

Program MSE  
MSE Day 18.11.2022

## ELN Concept MSE

Susan Anson

HELMHOLTZ

# Why use an ELN?

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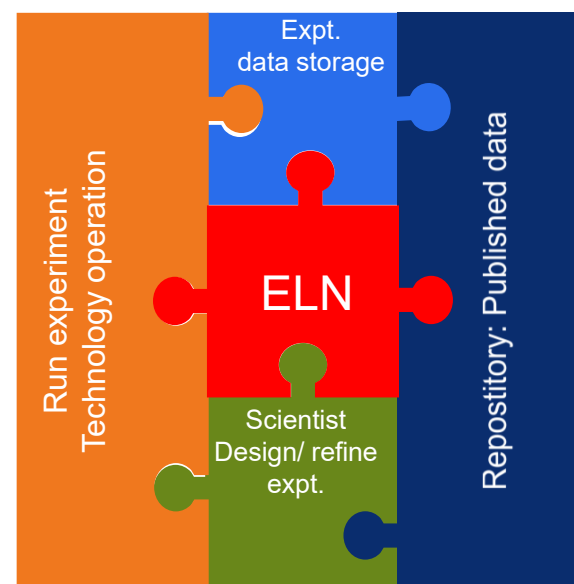
- An ELN is a support tool for good scientific practice
- Scientists and their employers are committed to the rules of good research practice as described in:
  - The Helmholtz Open Science Policy adopted 20.09.2022 <https://os.helmholtz.de/en/open-science-in-helmholtz/open-science-policy/>
  - DFG Code of Conduct Guidelines for Safeguarding Good Research Practice was adopted on 3 July 2019 <https://wissenschaftliche-integritaet.de/en/>
  - DFG Vorschläge zur Sicherung guter wissenschaftlicher Praxis/ Proposals for Safeguarding Good Scientific Practice First edition 1998, revised 2013

## Why now?

- The sheer amount and complexity of research data produced and analysed, requires efficient Research Data Management (RDM).
- RDM covers the collection, organisation, analysis, preservation and storage of data in a FAIR manner.
  - FAIR data= Findable, Accessible, Interoperable, Reusable.

# ELN – central to research data management

- Software in which all details of an experiment can be stored for future use- ideally open source, sustainably maintained
- Structured and secure storage of data:
  - Include structured and standardised **meta-data** descriptions
  - Allow for upload of data to a server or data repository
  - Each experiment has an automatically generated Identifier
  - automatic back up of data on an independent server
- search function
  - need a consistent **ontology** so that the information is searchable, and interoperable
- Controlled access rights – self only, research group members....



Over-simplified life-cycle of an experiment

## Other good reasons to use an ELN

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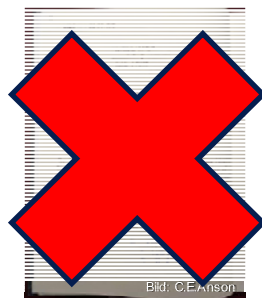
- After the initial effort it should make your life easier!
- Detailed, searchable, secure, consistent, electronic documentation of each experiment
- Platform for collaboration between partners
- Save time when writing a publication
- Help acquire research funding
  - ELN is a key component of a sound data management plan – required when submitting funding proposal e.g. DFG proposal

# ELN concept of MSE

June 2022

<10% MSE scientists use an ELN

- 10 - 15 % by the end of 2022
- 35 % by the end of 2023
- > 80 % by 2027



SampleDB Search... Instruments Actions Objects More Help

Sample #1: OMBE-1

Information

Instrument OMBE 1  
Action Updated Sample Create

Sample Information  
Sample Name OMBE-1  
Creation Date Feb 24, 2017, 12:56:00  
Checklist X  
Dropdown Option B  
Substrate GaAs

Multilayers

Multilayer  
Film Layer Repetitions 1

Films

Film  
Film Name Seed 1  
Film Thickness 5 Å  
Oxygen Flow Ovacor  
Substrate Temperature 130°C

GitLab repository page for 'kadi'. The page shows project information, including 1,680 commits, 1 branch, 27 tags, 1.7 MB files, 155.2 MB storage, and 27 releases. It also displays a commit history table with columns for Name and Last commit. The commit history shows a commit by 'kadi' with the message 'Merge branch 'external\_upload\_master' into 'master''.

Herio ELN interface showing a workflow for extrusion. The workflow includes steps for 'Extrusion' and 'Ideal temperature curve for furnace'. The 'Extrusion' step is detailed with performance metrics: 'Performance: 11/9/2022', 'Published: 11/14/2022', 'Edited: 11/14/2022', '2022-11-09-ind', and 'Diameter of used materials: 49mm'. The 'Ideal temperature curve for furnace' step includes a graph showing temperature over time.

## Which ELN should I use?

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- There is not (yet) a single ELN suitable for everyone
- Free to choose the one you prefer
- Criteria to consider are:
  - suitability and adaptability to one's own research and the nature of the research data,
  - the availability of dedicated support and open source software,
  - location and security of stored data,
  - the transfer of data to suitable repositories,
  - compatibility/interoperability with other ELNs,
  - availability of exit strategies, e.g. transfer to other ELNs in the case of discontinuation

## Who can help? ELN contacts in MSE

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- **KIT:** Chemotion/LabIMotion (contact: N. Jung, S. Bräse)\* and Kadi4Mat (M. Selzer)\*, eLabFTW (Matthias Schwotzer)
- **Hereon:** Herbie (C. Eschke, F. Kirchner)\*                      \*Developed in MSE Helmholtz centres
- **FZJ:** SampleDB (F. Rhiem, D. Weber)\*
- ELN finder: <https://eln-finder.ulb.tu-darmstadt.de/home>
- → Developers are already connected in several initiatives and collaborate to be able to exchange data interoperably



## MSE Participation in NFDI Consortia

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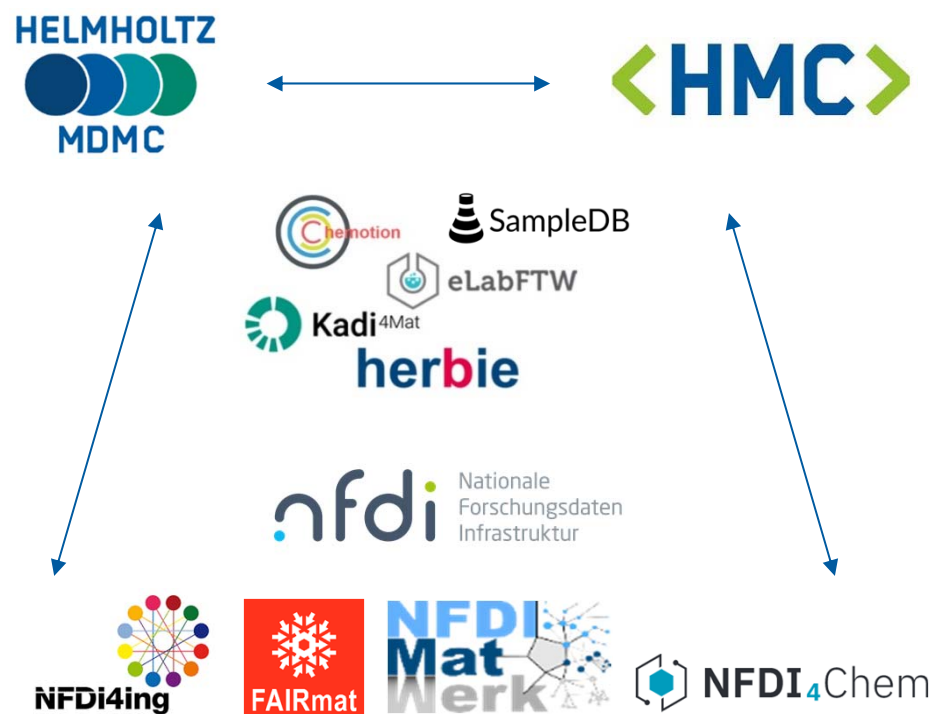
<b>NFDI platform</b>	<b>Linked data repositories</b>	<b>Contacts</b>
DAPHNE4NFDI		KIT: J.-D. Grunwaldt (RF Energy), F. Weber (NACIP)
FAIRmat	Nomad_Laboratory	KIT: C. Wöll
NFDI4Cat		KIT: O. Deutschmann, F. Studt (RF Energy both)
NFDI4Chem	Nine; currently active: chemotion-repository; radar4chem	KIT: N. Jung
NFDI4Ing	Several	KIT: A. Streit (EDF), B. Nestler, M. Selzer Hereon: C. Eschke, F. Kirchner FZJ: J. Mayer
NFDI4Matwerk		KIT: A. Streit (EDF), P. Gumbsch FZJ: J. Mayer, S. Sandfeld



# Towards a new generation of ELNs

## Collaborations to address challenges

- Improving interoperability
- Development of metadata schemas and ontologies
- Improved functionality
- Within Helmholtz
  - Discussion panels e.g. ELN working group
  - JL MDMC, HMC platform
- National level
  - Direct involvement with NFDI initiative
- European level
  - NEP/NFFA European pilot infrastructure project
  - EOSC-Pillar



# ELN Implementation Concept MSE: Summary

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## Background

- FAIR Research Data Management (RDM) is prerequisite to day-to-day laboratory work
  - Electronic Laboratory Notebooks (ELNs) are a key enabling tool for RDM
  - DFG Guidelines for Safeguarding good scientific practice require ELNs
  - Leading researchers in MSE are involved in virtually all the Materials Science relevant NFDI consortia of which several develop and host ELNs and data repositories
- use of **ELNs is a central and crucial step in the digitalization of Materials Science!**

## Aim is that MSE researchers use an ELN

- 10 - 15 % by the end of 2022
- 35 % by the end of 2023
- At least 80 % by the end of the PoF4 funding period

**Advice and assistance is available – Please ask!**

# Thank you for your attention

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## Acknowledgements:

in particular: Nicole Jung, Michael Selzer, Matthias Schwotzer, Dieter Weber, Florian Rhiem, Catriona Eschke, Rossella Aversa, Alex Welle, Christof Wöll

- Some case studies of ELNs are presented in the poster exhibition

[Susan.anson@kit.edu](mailto:Susan.anson@kit.edu)