What is NFDI4Cat?

NFDI4Cat is a community-driven and user-oriented initiative to secure the digital future of catalysis.

NFDI4Cat
NFDI for Catalysis-Related Sciences

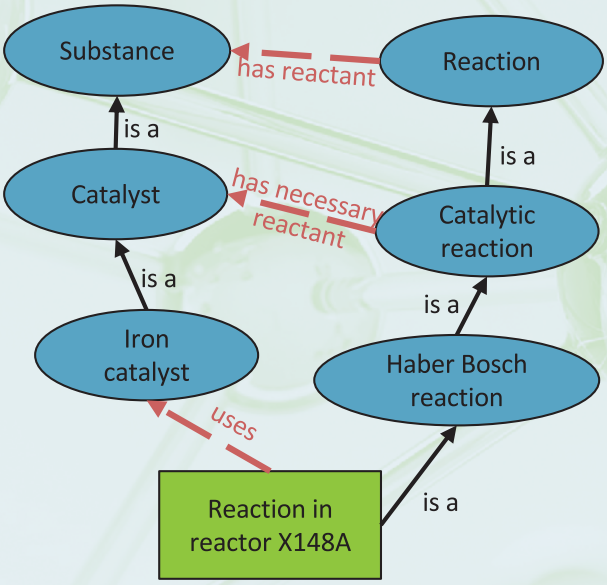
Ontologies for Catalysis

Data **FAIR**ness (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable) is important to align data structures. This can be done by ontologies, that provide an interconnectivity between different data sources.

Ontologies consist of:

- **Classes** to express concepts
- **Relations** between classes
- **Individuals** representing real existing cases of the classes
- **Axioms**, *like all catalytic reactions need one or more catalyst*

Once, an ontology is set up, reasoning helps to enhance the annotation of data.



Applying a reasoner on the information *"The reaction in reactor X148A uses iron catalysts"* can yield with the help of an ontology as shown in the image above: *"The reaction in reactor X148A is a Haber-Bosch reaction which in turn is a catalytic reaction and uses iron catalyst as catalyst."*

DFG Deutsche Forschungsgemeinschaft
German Research Foundation

nfdi Nationale Forschungsdaten Infrastruktur

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Enabling Knowledge Transfer

Catalysis research data often contains plenty of different data, data types and (measured) concepts. In addition, knowledge on the data often is “hidden“, often allowing only the researchers who conducted the respective recorded experiments to fully understand their data.

Shaping your Data

Detecting patterns in research data is not only the often applied task of researchers, but also done by machine learning applications. To be able to search for such shapes, one needs to classify their data.

Modeling Reactions in Ontologies

Modeling a catalyst is complex, as the exact reaction conditions that are needed for catalytic activity of the substance are required. Thus, modeling a catalyst requires modeling reactions. The figure on the right is such an ontology used as a model of a methanation reaction. Educts and products are modeled as arrays of mixture components. This allows for simple data entry, as direct connections (dashed arrows) from the reaction to components are logically inferred by a reasoner. The reaction conditions are modeled as data properties; however, their modeling is not shown here for simplicity.

Extended & Annotated Data

After modeling the data, the model can be used to enrich the data. First, the data is connected to related data. Second, data is annotated, with information such as links to data repositories or Wiki’s and thesauri for textual definition(s).

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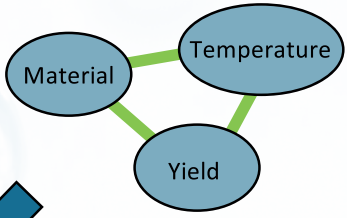
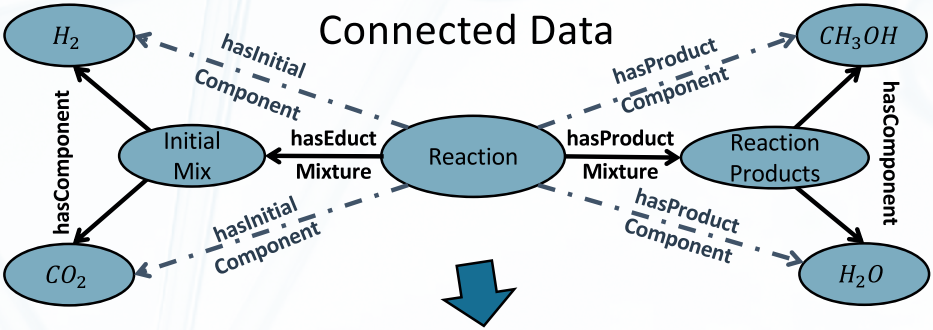
Meas	Mat	Temp	Pres	X	Y
1	Co-Ni	277,9	1,02	69,4	28,5
2	Al-Ni	262,3	1,04	7,4	8,4
3	Fe-Co	271,4	1,05	28,2	28,1
4	Al-Fe	251,4	1,03	52,0	61,4
5	Co-Al	293,7	1,01	68,8	8,9

Data

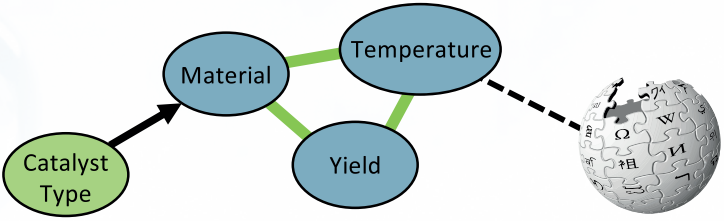
Shape



Connected Data



Annotated Data



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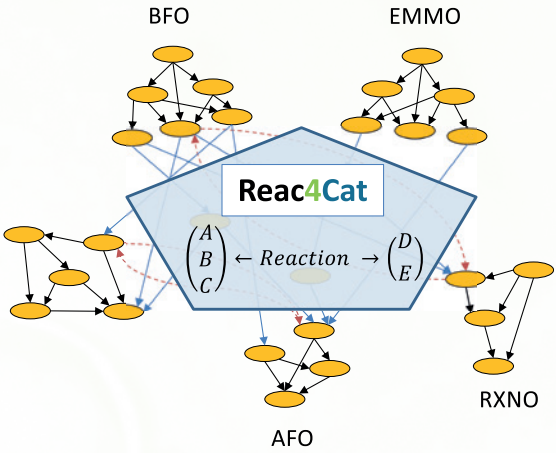
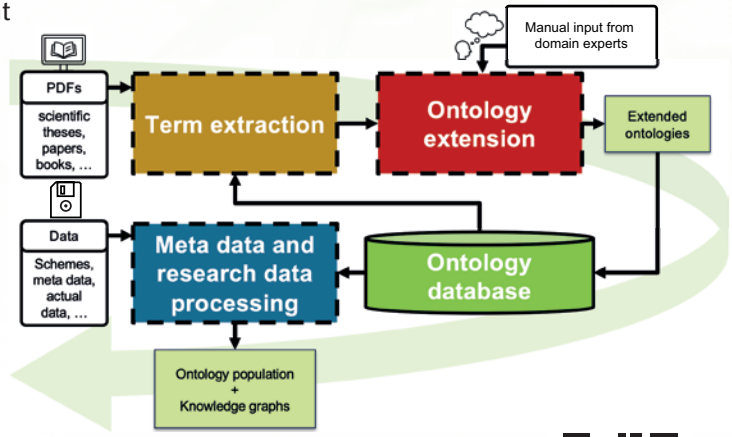


Cross Connecting Data

Interconnecting your data (e.g., regarding catalyst deactivation) with complementary data (e.g., spectroscopic analysis data) increases the value of your data. Anonymization of your data is possible. To enable you to interconnect your data, we try to integrate our ontology models into the world of ontologies. While there are some ontologies already present, no ontology is currently available for the scope of catalysis research.

Future & Related Work

To mitigate manual and recursive work, we also develop methods for your adaptation in your research data workflows. For example, term extraction can be used in a method to aid in finding the right concepts for extending your ontology and map it to already existing ones.



More info, guidelines, related publications, and much more here:
zenodo.org/communities/nfdi4cat