



**NFDI<sub>4</sub>Chem**

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DATA.

## **Progress Report NFDI4Chem**

In the National Research Data Infrastructure (NFDI)

The NFDI4Chem writing team

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## Table of Content

|                                     |   |
|-------------------------------------|---|
| B-1 Progress Report Template Part 1 | 3 |
| 1 General Information               | 3 |
| 2 Summary                           | 4 |
| 3 Composition of the consortium     | 6 |

# B-1 Progress Report Part 1

## 1 General Information

### Name of the consortium:

NFDI4Chem - Chemistry Consortium in the NFDI

### Research domains<sup>1</sup> or research methods addressed by the consortium:

**NFDI4Chem aims to develop and maintain a sustainable research data management (RDM) infrastructure in Germany by applying digitalisation principles to all key steps of research in chemistry**, supporting scientists in their efforts to collect, store, process, analyse, disclose and re-use research data. Measures to promote Open Science and RDM according to FAIR data principles are at the heart of NFDI4Chem to serve the community with a holistic approach to research data access. NFDI4Chem aims to represent all disciplines of chemistry in academia. We collaborate closely with thematically related consortia. In the initial funding phase, NFDI4Chem **focuses on molecules and data for their characterisation and reactions, both experimental and theoretical**. The relevant DFG review boards are:

- 321 Molecular Chemistry
- 323 Physical Chemistry
- 324 Analytical Chemistry
- 325 Biological Chemistry and Food Chemistry
- 326 Polymer Research
- 327 Theoretical Chemistry

### URL of the consortium website and repositories used for publishing output

**Website:** [www.nfdi4chem.de](http://www.nfdi4chem.de)

**Repositories:** For the research data repositories, refer to this list with direct links:

<https://www.nfdi4chem.de/index.php/repos/>

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<sup>1</sup> Please provide the respective names and numbers of the DFG review boards when listing the research domains.

## 2 Summary

The progress of the NFDI4Chem consortium in data management in chemistry is outlined in our latest report, highlighting the steps we have taken to integrate a data-centric approach within the chemistry community.

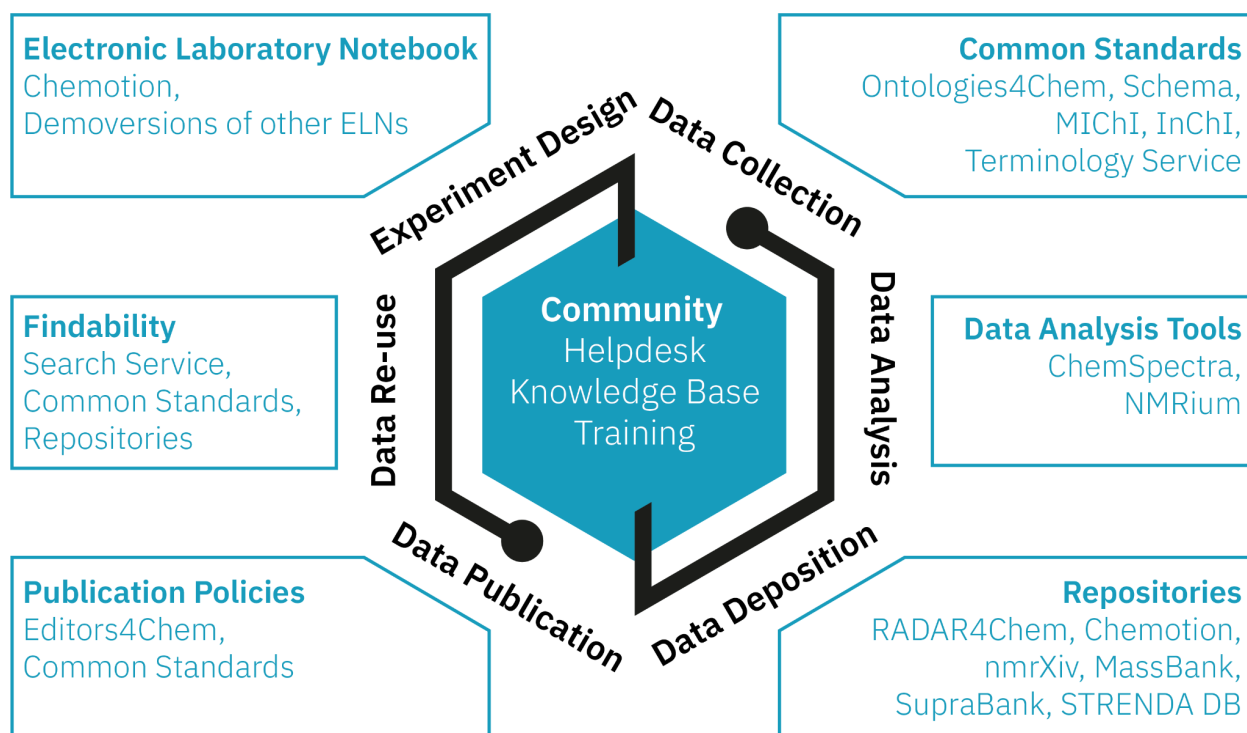
The shift towards digital tools in research documentation is evident in our work with Electronic Laboratory Notebooks (ELNs). **Chemotion ELN** represents our efforts in this domain, providing a platform for systematic data storage that enables straightforward retrieval and sharing of data. To facilitate research collaboration, we have provided guidelines and best practices for data sharing within the Chemotion ELN. Much of our effort has gone into the development and improvement of repositories. The Chemotion and **RADAR4Chem** repositories are primary examples. The Chemotion repository, designed for sustainable chemical research, provides organised storage of reaction information and analytical data, while RADAR4Chem provides storage for all types of chemical data. The emphasis on general chemical repositories, as well as the development of specific repositories such as nmrXiv, is based on the recognised need for structured data storage and retrieval in contemporary chemical research.

Engaging with the community and providing educational resources has been an important part of our agenda to foster **cultural change in the community** towards FAIR data. We have organised 21 workshops, reaching over 600 participants at various institutions in Germany and extending to international locations. These workshops are aimed at a broad audience, from researchers to data stewards. Our initiatives such as the FAIR4Chem award and the first Chemistry Data Days underline our approach to community engagement. In addition, our monthly Stammtisch discussions on various topics aim to keep the community informed and provide a platform for dialogue.

We have successfully established the **Editors4Chem** initiative with all chemistry publishers to promote standardised data management practices within the chemistry community. Through this partnership we have been able to reach a wider audience and ensure that the benefits of structured data management are understood and adopted by researchers, editors and publishers alike. Ontologies play a crucial role in ensuring that data is not only structured but also semantically meaningful. Our **Ontologies4Chem** workshops and collaboration with the Royal Society for Chemistry (RSC) on ontology development and curation are indicative of our commitment to this area. Our review article "Ontologies4Chem: the landscape of ontologies in chemistry" provides a comprehensive overview of the current state of ontologies in the field. To ensure that the data and resources we provide are easily accessible, we have developed the NFDI4Chem **Search Service**. This service allows users to quickly search and retrieve data from

our repositories. Furthermore, all our efforts, resources and tools are consolidated and made available through our portal [www.nfdi4chem.de](http://www.nfdi4chem.de), ensuring that users have a one-stop solution for all their data management needs in chemistry.

Our engagement with the wider scientific community is also reflected in our academic contributions. We have published 15 journal articles on topics ranging from molecular representations to research data management practices. Our tools and services have been presented at over 65 national and international conferences. Our presence on platforms such as X/Twitter and LinkedIn demonstrates our efforts to stay connected and share updates with peers worldwide. The progress report provides a comprehensive overview of NFDI4Chem's activities in the area of data management in chemistry (Figure 1). Through our repository initiatives, work with ELNs, outreach programmes and academic publications, we are addressing the evolving needs of the chemistry research community. As we continue our efforts, our focus remains on providing tools and resources that facilitate efficient data management and collaboration in chemistry.



**Figure 1:** Efforts to help chemists publish FAIR data. NFDI4Chem offers technical services and platforms throughout the whole data life cycle from experiment design to re-use, as well as research data management support for the community. ELN - Electronic Laboratory Notebook; MICHl - Minimum Information for Chemical Investigations; InChI - International Chemical Identifier.

### 3 Composition of the consortium

| Applicant institution                    | Location | Duration      |
|--|----------|---------------|
| Friedrich Schiller University Jena (FSU) | Jena     | since 10/2020 |

| Spokesperson   | Institution, location  | Duration      |
|--|--|---------------|
| Prof. Dr. Christoph Steinbeck<br><a href="https://orcid.org/0000-0001-6966-0814">orcid.org/0000-0001-6966-0814</a> | Friedrich Schiller University,<br>Institute for Inorganic and Analytical<br>Chemistry, Lessingstr. 8, 07743 Jena | since 10/2020 |

| Co-applicant institutions   | Location                     | Duration      |
|---|------------------------------|---------------|
| Karlsruhe Institute of Technology (KIT)                                   | Karlsruhe                    | since 10/2020 |
| FIZ Karlsruhe - Leibniz Institute for<br>Information Infrastructure (FIZ) | Eggenstein-<br>Leopoldshafen | since 10/2020 |
| Leibniz Institute of Plant Biochemistry (IPB)                             | Halle (Saale)                | since 10/2020 |
| RWTH Aachen University (RWTH)   | Aachen                       | since 10/2020 |
| Johannes Gutenberg University Mainz (JGU)                                 | Mainz                        | since 10/2020 |
| German National Library of Science and Technology (TIB)                   | Hannover                     | since 10/2020 |

| Co-spokespersons   | Institution, location  | Task area(s)          | Duration      |
|--|--|-----------------------|---------------|
| Dr. Nicole Jung<br><a href="https://orcid.org/0000-0001-9513-2468">orcid.org/0000-0001-9513-2468</a>     | Karlsruhe Institute of Technology,<br>Institute of Organic Chemistry<br>Kaiserstraße 12, 76131 Karlsruhe                                 | TA2 - Smart<br>Lab    | since 10/2020 |
| Dr. Felix Bach<br><a href="https://orcid.org/0000-0002-5035-7978">orcid.org/0000-0002-5035-7978</a>      | FIZ Karlsruhe - Leibniz Institute<br>for Information Infrastructure,<br>Hermann-von-Helmholtz-Platz 1,<br>76344 Eggenstein-Leopoldshafen | TA3 -<br>Repositories | since 10/2020 |
| Matthias Razum<br><a href="https://orcid.org/0000-0002-5139-5511">orcid.org/0000-0002-5139-5511</a>      | FIZ Karlsruhe - Leibniz Institute<br>for Information Infrastructure,<br>Hermann-von-Helmholtz-Platz 1,<br>76344 Eggenstein-Leopoldshafen | TA3 -<br>Repositories | since 10/2020 |
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|  |  |   |               |
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| Participating institutions                             | Location          | Duration             |
|--|-------------------|----------------------|
| Beilstein-Institut (BI)                                | Frankfurt am Main | since 10/2020        |
| Bundesanstalt für Materialforschung und -prüfung (BAM) | Berlin            | since 06/2023        |
| Deutsche Pharmazeutische Gesellschaft e.V. (DPHG)      | Frankfurt am Main | since 10/2020        |
| Fritz Haber Institute of the Max Planck Society (FHI)  | Berlin            | since 10/2020        |
| Leibniz Institute of Photonic Technology (IPHT)        | Jena              | since 08/2021        |
| Georg August University Göttingen (GAU)                | Göttingen         | since 10/2020        |
| Gesellschaft Deutscher Chemiker e.V. (GDCh)            | Frankfurt am Main | since 10/2020        |
| Julius Maximilians University Würzburg (JMU)           | Würzburg          | since 10/2020        |
| Ludwig-Maximilians-Universität München (LMU)           | München           | since 10/2020        |
| Physikalisch-Technische Bundesanstalt (PTB)            | Braunschweig      | since 10/2020        |
| Technische Universität Braunschweig (TU Br)            | Braunschweig      | since 10/2020        |
| TU Dortmund University (TU Do)                         | Dortmund          | since 10/2020        |
| Technische Universität Dresden (TU Dr)                 | Dresden           | since 10/2020        |
| Helmholtz Centre for Environmental Research (UFZ)      | Leipzig           | since 10/2020        |
| University of Stuttgart (USt)                          | Stuttgart         | since 06/2022        |
| University of Cologne (UzK)                            | Köln              | 10/2020 -<br>12/2021 |

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