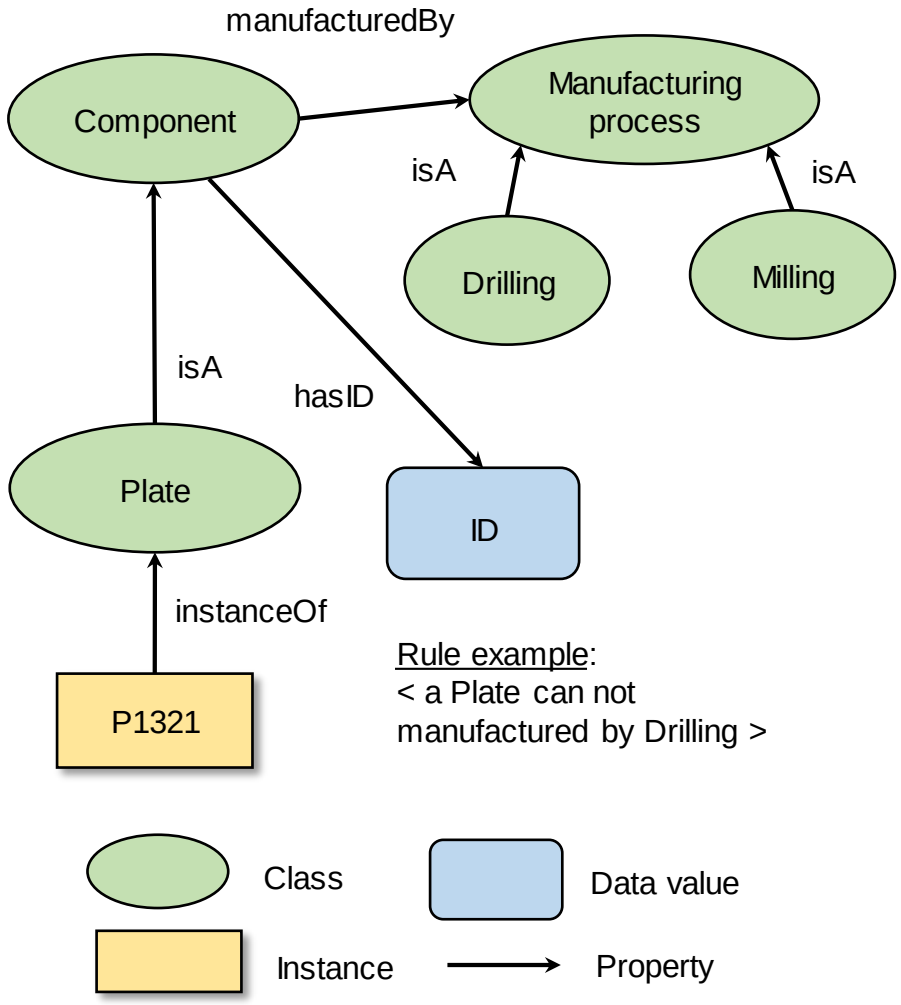
Relations are distinguished

- object-related relations describe relations between two classes
- data-related relations assign certain properties to classes, for example in the form of strings or numbers



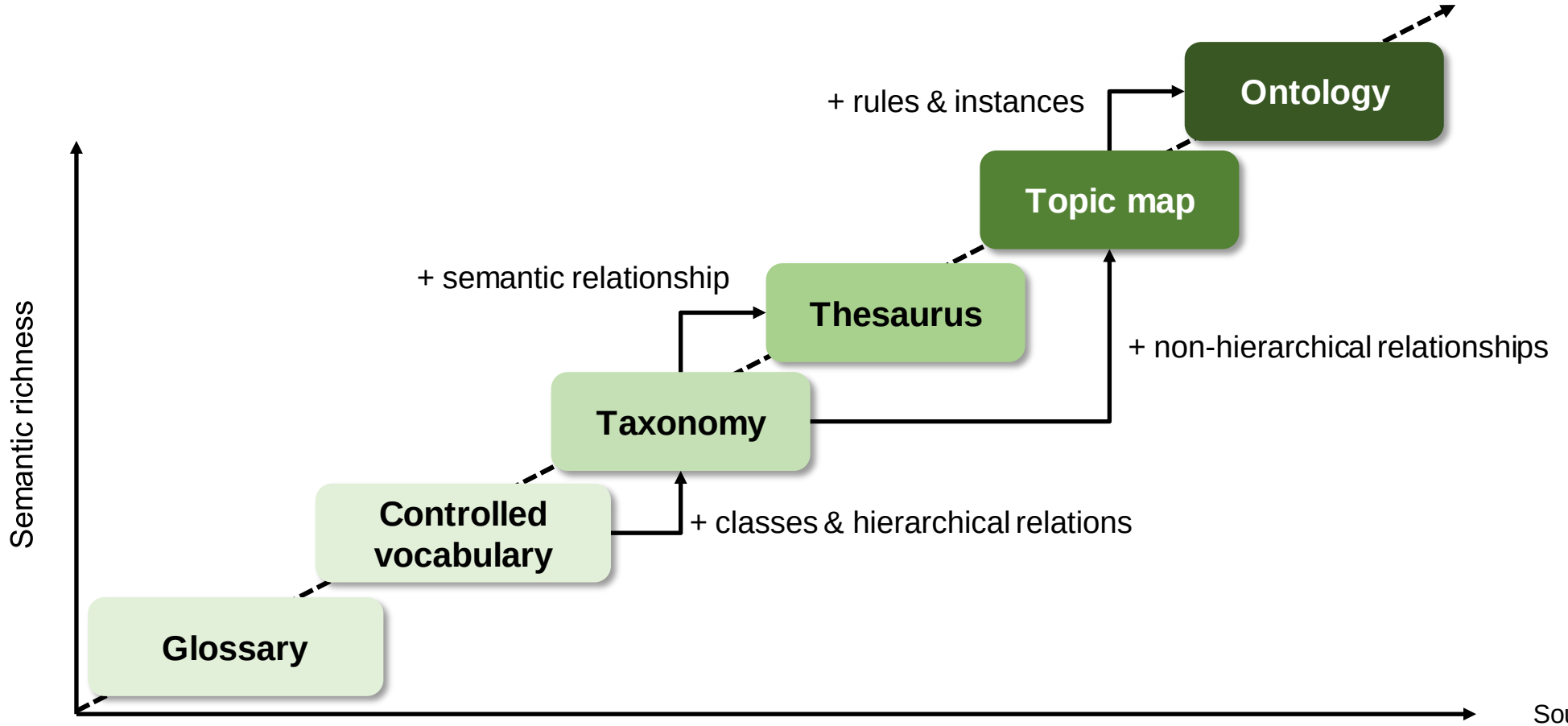
Ontology

- Ontology is a formal explicit specification of a shared conceptualization
- Allows the modeling of complicated knowledge contexts
- Usually consist of four components:
  - Classes describe the various concept categories; often in the form of a taxonomy.
  - Relations describe relationships between two classes or between a class and properties.
  - Instances represent real existing elements within a domain. Instances of a class with similar characteristics are grouped together in a class.
  - Rules are used to describe circumstances in the domain, which must always be true.



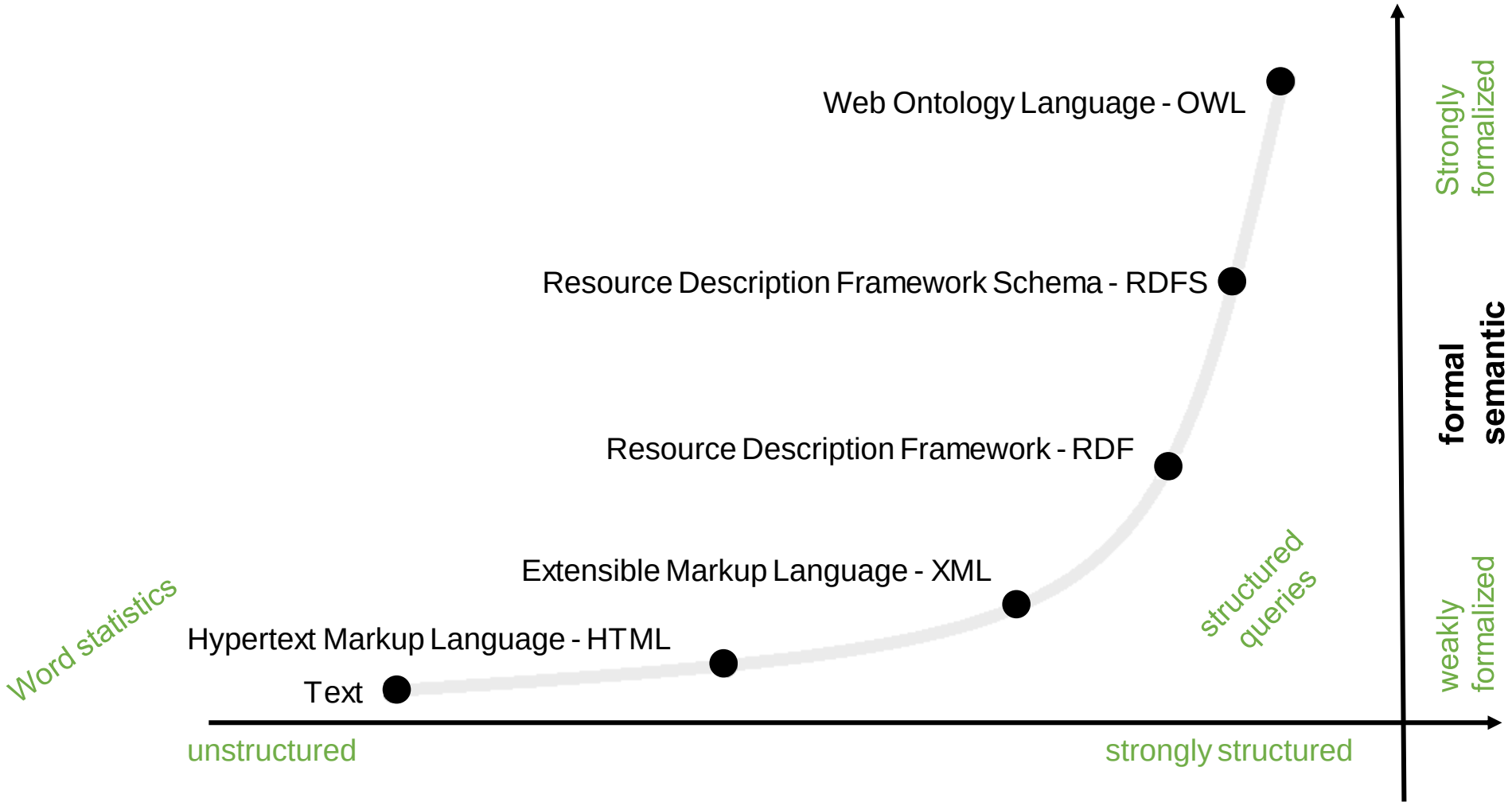
Formalization - Semantic staircase

Ontologies are a form of knowledge representation to provide formalized knowledge for machine services. They are knowledge models that describe parts of the world.



Source: Dengel, 2012

Knowledge presentation with semantic technologies

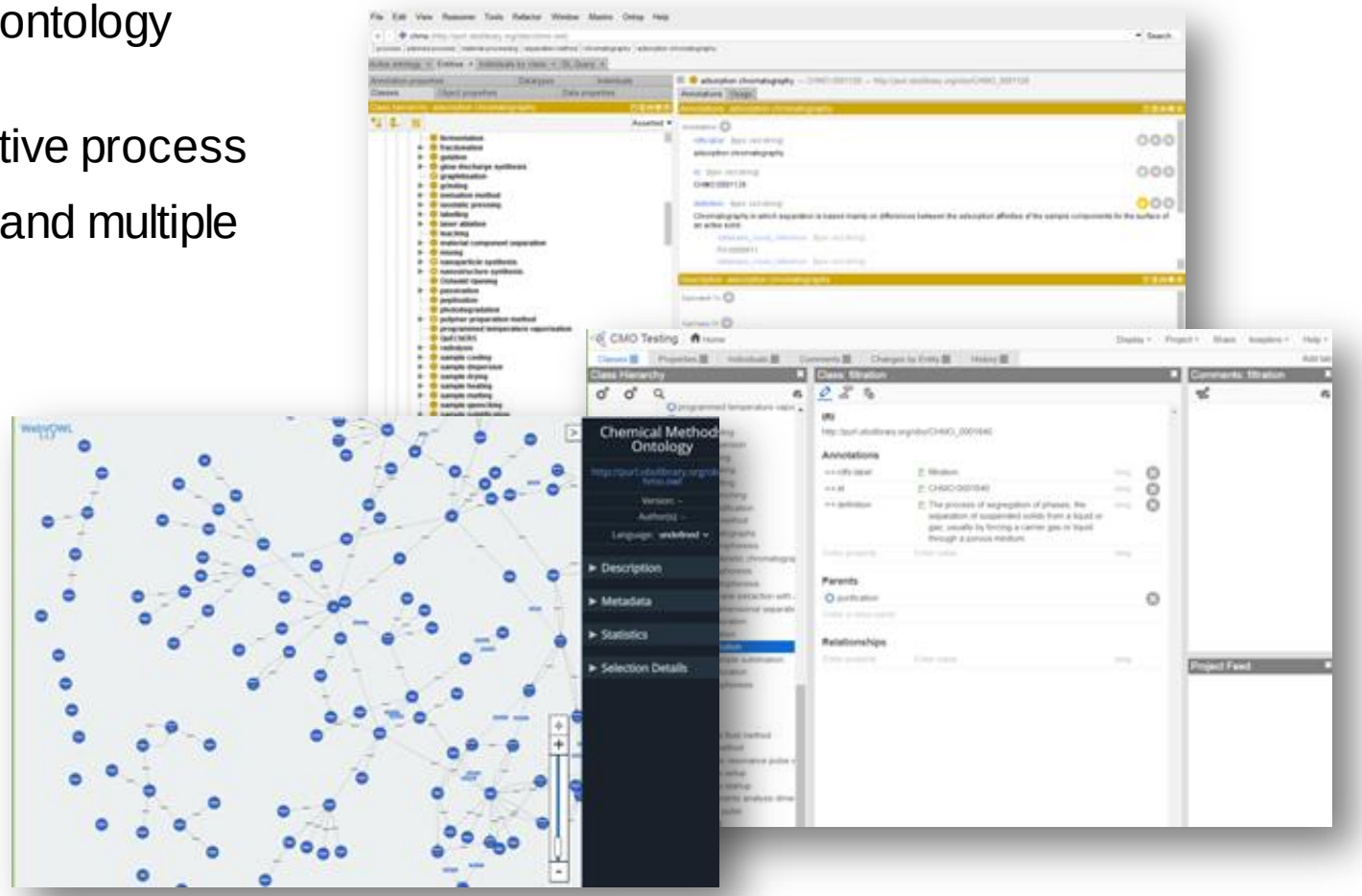


Development of an Ontology: Methods and Tools

- There is no single correct approach to ontology modeling
- Ontology modeling is a multi-step iterative process
- There are always alternative solutions and multiple ontology variants

Ontology curation tools

- Protegé
- Web-Protegé
- WebVowl



Looking forward: Existing ontologies for our domains

chmo	Chemical Methods	CHMO, the chemical methods ontology, describes methods used to collect data in chemical experiments
rxno / mop	Name reaction ontology	It contains more than 500 classes representing organic reactions such as the Diels–Alder cyclization. MOP contains the underlying molecular processes, for example cyclization, methylation and demethylation.
Chebi	Chemical Entities of Biological Interest	A structured classification of molecular entities of biological interest focusing on 'small' chemical compounds
cheminf	Chemical Information	Includes terms for the descriptors commonly used in cheminformatics software applications and the algorithms which generate them
chiro	CHEBI Integrated Role	CHEBI provides a distinct role hierarchy. Chemicals in the structural hierarchy are connected via a 'has role' relation. CHIRO provides links from these roles to useful other classes in other ontologies.
fix	Physico-chemical methods and properties	An ontology of physico-chemical methods and properties
rex	Physico-chemical process	An ontology of physico-chemical processes, i.e. physico-chemical changes occurring in course of time

Looking forward: Existing ontologies for our domains

CORA	Core Ontologies for Robotics and Automation	IEEE1872-owl is an OWL specification of the Core Ontology for Robotics and Automation (CORA) and other ontologies ontologies that give support to CORA in IEEE 1872-2015 standard. https://doi.org/10.1109/IEEESTD.2015.7084073
MSDL	Manufacturing Service Description Language	Manufacturing Service Description Language (MSDL) is an ontology for representation of manufacturing services. MSDL provides the primitive building blocks required for description of a wide spectrum of manufacturing services. Description Logic is used as the knowledge representation formalism of MSDL in order to make it amenable to automatic reasoning. https://doi.org/10.1115/DETC2006-99600
MobiVoc	Open Mobility Vocabulary	MobiVoc is a standardized vocabulary for mobility data. Currently, the following topics are covered: Electric Charging Points, Parking Facilities, Highway Roadworks sites.
SEAS	Thermodynamic System ontology	The SEAS Thermodynamic System ontology defines systems that may exchange heat.
OntoCape	Process engineering domain	OntoCAPE is a large-scale ontology for the domain of Computer Aided Process Engineering (CAPE).

Where can you find ontologies?

Ontology Registries

- Obofoundry
- Bioportal
- Ontology Lookup Service OLS
- Linked Open Vocabularies LOV

Introduction to Ontologies
–
What is it all about?

Dr. Oliver Koepler, Leibniz Information Centre for Science and Technology TIB
Cord Wiljes, Bielefeld Center for Data Science, Bielefeld University
Dr. Iryna Mozgova, Leibniz University Hannover

LEIBNIZ INFORMATION CENTRE
FOR SCIENCE AND TECHNOLOGY
UNIVERSITY LIBRARY

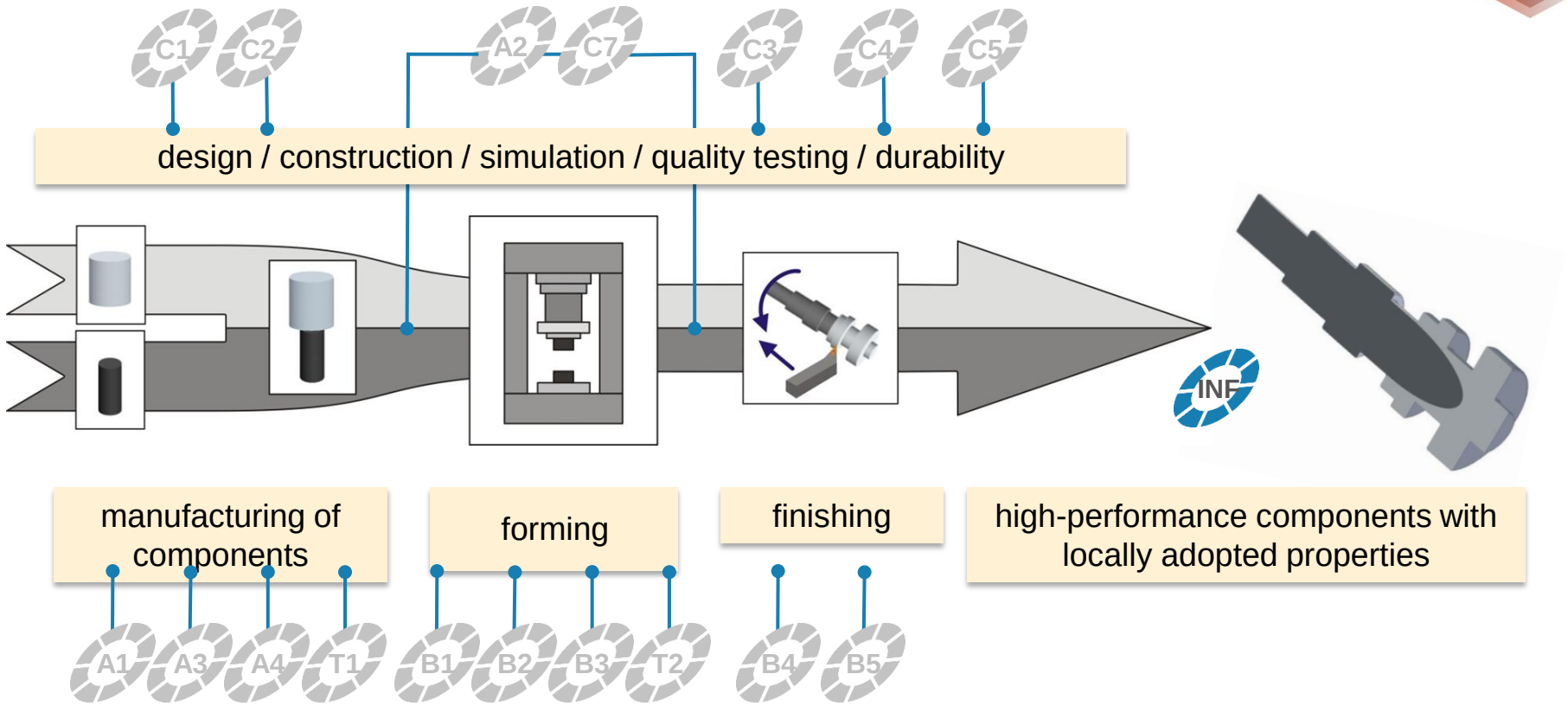
TIB

Ontologies in the CRCs 1153 and 1368 in the scope of engineering sciences

Tatyana Sheveleva,
19. January 2021
Joint Webinar Ontologies in Science and Technology

Leibniz Association

Collaborative Research Centre 1153 Tailored-Forming



IFUM Institut für Umformtechnik und Umformmaschinen

IFW Institut für Fertigungstechnik und Werkzeugmaschinen

match Institut für Montagetechnik

IW Institut für Werkstoffkunde

IMKT Institut für Maschinenkonstruktion und Tribologie

IPH Institut für Integrierte Produktion Hannover

iPeG Institut für Produktentwicklung und Gerätebau

LZH Laser Zentrum Hannover e.V.

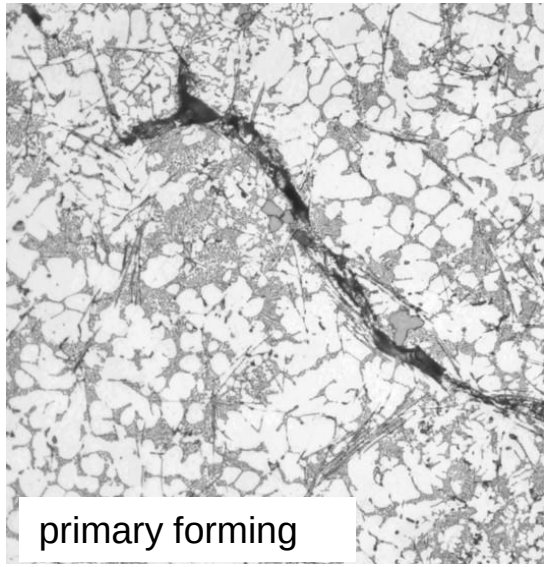
imr Institut für Mess- und Regelungstechnik

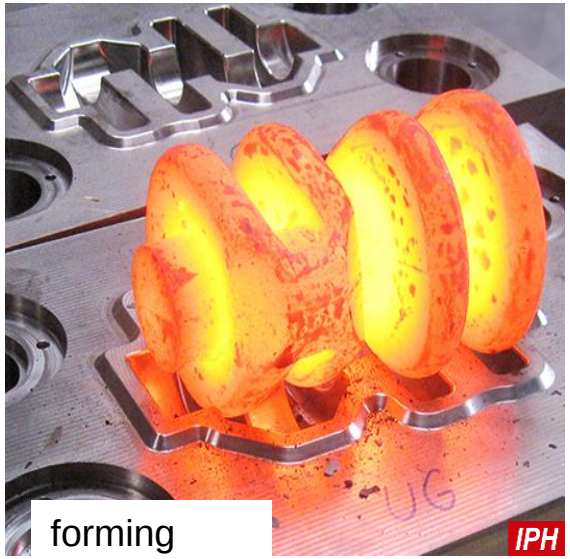
Institut für Kontinuumsmechanik

IDS Institut für Dynamik und Schwingungen

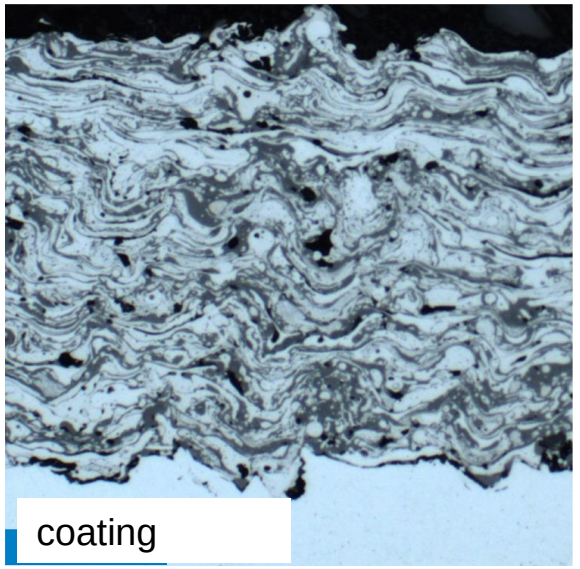
TIB Leibniz-Informationszentrum Technik und Naturwissenschaften Universitätsbibliothek

Collaborative Research Centre 1368 Oxigen-free Production


primary forming



forming


coating

separation

Leibniz Universität Hannover

LZH LASER ZENTRUM HANNOVER e.V.

TU Clausthal
Institut für
Mechanische Verfahrenstechnik

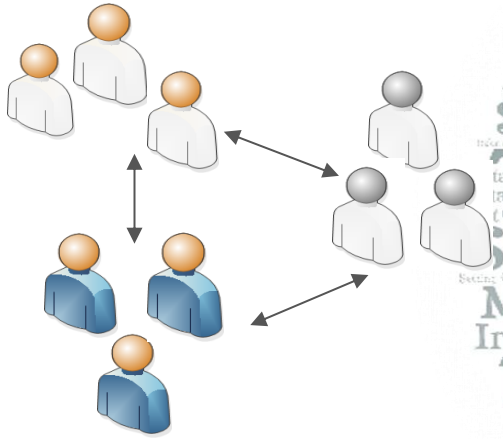
IW IFW IMPT IPH iPeG Institut für Technische Mechanik

TU Clausthal
Institut für Energieforschung und
Physikalische Technologien

IFUM match ITA IVS Clausthaler Zentrum für Materialtechnik SWZ Clausthal - Göttingen Simulation Science Center

Challenges of the Collaborative Research Centres

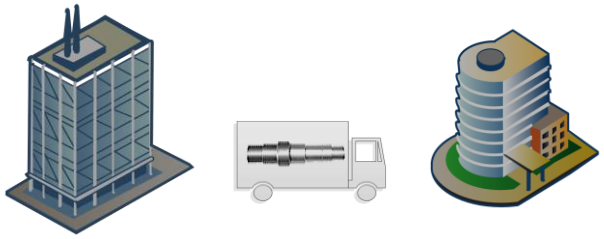
Research Groups



Research Activities

Research Objectives

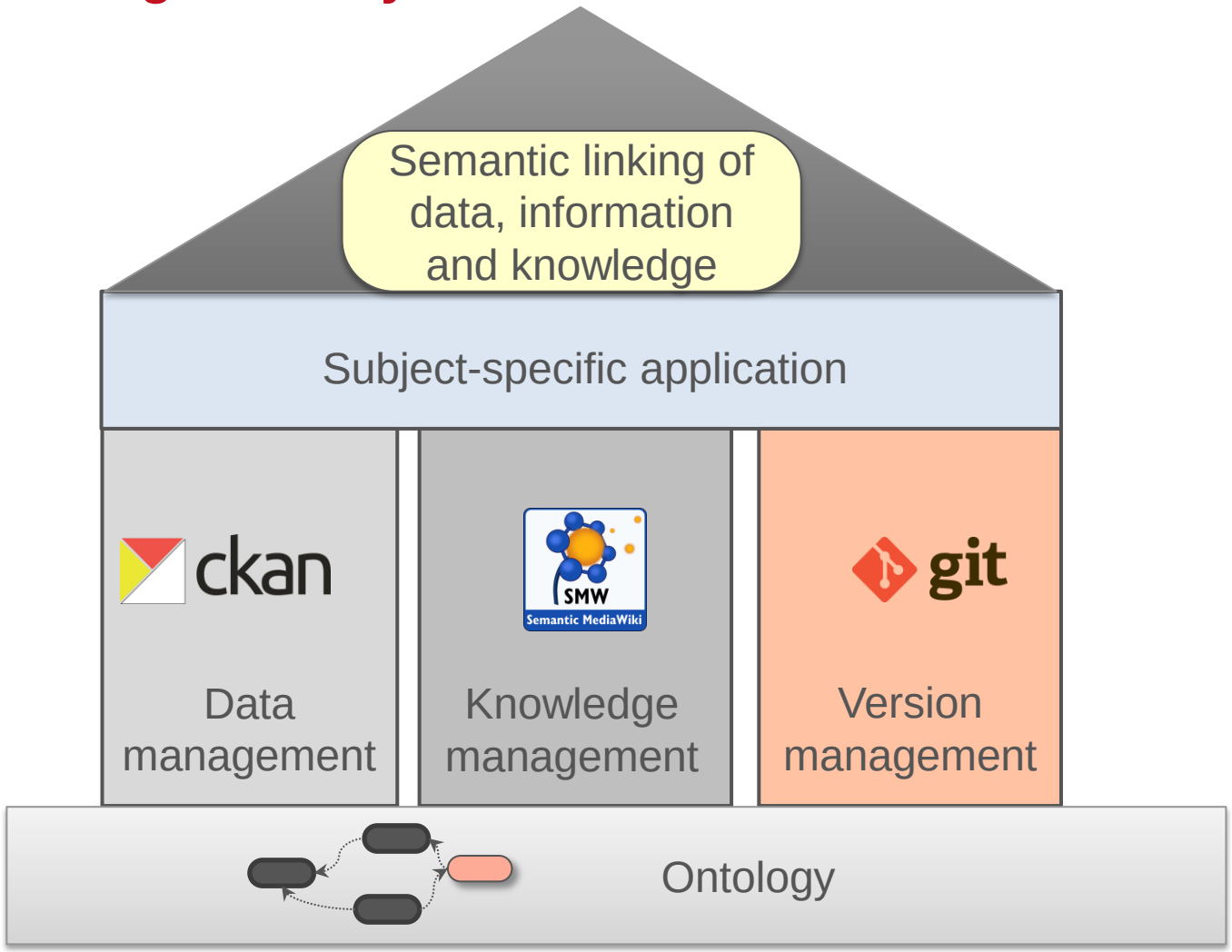
Transfer



Research Equipment

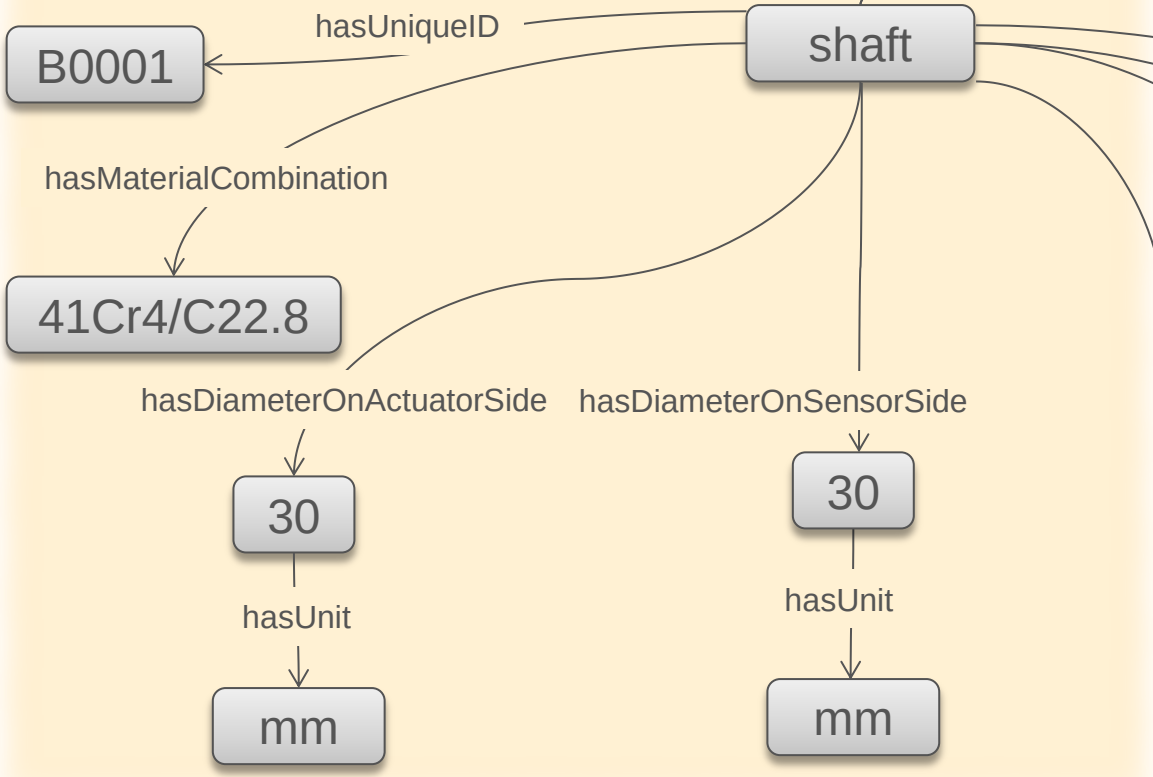
Image source: https://www.hoffmann-group.com/DE/de/hom/Monozerspanung/VHM-Fr%C3%A4ser/VHM-Fr%C3%A4ser-AlCrN/p/202275

Research Data Management System

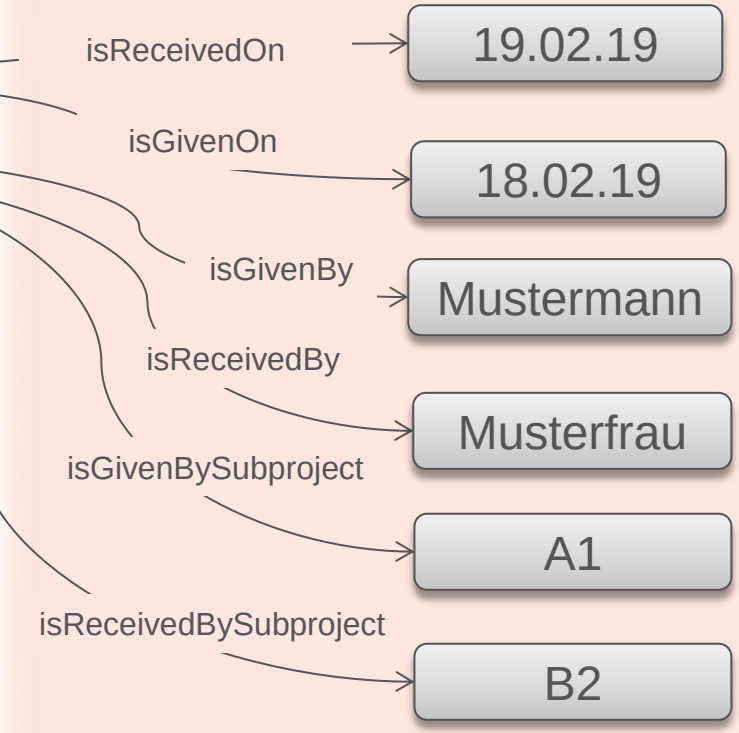


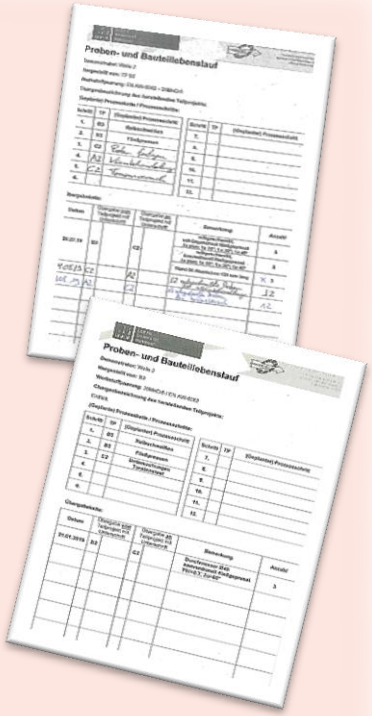
Sample Description and Tracking

Sample Characterization



Sample Tracking

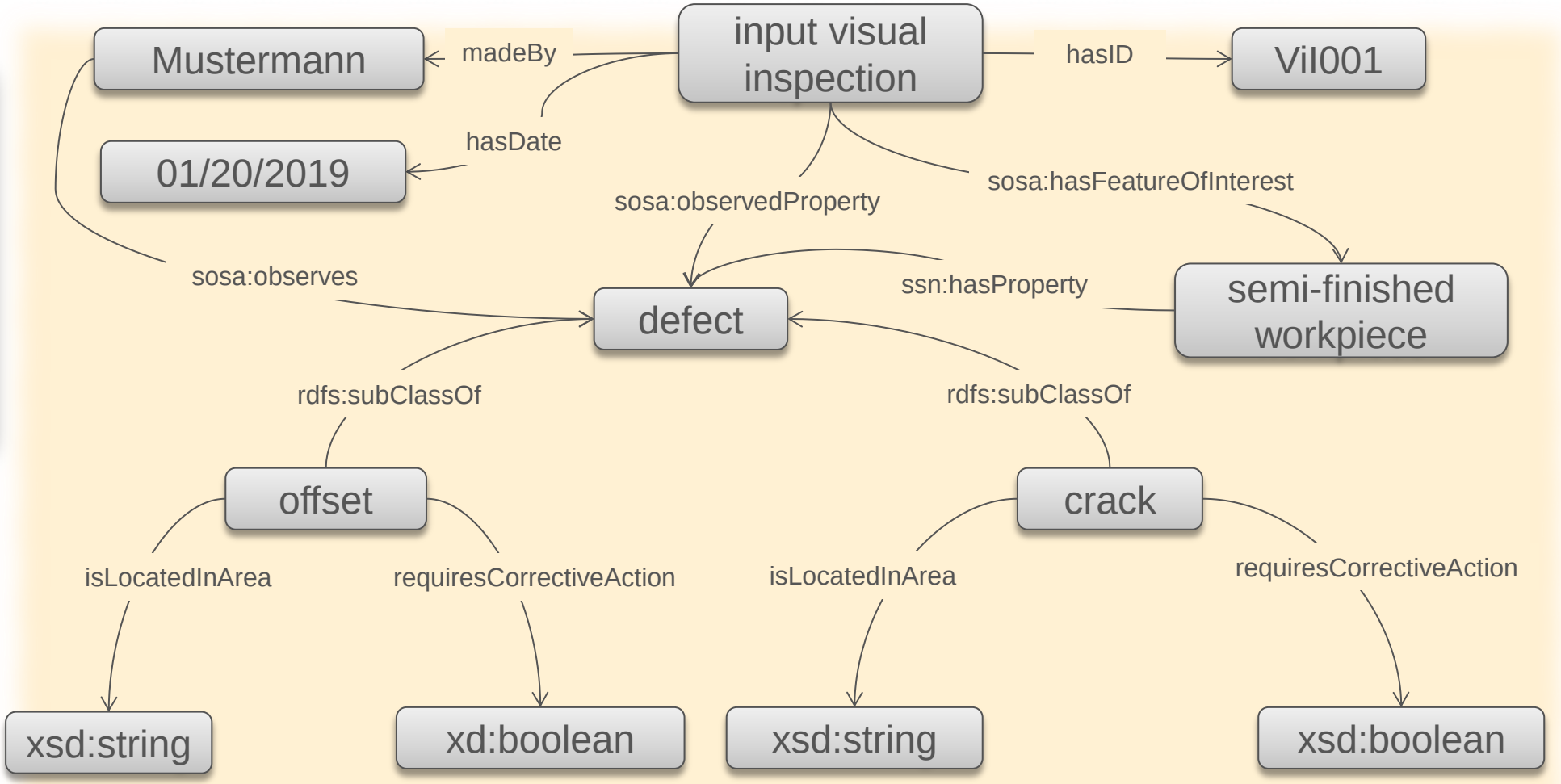




Input/Output Visual Inspection of Samples

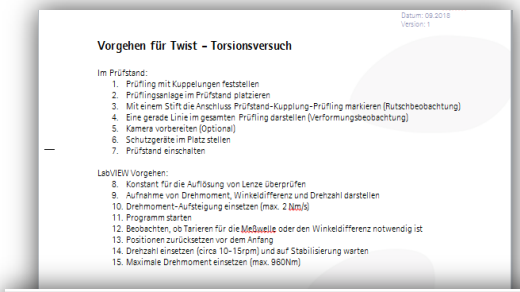
Defective Sample

Semantically Annotated Input Visual Inspection



Semantic Annotation of Research Activities

Unstructured Documentation of a Torsion Test



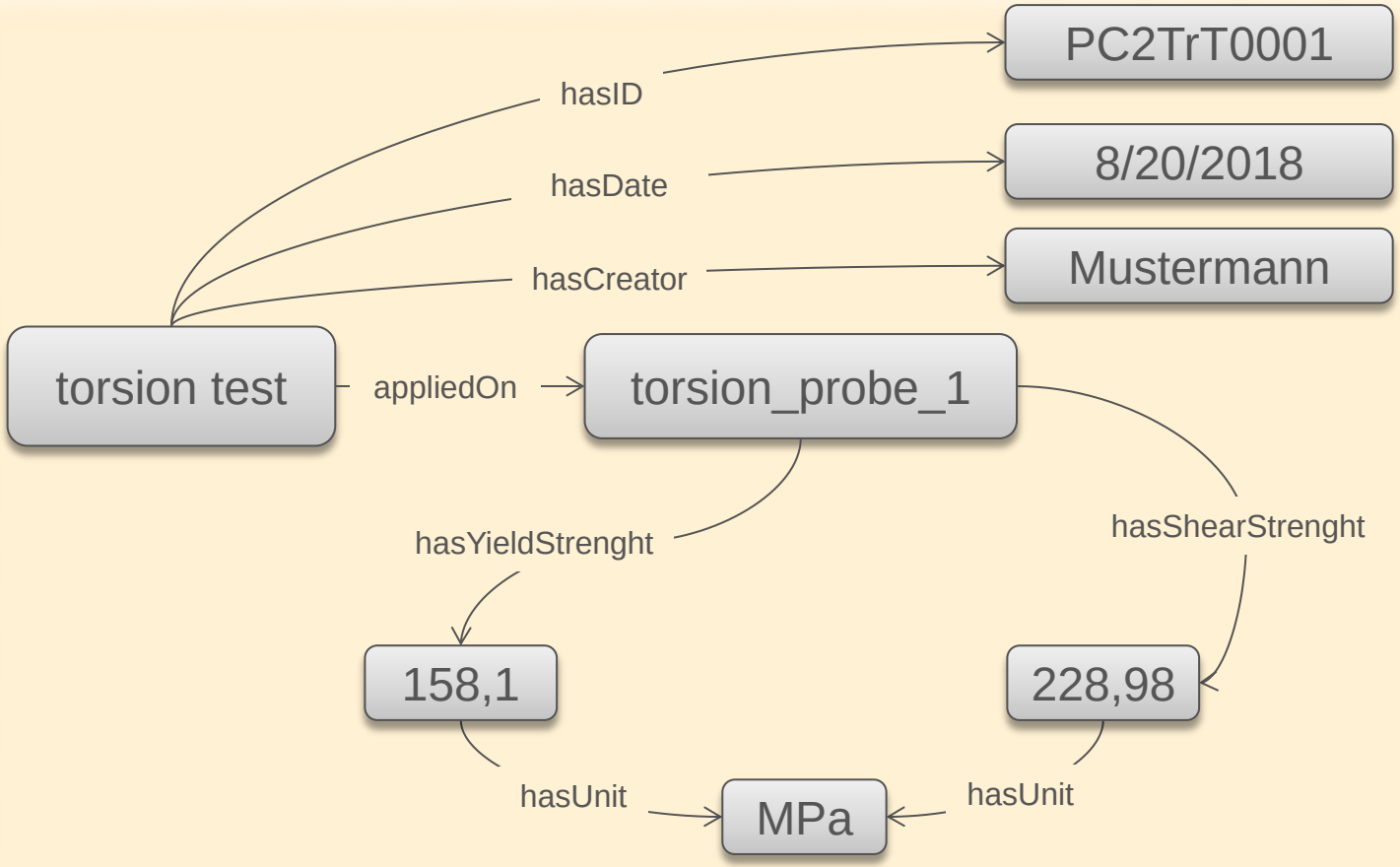
Vorgehen für Twist – Torsionsversuch

Im Prüfstand:
1. Prüfling mit Kuppelungen feststellen
2. Prüfungsanlage im Prüfstand platzieren
3. Mit einem Stift die Anschluss Prüfstand-Kupplung-Prüfling markieren (Rutschbeobachtung)
4. Eine gerade Linie im gesamten Prüfling darstellen (Verformungsbeobachtung)
5. Kamera vorbereiten (Optional)
6. Schutzgeräte im Platz stellen
7. Prüfstand einschalten

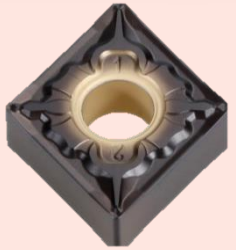
LabVIEW Vorgehen:
8. Konstant für die Auflösung von Lenze überprüfen
9. Aufnahme von Drehmoment, Winkeldifferenz und Drehzahl darstellen
10. Drehmoment-Aufsteigung einsetzen (max. 2 Nm/s)
11. Programm starten
12. Beobachten, ob Tarieren für die Meßwelle oder den Winkeldifferenz notwendig ist
13. Positionen zurücksetzen vor dem Anfang
14. Drehzahl einsetzen (circa 10-15rpm) und auf Stabilisierung warten
15. Maximale Drehmoment einsetzen (max. 980Nm)

Datum	Material	Probe modell	Rp0,2 [MPa]	Scherfestigkeit [MPa]
9/20/2018	Stahl S355	Torsionsprobe_1	-	494.27
9/27/2018	Stahl S355	Torsionsprobe_1	-	486.09
10/9/2018	20MnCr5 / AW6082	Einfache Welle 30mm	-	nicht erreicht
12/17/2018	20MnCr5 / AW6082	Einfache Welle 30mm	-	nicht erreicht
1/8/2019	20MnCr5 / AW6082	Torsionsprobe_3	158.1	228.98
1/15/2019	20MnCr5 / AW6082	Torsionsprobe_3	165.5	236.5
1/16/2019	20MnCr5 / AW6082	Torsionsprobe_3	167.9	225
1/30/2019	20MnCr5 / AW6082	Torsionsprobe_3	165.9	230.89
1/30/2019	20MnCr5 / AW6082	Torsionsprobe_3	148.4	229.21
1/31/2019	20MnCr5 / AW6082	Torsionsprobe_3	121.3	224.09
1/31/2019	Stahl-Stahl	Torsionsprobe_4	-	568.9
1/30/2019	20MnCr5 / AW6082	Torsionsprobe_4	-	-
2/1/2019	20MnCr5 / AW6082	Torsionsprobe_6	-	148.32
2/4/2019	20MnCr5 / AW6082	Torsionsprobe_5	158.8	175.01
2/19/2019	20MnCr5 / AW6082	Torsionsprobe_5	153.7	224.51
2/21/2019	20MnCr5 / AW6082	Torsionsprobe_5	172.1	205.98
3/4/2019	20MnCr5 / AW6082	Torsionsprobe_7	50	129.38
3/5/2019	20MnCr5 / AW6082	Torsionsprobe_7	60	136.50
3/7/2019	20MnCr5 / AW6082	Torsionsprobe_7	45	126.28
3/6/2019	20MnCr5 / AW6082	Torsionsprobe_7	65	131.16

Semantic Annotation of a Torsion Test



Semantic Description of Research Equipment



turning machine

isUsedByMachine

indexable insert

hasTypeDesignation

isUsedBySubproject

isUsedBySubproject

hasManufacturer

CTX 420 linear

B4

Garant

appliesFeedForce

appliesCuttingForce

hasISODesignation

appliesCuttingDepth

10

10

CNMG120408

2,5

hasUnit

hasUnit

hasPlateGeometry

hasUnit

kN

kN

xsd:string

mm

Image source: Gildemeister

Reuse of Existing Ontologies

Semantic Sensor Network Ontology (SSN)	SSN ontology is an ontology for describing sensors and their observations, the involved procedures, the studied features of interest, the samples used to do so, and the observed properties, as well as actuators. Source: <www.w3.org/TR/vocab-ssn/>.
ExtruOnt	ExtruOnt ontology provides different types of information related with an extruder, which are reflected in distinct modules that constitute the ontology. Source: DOI:10.3233/SW-200376.
Basic Formal Ontology (BFO)	BFO is a small, upper level ontology that is designed for use in supporting information retrieval, analysis and integration in scientific and other domains. BFO does not contain physical, chemical, biological or other terms which would properly fall within the coverage domains of the special sciences. Source: <basic-formal-ontology.org>.
Ontology of units of Measure (OM)	OM ontology provides classes, instances, and properties that represent the different concepts used for defining and using measures and units. It includes, for instance, common units such as the SI units metre and kilogram, but also units from other systems of units such as the mile or nautical mile. Source: <Ontology of units of Measure - Summary | NCBO BioPortal (bioontology.org)>.
Provenance Ontology (Prov-O)	Prov-O is a lightweight ontology that can be adopted in a wide range of applications. It can be specialized for modeling application-specific provenance details in a variety of domains. Source: <https://www.w3.org/TR/prov-o/>.

Sources

- W3C Recommendation 25 February 2014: RDF Schema 1.1. https://www.w3.org/TR/rdf-schema/
- W3C Recommendation 19 October 2017: Semantic Sensor Network Ontology. https://www.w3.org/TR/vocab-ssn/

Image Sources

- Indexable insert CNMG120408-HB7020: https://www.hoffmann-group.com/DE/de/hom/Modulare-Zerspanung/WP-Drehen-GARANT/CNMG-120408/p/250060-HB7020#anchor_applicationTable
- Air circulation chamber furnace THERMOCONCEPT KU 15/06 A: https://www.thermconcept.com/virthos.php?//Produkte/Waermebehandlung%20Metall/Anlassen%2C%20Verg%C3%BCten%2C%20Auslagern%2C%20Vorw.../Umluft-Kammer%C3%B6fen%20bis%201000l
- Surface measuring device Alicona InfiniteFocus: https://www.alicona.com/en/products/infinitefocus/
- Milling cutter Holex 202275 8: https://www.hoffmann-group.com/DE/de/hom/Monozerspanung/VHM-Fr%C3%A4ser/VHM-Fr%C3%A4ser-AlCrN/p/202275
- Turning machine CTX 420 linear: Gildemeister

LEIBNIZ INFORMATION CENTRE
FOR SCIENCE AND TECHNOLOGY
UNIVERSITY LIBRARY

TIB

Acknowledgements

The authors gratefully acknowledge the support from the Collaborative Research Centre (CRC) 1153 Process Chain for Manufacturing of Hybrid High Performance Components by Tailored Forming, Project number 252662854 (INF) and from the Collaborate Research Centre (CRC) 1368, Project number 394563137 (INF), funded by the German Research Foundation (DFG).

Contact
Tatyana Sheveleva
T +49 511 762-18838, tatyana.sheveleva@tib.eu

Leibniz Association

OntoCAPE in NFDI4Cat

Norbert Kockmann

Dortmund, 19.01.2021

Outline

- NFDI4Cat Overview
  - data value chain in catalysis and process engineering
  - ontology, meta data structure, and repositories
- NFDI4Cat Ontologies
  - OntoCAPE
  - heat exchangers
  - chemical reactors and reactions
- Common ontologies in chemistry, engineering and catalysis
- Summary

The Consortium NFDI4Cat and Partners

- Who is NFDI4Cat?

NFDI4Cat Core Consortium

Roof Organization DECHEMA

Data Driven Catalysis Research
homogeneous, heterogeneous, bio-, photo-, electro-catalysis

Catalysis Competence Partners
Universities, Max-Planck-Institutes, Helmholtz-Institutes, Leibniz Institutes

Learned Societies:
GeCatS, ProcessNet, Bunsengesellschaft, DGMK, VDI, GDCh

Data Science Competence Partners
HPC: HLRS Stuttgart, Mathematics: MPI-DCTS Magdeburg
Data structures: Berlin Big Data Center (BBDC), Fraunhofer FOKUS Berlin (Berlin)
ML Methods: Berlin Center for Machine Learning (BZML)

Cooperation Partners within NFDI

NFDI4Ing
Common Topics: engineering aspects of catalysis, multiscale modelling

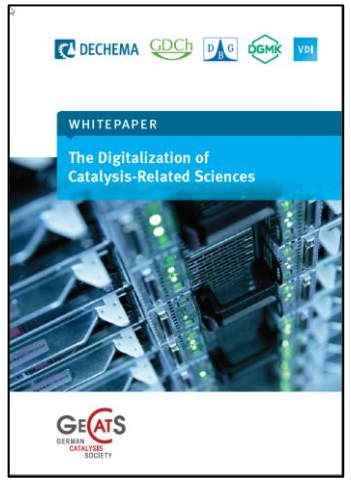
FAIRMat
Common Topics: theoretical chemistry/ chemistry of materials interfaces

DAPHNE
Common Topics: analytical data of materials material interfaces

NFDI4Chem
Common Topics: chemistry of molecular compounds, analysis data, ELN

Advisory Role of Chemical Industry

BASF, EVONIK, covestro, CLARIANT, thyssenkrupp, hte, THE LINDE GROUP



From meta data to repositories

- Meta data in the data value chain
- Repositories

Syngas Plant, Linde Engineering

Process Simulation

Multiscale Modelling

Process Design Data, Energy & Cost data (Process Synthesis and Design)

FAIRmat

Molecular Modelling

NFDI4Ing

Data Exchange with Theory

Heat & Transport Data, Kinetic Data (Reactor Analysis and Design)

NFDI4Chem

Synthesis Data (Catalyst Synthesis, Catalyst Conditioning)

Operando Data (Active Site, Mechanism)

Performance Data (Rate, Selectivity, Lifetime)

Characterisation Data (In-Situ Characterisation, Crystal Structure)

Feedback Loops

EngMeta

HLRS

repositories I

DAPHNE

repositories II

NFDI4Cat – first steps into ontologies

- OntoCAPE as a starting point
- RWTH Aachen,

www.avt.rwth-aachen.de/cms/AVT/Forschung/Sonstiges/Software/~ipts/OntoCape/

- aspect system
- different aspect systems define process unit

Diss J. Morbach, **2009**

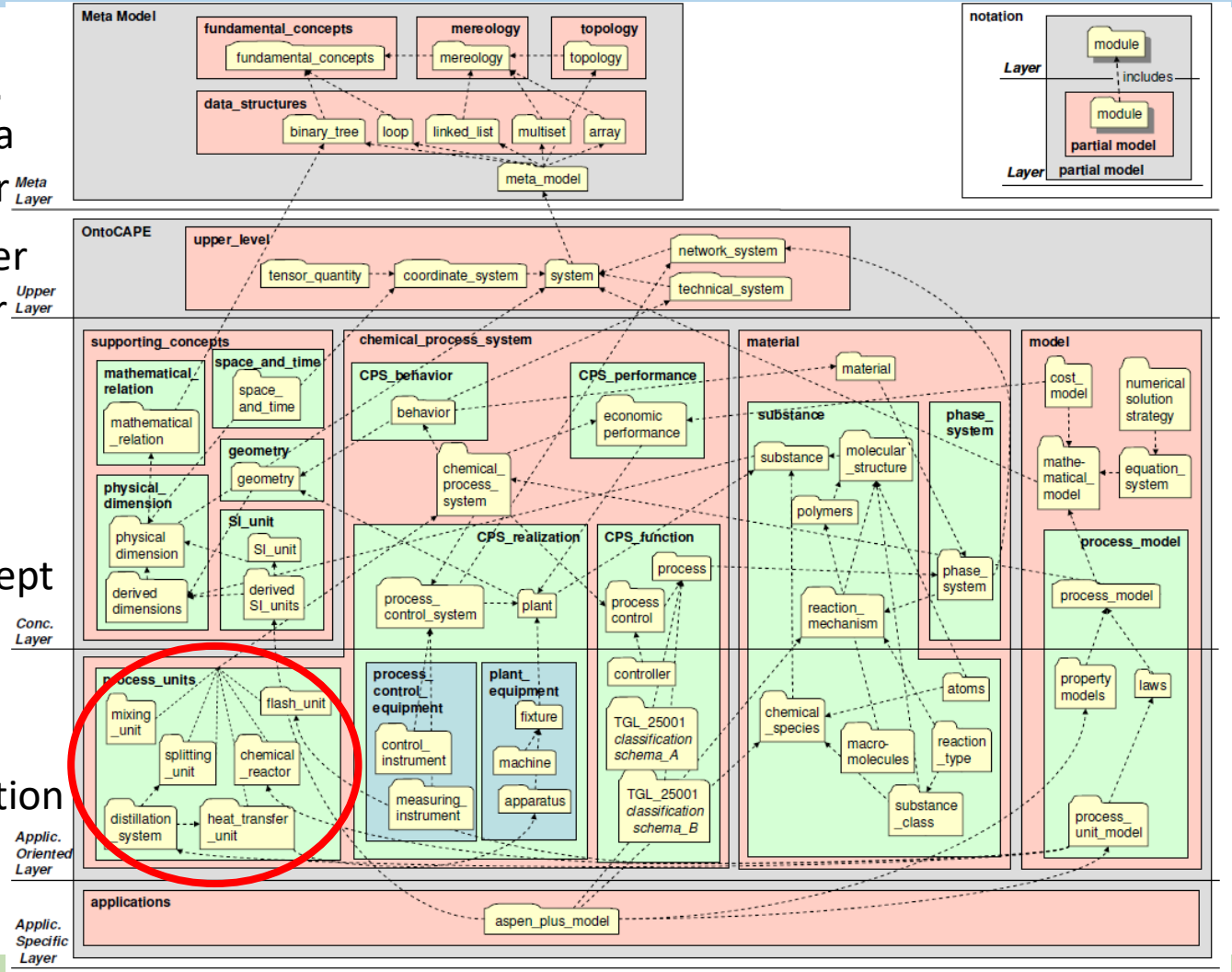
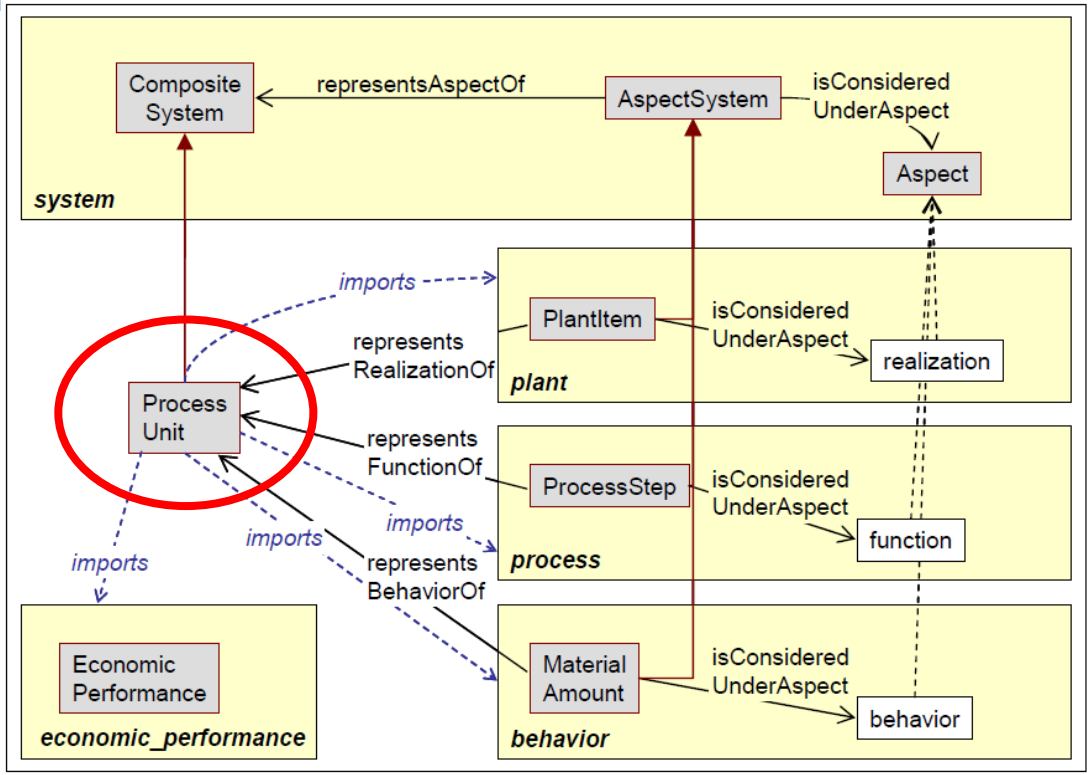


Fig. 5: Structure of OntoCAPE

NFDI4Cat – first steps into ontologies

- OntoCAPE with aspect system
- modular consideration
  - The class process step represents the desired function
  - The class plant item reflects its physical realization
  - A material amount describes the physicochemical behavior of a chemical process system



- “an aspect system is a special type of subsystem, which contains only those components of the overall system that are considered under the respective aspect”

Diss J. Morbach, **2009**

NFDI4Cat – first steps into ontologies

- OntoCAPE with aspect system
- different aspect systems define process unit
- modelling as subclasses of system of each module
- modular consideration of aspects for each unit

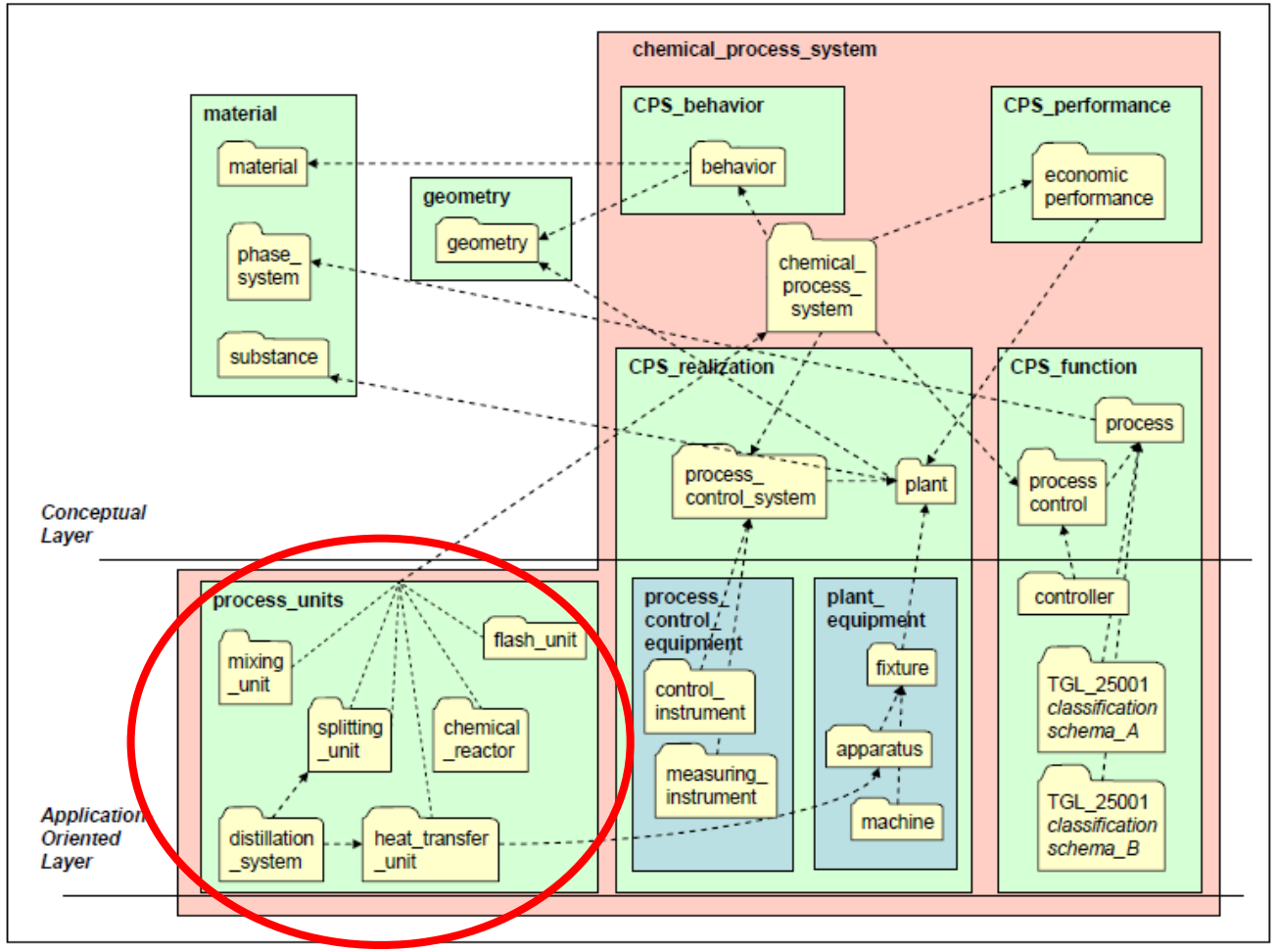
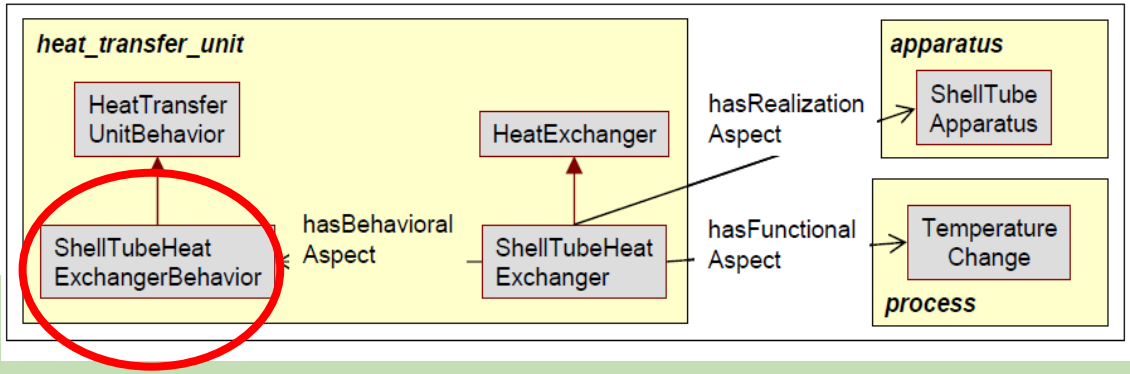


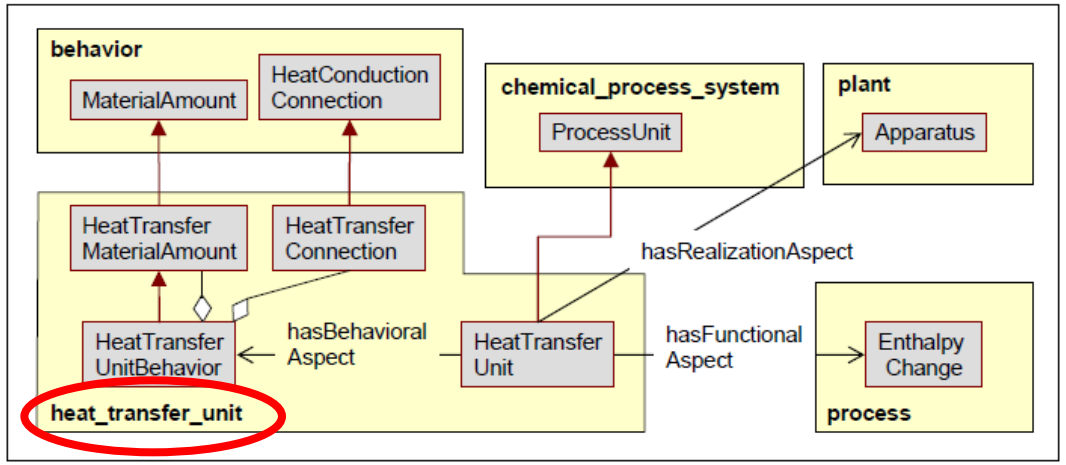
Fig. 1: Overview on the partial model **chemical_process_system**

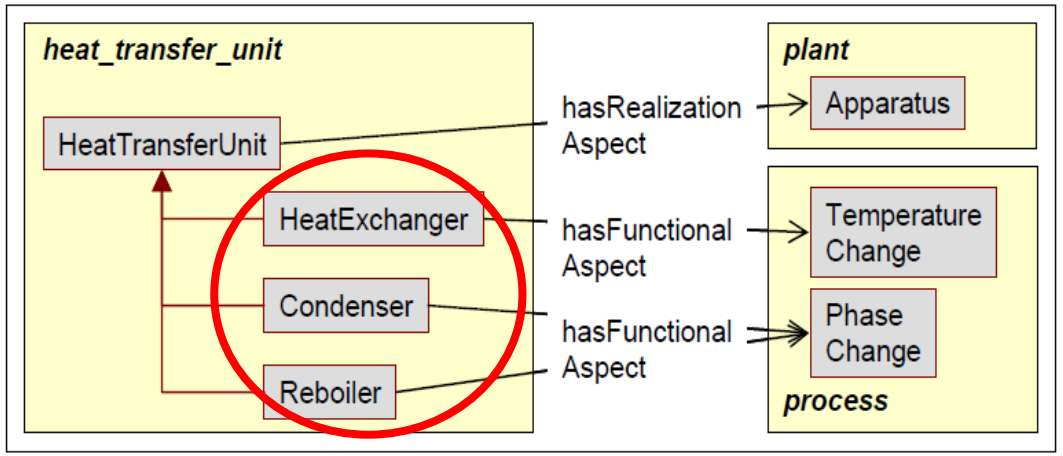
Diss J. Morbach, **2009**

OntoCAPE – Heat transfer unit

- Process unit which has functional aspect of enthalpy change
- Three specializations of heat transfer unit
  - Heat Exchanger, Condenser, Reboiler
- Class „shell tube heat exchanger“ implemented as pars pro toto of heat exchangers







Diss J. Morbach, **2009**

OntoCAPE – Heat transfer unit behavior

- depicts the behavioral viewpoint of a *chemical_process_system* which mainly characterizes the physicochemical phenomena occurring when materials are processed in an equipment

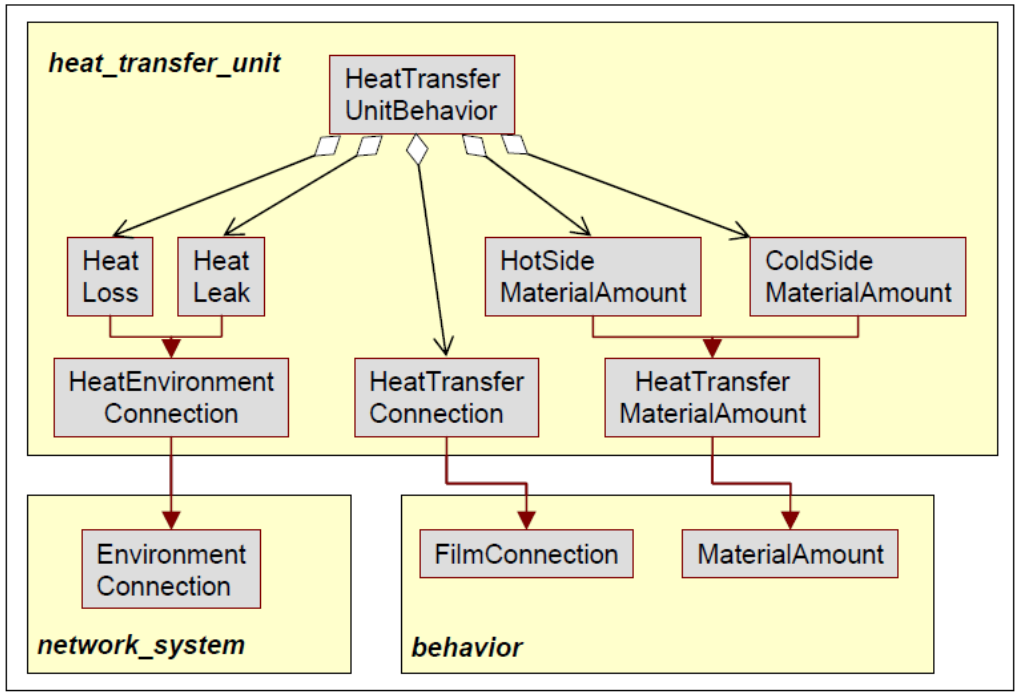


Fig. 76: Exemplary elaboration of *heat transfer unit behavior*

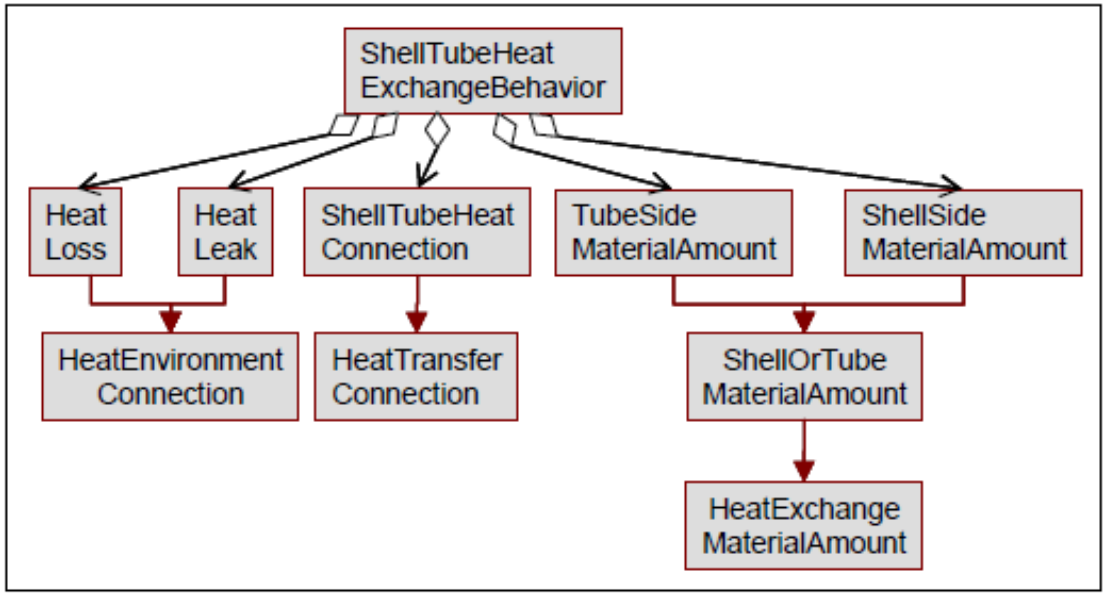
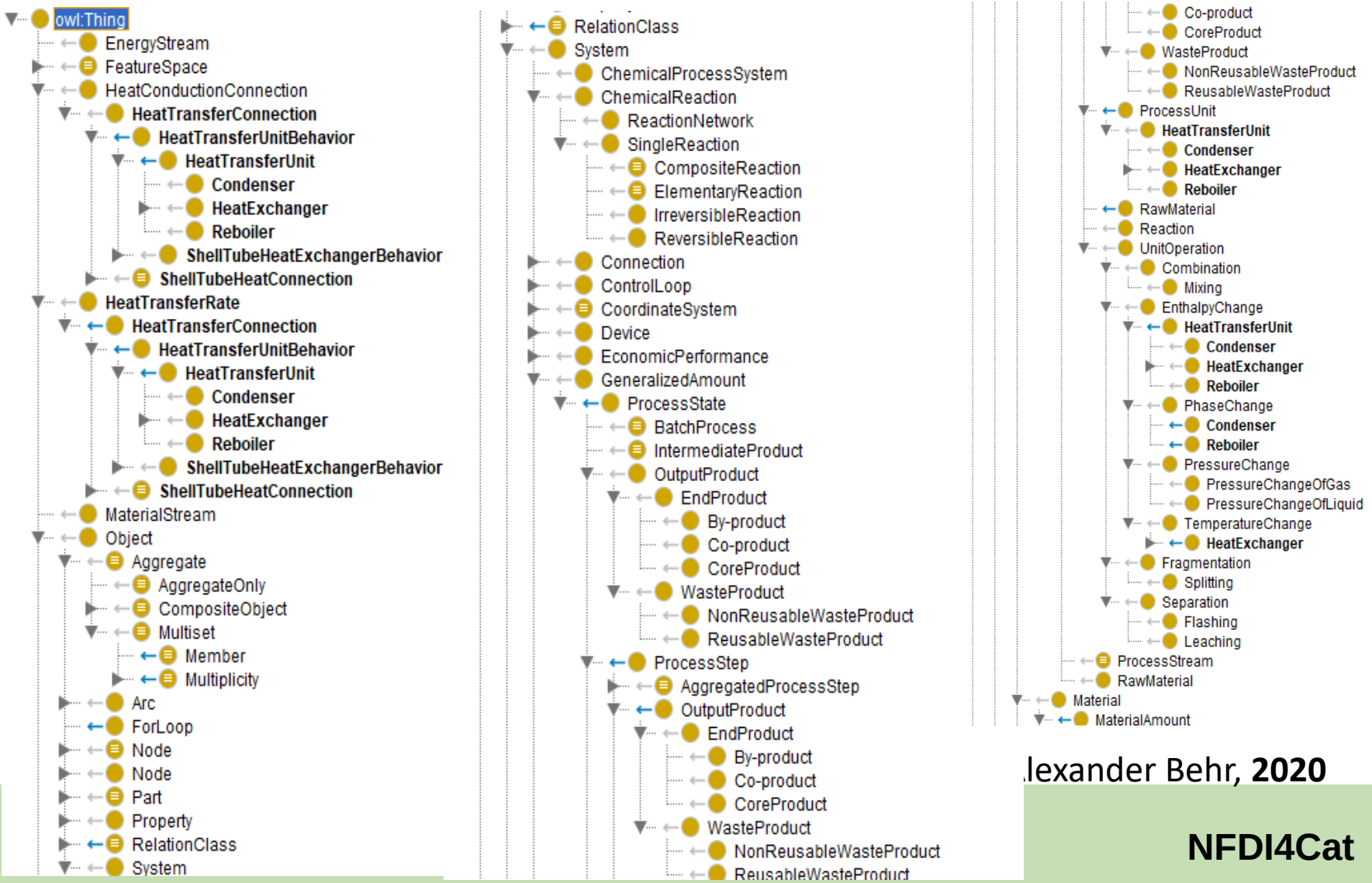


Fig. 77: Description of a *shell tube heat exchange behavior*

Diss J. Morbach, **2009**

OntoCAPE – representation in *protégé*

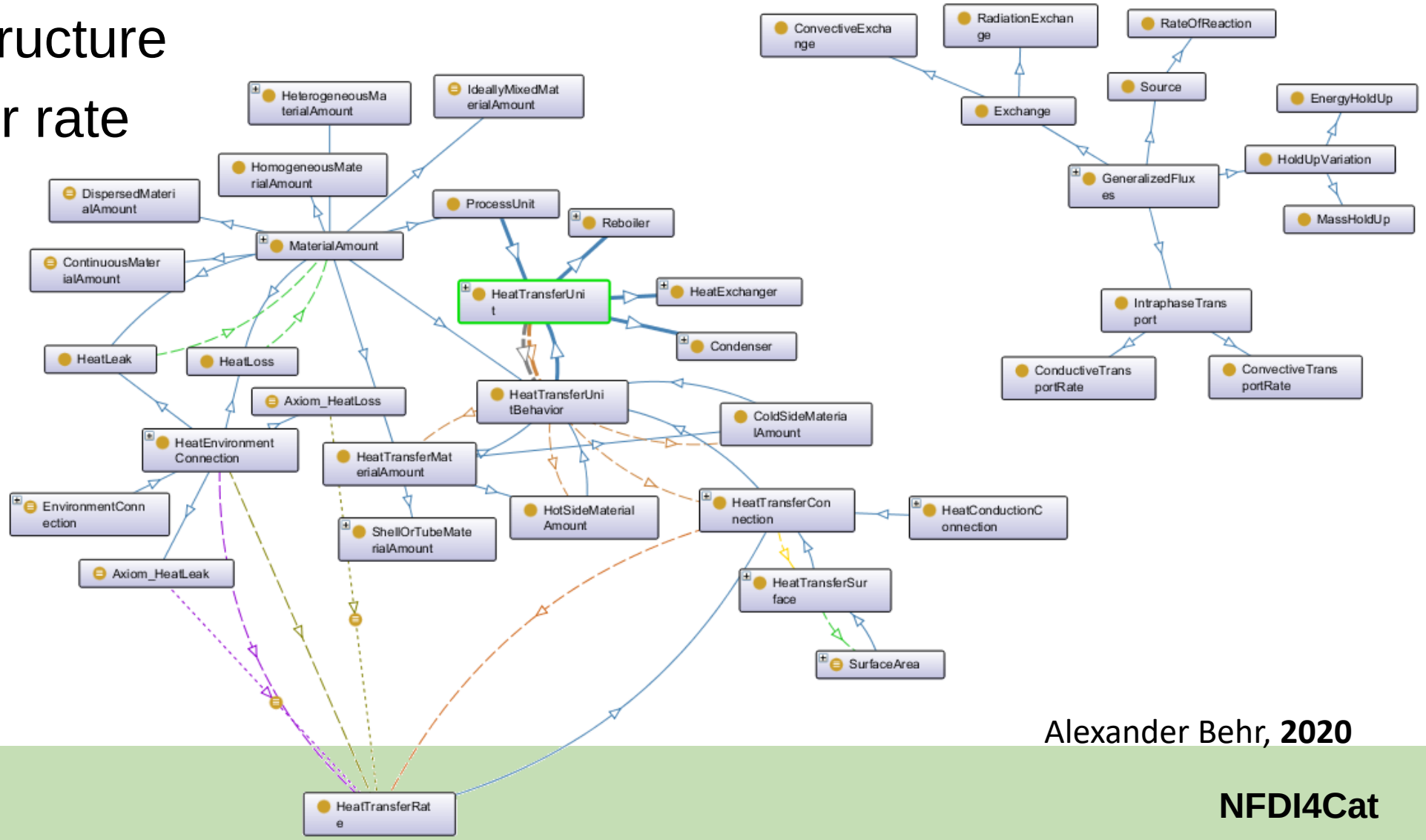
- heat transfer
- transfer unit
- list display



lexander Behr, **2020**

OntoCAPE – representation in *protégé*

- mindmap structure
- heat transfer rate



Alexander Behr, **2020**

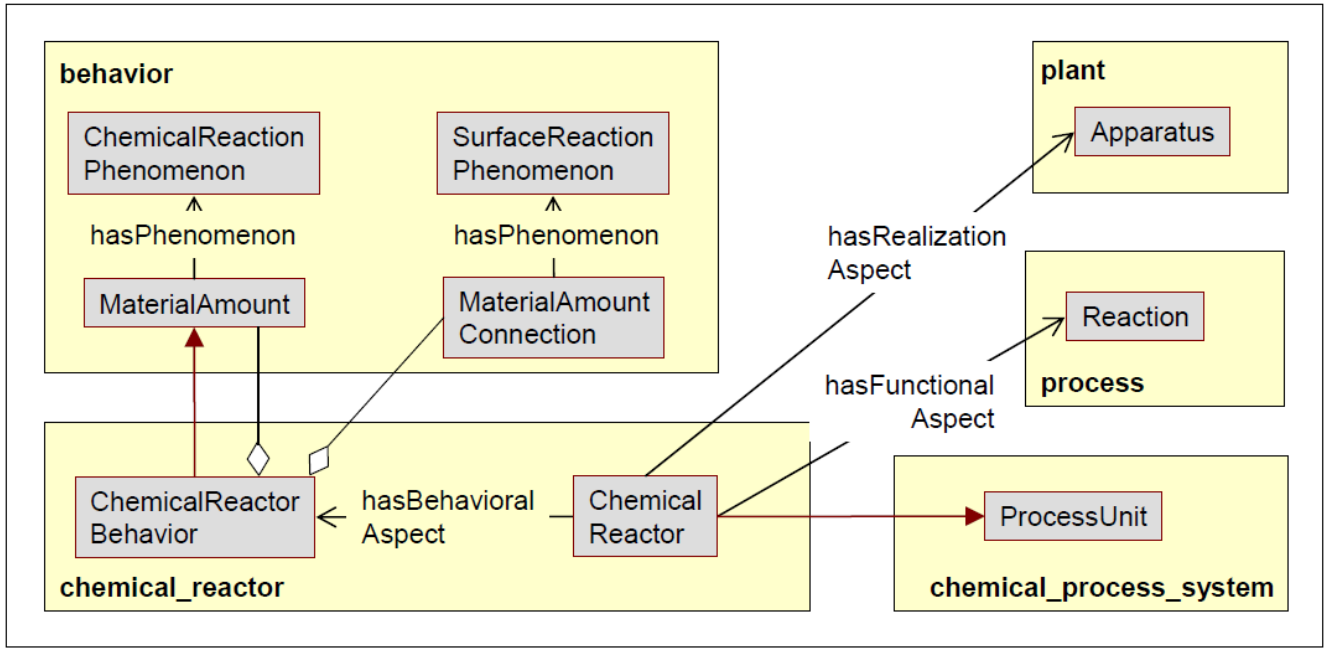
OntoCAPE – reactor unit

- definition

  “A *chemical reactor* realizes a *reaction* function within an *apparatus* and demonstrates *chemical reaction behavior* in some *material amounts* or at some *material amount connections*.”

- but

  No characterization on distribution is specified with this concept;
  specialized reactors such as of CSTR or plug-flow based reactors can be defined by refining the present definition.



Diss J. Morbach, **2009**

OntoCAPE – Chemical reaction mechanism(s)

- property of material -> substance module
- example in documentation
  - reaction

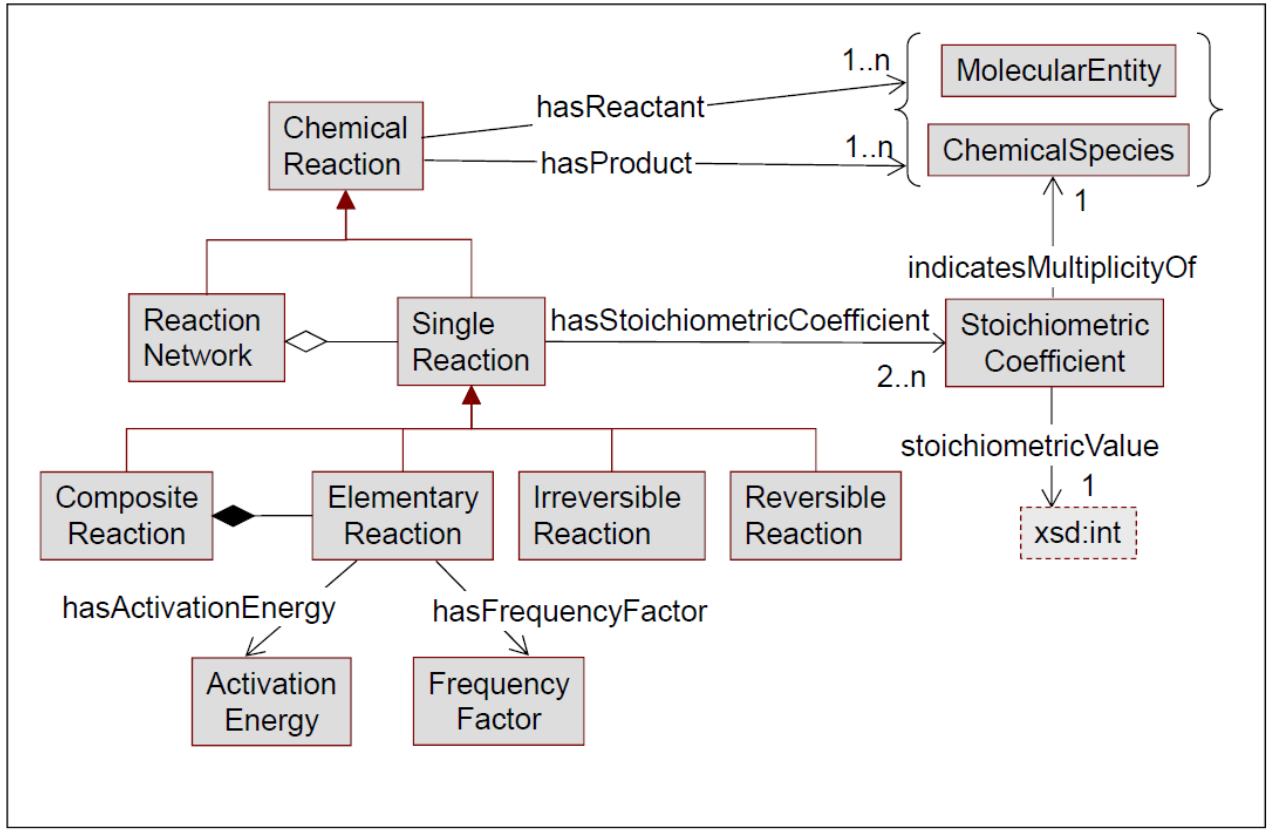
$$2\ H_2 + 2\ NO \rightarrow N_2 + 2\ H_2O$$

  - elementary reactions:

$$2\ NO \rightarrow N_2O_2$$

$$H_2 + N_2O_2 \rightarrow N_2O + H_2O$$

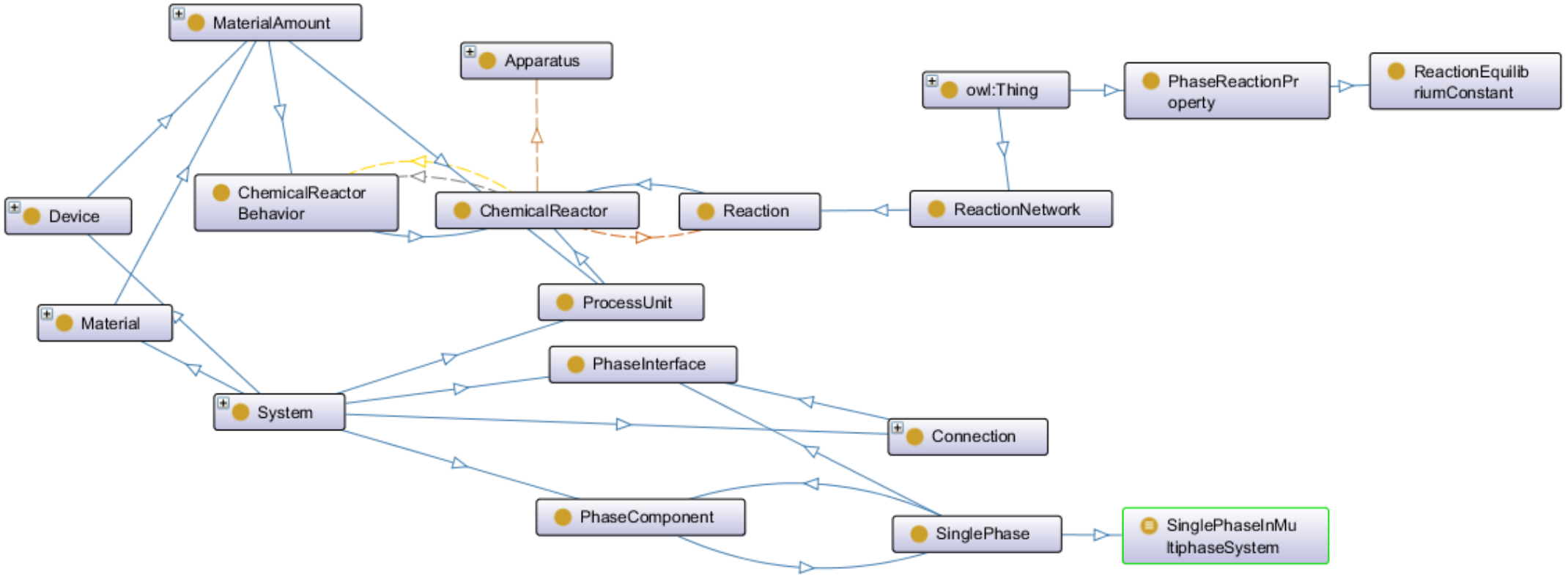
$$H_2 + N_2O \rightarrow N_2 + H_2O$$



Diss J. Morbach, **2009**

OntoCAPE – Chemical reactor module

- mindmap structure



Alexander Behr, **2020**

Summary and Outlook

- NFDI4Cat addresses catalytical and process sciences
- ontology development has just started
- OntoCAPE as base for process engineering
- protégé as ontology editor

- collection of domain knowledge
- structuring the knowledge
- connecting with chemists and (mechanical) engineers

NFDI for Catalysis-Related Sciences

Homepage: http://gecats.org/NFDI4Cat.html

You would like to interact, be part of the community
or do you have questions?

Get in touch with us: Dr. Nils Bohmer (DECHEMA e.V.)
Phone +49-69-7564-620
Email info@nfdi4cat.de
LinkedIn www.linkedin.com/company/nfdi4cat
Twitter @Nfdi4Cat

SCAN ME

Joint Webinar
Ontologies in Science and Technology

19 January 2021, 3 pm

https://nfdi4chem.de

https://twitter.com/nfdi4chem

contact@nfdi4chem.de

https://lists.nfdi.de/postorius/lists/

https://www.youtube.com/channel/UCQIKQDjyYFzlUFrDfR9vVJg

https://nfdi4ing.de

https://twitter.com/nfdi4ing

contact@nfdi4ing.de

http://nfdi4cat.org

https://twitter.com/nfdi4cat

info@nfdi4cat.org

https://www.linkedin.com/company/nfdi4cat

Next steps

Want to dive deeper? Want to be part of modelling the world (of your research)?

- Ontology workshop (NFDI4Chem) in summer

https://nfdi4chem.de/index.php/events/
https://nfdi4chem.de/index.php/network/

https://nfdi4ing.de/events/

http://nfdi4cat.org

Stay in contact
https://forms.gle/Zwwy66kfYH4YZobQ6

Evaluate the event
https://forms.gle/PaMUhH4pDsY2oyYP9

Ressources mentioned during discussion

- Git: https://git-scm.com/book/en/v2/Getting-Started-About-Version-Control, https://stackshare.io/stackups/git-vs-gitlab
- Finding Ontologies: https://lov.linkeddata.es/dataset/lov, https://bartoc.org/
- Protege, tool for building ontologies: https://protege.stanford.edu/
- CEDAR, tool for creating metadata templates which include ontologies: https://more.metadatacenter.org/, https://more.metadatacenter.org/tools-training/cedar-metadata-tools
- Ontology matching: http://oaei.ontologymatching.org/
- OntoCape, large-scale ontology for the domain of Computer Aided Process Engineering: https://www.avt.rwth-aachen.de/cms/AVT/Forschung/Sonstiges/Software/~ipts/OntoCape/
- TIB Ontologies Management Initiative: https://github.com/tibonto
- NFDI4Chem – Chemistry Consortium in the NFDI: https://github.com/nfdi4chem
- Example for a service that allows easy creation of data based on ontologies: https://www.wikidata.org/
- Chemotion ELN / Repository: https://chemotion.net/
- https://www.stardog.com/
- Neo4J Graph Database: https://neo4j.com/

Team

Susanne Arndt, *Bestandsentwicklung und Metadaten, TIB*
Felix Bach, *Scientific Data Management, SCC, KIT*
Stephan Hachinger, *Research Data Management, Leibnitz-Rechen-Zentrum*
Kevin Hermann, *IPeG, LUH*
Johanna Hickmann, *University Library, TU Berlin*
Dorothea Iglezakis, *FoKUS, University of Stuttgart*
Oliver Koepler, *Lab Linked Scientific Knowledge, TIB*
Angelina Kraft, *Research Data Services, TIB*
Giacomo Lanza, *Research Data Management, PTB*
Johannes Liermann, *Zentrale Analytik Chemie, Uni Mainz*
Iryna Mozgova, *IPeG, LUH*
Patrick Mund, *Fertigungsmesstechnik und Qualitätsmanagement, RWTH Aachen*
Johannes Munke, *Research Data Management, Leibniz-Rechenzentrum*
Steffen Neumann, *Bioinformatik & Forschungsdaten, Leibniz-Institut für Pflanzenbiochemie*
Mehtap Özaslan, *Technical Electrocatalysis, TU Braunschweig*
Christian Popp, *Project Manager NFDI4Chem, Uni Jena*
Tatyana Sheveleva, *Lab Linked Scientific Knowledge, TIB*
Džulia Terzijska, *Research Services, KIT Library*
Kerstin Wedlich-Zachodin, *Research Services, KIT Library*
Cord Wiljes, *Kompetenzzentrum Forschungsdaten, Universität Bielefeld*