

Towards a National Research Data Infrastructure for Chemistry in Germany

The NFDI4Chem Consortium



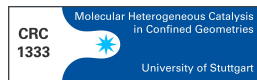
The NFDI in General



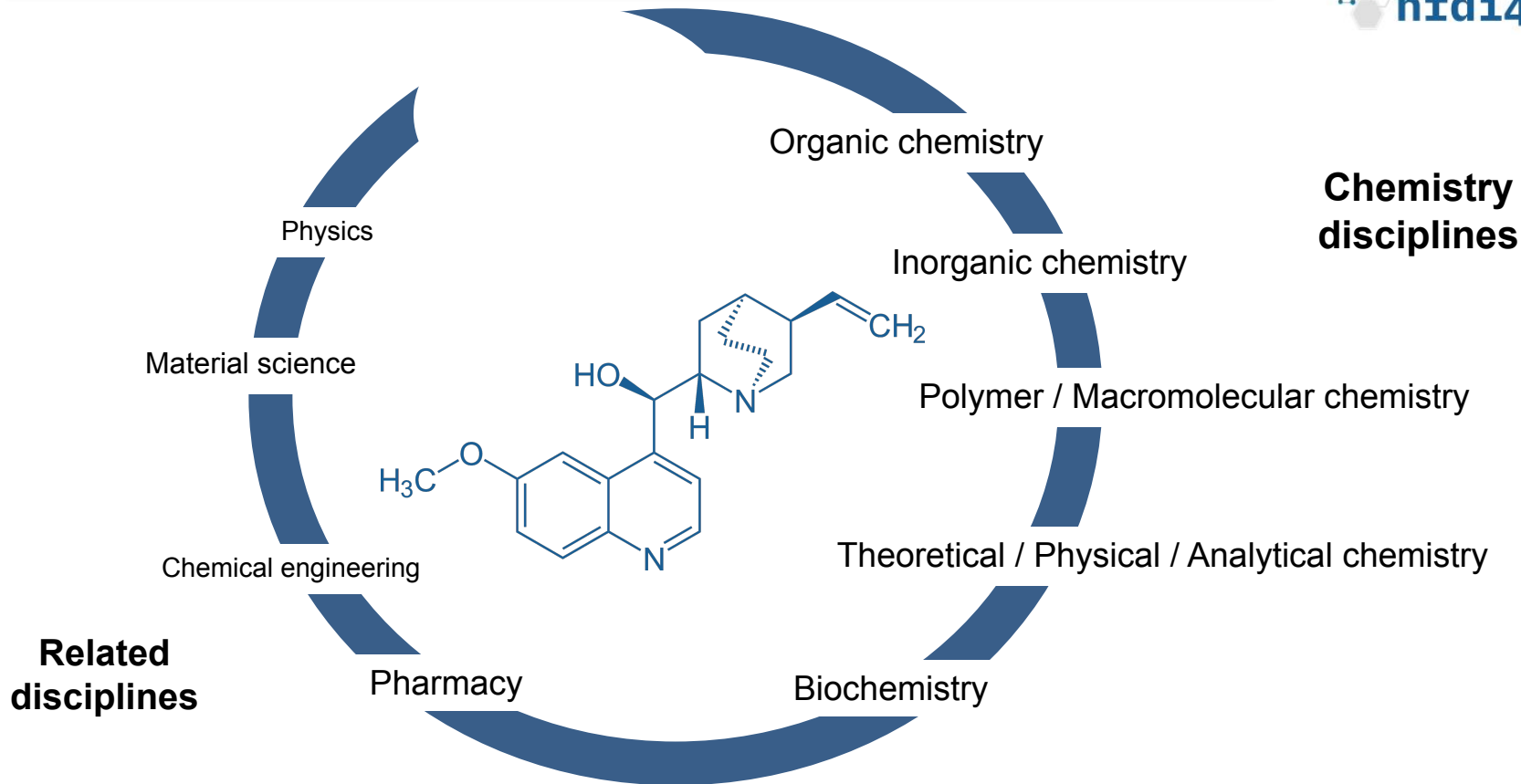
Federal Government and the States will fund a National Research Data Infrastructure for Germany

- **N**ationale **F**orschungs**d**aten**i**nfrastruktur (NFDI)
- 85 Mio Euro funding per year in production phase
- Eventually, 30 consortia in all areas of science funded
- Initial conference was May 2019 with 57 consortia
- Initial proposals from about 5 consortia due in Oct 2019
- 5 Mio per consortium per year

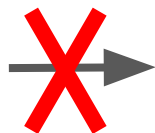
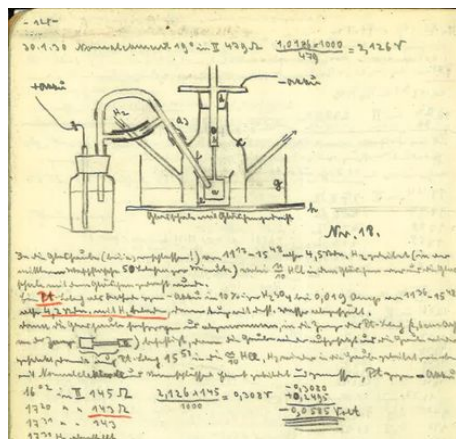
The NFDI4Chem: Who we are



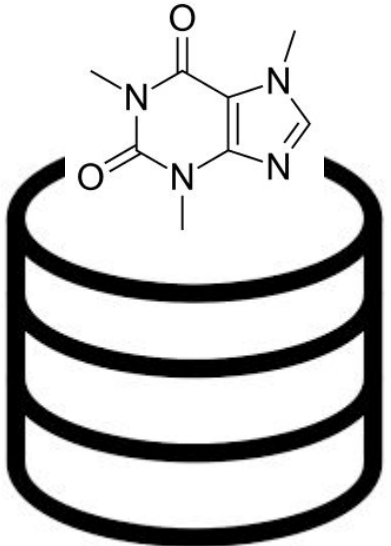
Our scientific community



Chemistry



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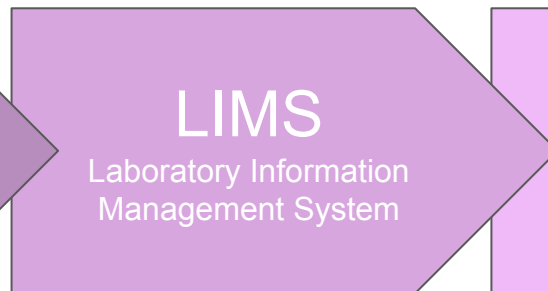
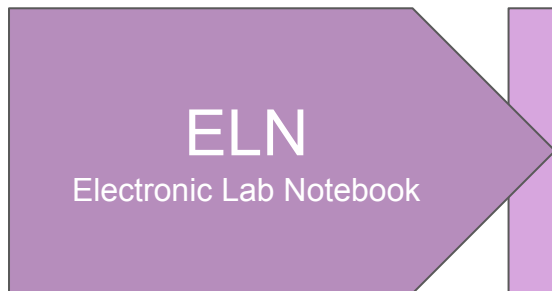
#239234240

FAIR early data acquisition in the lab is poorly established

Chemistry



The missing components:



Key objectives



Objective 1: Connect existing **data repositories**, fill in missing research data repositories, and link them to international repositories.



Objective 2: **Minimum information (MI) standards for data and machine-readable metadata**, open data standards, in order to support the FAIR principles for research data.



Objective 3: Foster **Electronic Laboratory Notebooks (ELN)**, tools and APIs between between instrumentation and software towards a embedded, digital information architecture. Capture research data in well-annotated electronic form at the **earliest possible point in time in the research process**.



Key objectives



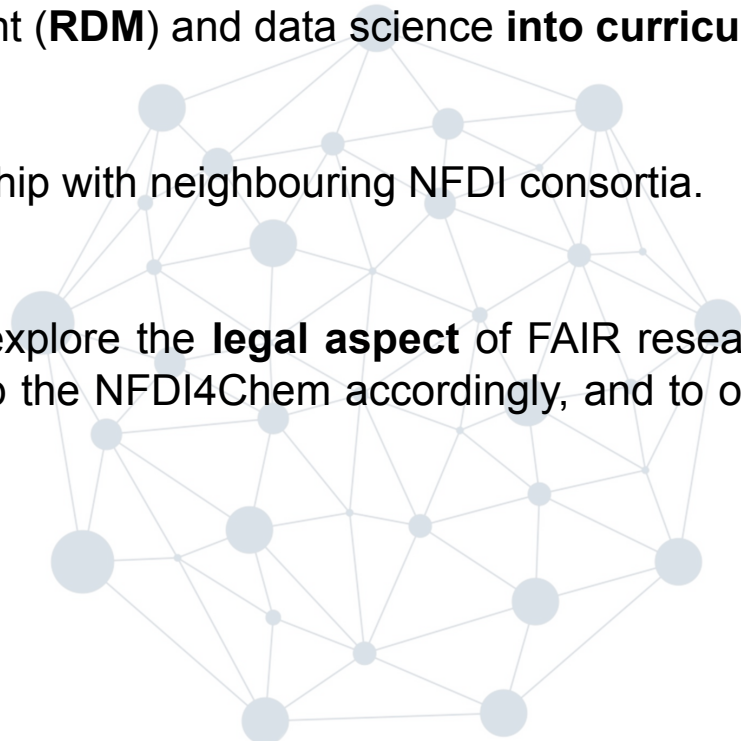
Objective 4: Create **awareness** for **FAIR data management**, initiate processes to **integrate** research data management (**RDM**) and data science **into curricula**.



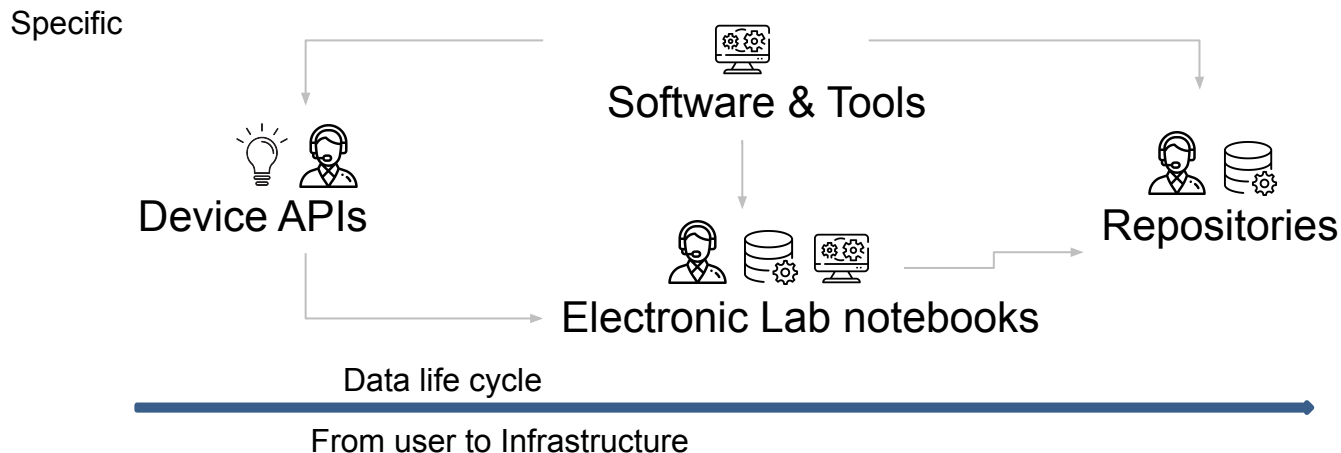
Objective 5: Maintain a close relationship with neighbouring NFDI consortia.



Objective 6: Engage with experts to explore the **legal aspect** of FAIR research data management, design and develop the NFDI4Chem accordingly, and to offer advice for the research community.



Digital change in chemistry



Generic

Standards &
Formats

Communities

Legal aspects

Data aspects

Data formats

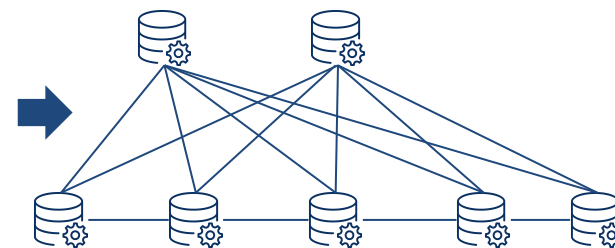
Open standards
Open formats
vs.
Heterogeneity
Proprietary

Metadata

Open standards
Open formats
vs.
Heterogeneity

Vocabularies

Mapping of
heterogeneous data
and metadata
formats to domain
specific vocabularies



FAIR principles

Generic



Standards &
Formats



Communities



Legal aspects

International network



- Development of standards is an international effort
- We need to negotiate:
 - Minimum Information Standards
 - Open Data formats
 - Methods for global data exchange
- Funding for international workshops on these topics will be part of NFDI.



NFDI4Chem will ...



1. Foster awareness of research data management in chemistry.
2. Manage data about molecules, their characterisation and reactions, both experimental and theoretical.



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