Chemistry Consortium NFDI4Chem

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Our vision

NFDI4Chem is a **grassroots movement** of researchers, infrastructure experts and actors of learned societies from all disciplines of chemistry. The vision of NFDI4Chem is the application of digitisation principles to all key steps of research in chemistry. In the initial phase, NFDI4Chem focuses on **molecules and data for their characterisation** and reactions, both experimental and theoretical.

Key objectives

Objective 1: Connect existing data repositories, develop missing ones, and link them to international repositories.

Objective 2: **Minimum information (MI) standards** for **data** and **machine-readable metadata**, as well as open data standards.

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

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

Objective 5: Exploit synergies with neighbouring NFDI consortia NFDI4Cat, FairMat, NFDI4MSE, NFDI4BioDiversity.

Objective 6: Explore the legal aspect of FAIR research data management.

Our contribution to the NFDI

- We provide data standards and open formats for all data related to molecule characterisation and reactions.
- We are the national hub for international standardisation efforts on molecule data and descriptive metadata.
- We develop digital lab environments with ELNs as central tool for embedded research data management.
- We develop vocabularies, ontologies to semantically annotate data.
- We explore legal aspects of research data management and develop services to advice and train researchers.

Expected synergies within the NFDI

- How to annotate data with metadata, adding semantics and context to data.
- Development of standards for machine-readable data and metadata.
- Integrated digital lab environments, application of ELNs.
- Exploration of new applications of research data with respect to big data and AI methods.

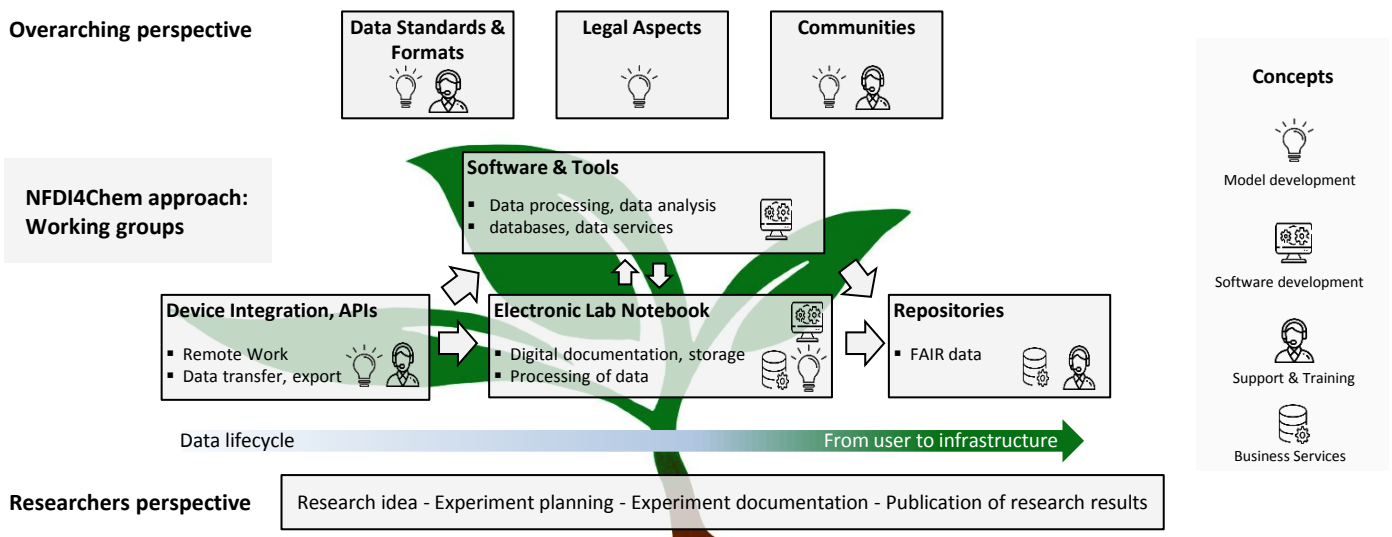
Researchers perspective (based on user surveys)

- Average researcher spends > 50 % of time with generation and analysis of research data.
- RDM is well accepted, but underdeveloped! 90 % of the community would publish more data when supported.

Wishes of community:

- Intuitive tools for data organisation and archiving
- Systematic way of data archiving
- Automated metadata parsing to make data findable
- Data archiving standards urgently needed

Digital and Cultural Change in Chemistry



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