



ELNs – electronic laboratory notebooks + data security of DDR @CXI

What is ELN?

- It is a tool that helps to streamline laboratory workflows and make data more accessible and organized.
- Digital platform that enables scientists and researchers to record, store, and manage their laboratory experiments, observations, and data electronically
- Replaces traditional paper-based lab. notebook
- Features & advantages:
 - ✓ Electronic templates for experiment entries
 - ✓ Ability to attach digital files (images, graphs, datasets)
 - ✓ Tools for collaboration and sharing data with other researchers
 - ✓ Advanced search functions (helps finding specific data or experiments quickly)
 - ✓ Security and backup to protect against data loss or unauthorized access

ELN – electronic laboratory notebook(s)

What is NOT ELN?

**ELN is not instrument (machine)
log book – it is separate tool**

ELN – electronic laboratory notebook(s)

- **OpenBIS**
- **Kadi4Mat**
- **NOMAD (Oasis)**

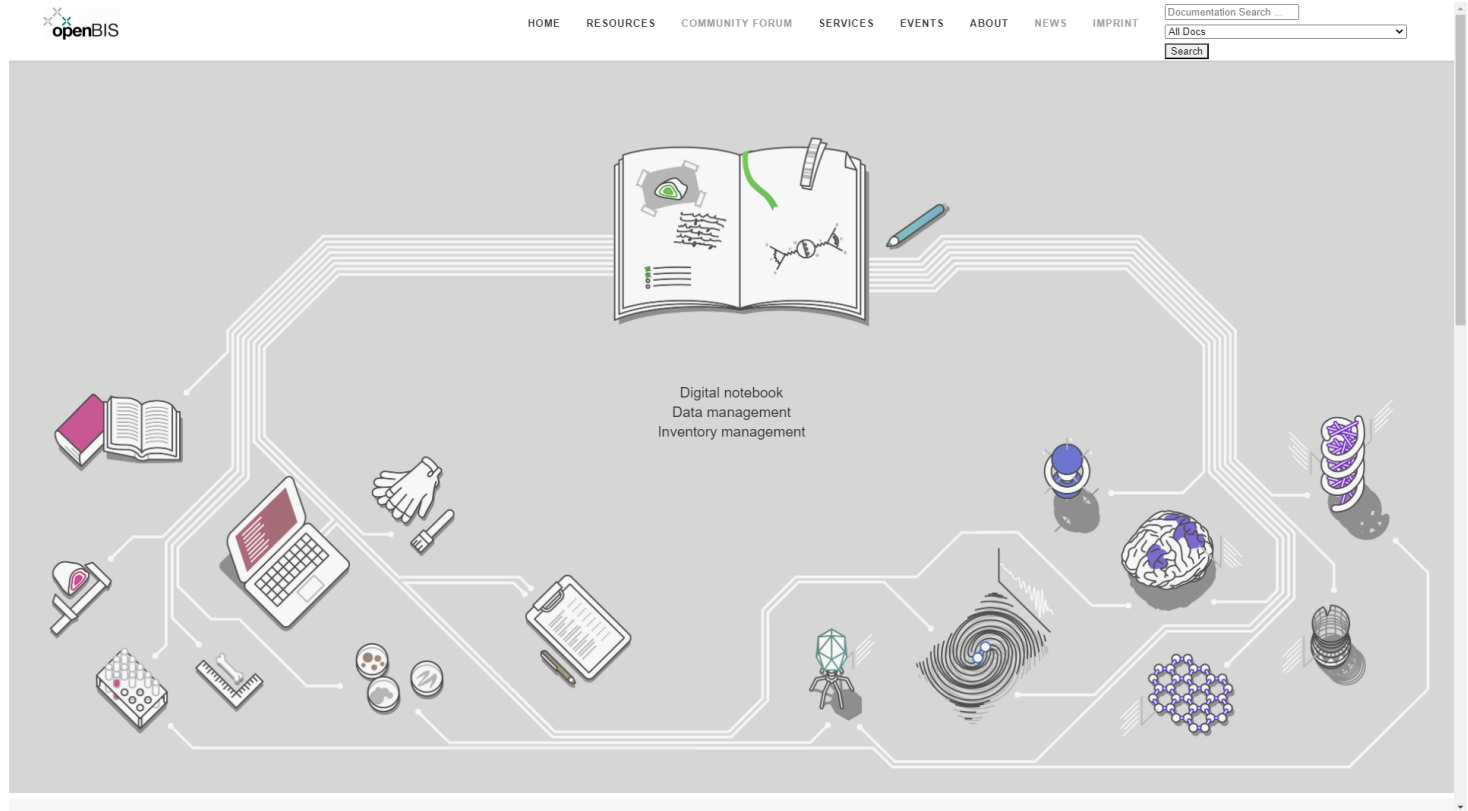
ELN – electronic laboratory notebook(s)

OpenBIS

- Developed at ETH Zürich (originally for biologists)
- Secured financing and further support
- Pretty complex system which contains (almost) every necessary function
- JupyterLab integration – useful for Python/R calculations
- <https://openbis.ch/>

ELN – electronic laboratory notebook(s)

OpenBIS



ELN – electronic laboratory notebook(s)

OpenBIS

Browse ▾ New ▾ Import ▾ Utilities ▾

Project Registration **Project Browser**

Code	Space	Description	Registrator
DEFAULT	DEFAULT		System User
DEFAULT_PROJECT	DEFAULT_LAB_NOTEB...	Default Project	System User
ORDERS	STOCK_ORDERS	Orders	System User
PRODUCTS	STOCK_CATALOG	Products	System User
PROTOCOLS	METHODS	Protocols	System User
PUBLIC_REPOSITORIES	PUBLICATIONS	Public Repositories	System User
REQUESTS	STOCK_CATALOG	Requests	System User
STORAGES	ELN_SETTINGS	Storages	System User
SUPPLIERS	STOCK_CATALOG	Suppliers	System User
TEMPLATES	ELN_SETTINGS	Templates	System User

Browse ▾ New ▾ Import ▾ Utilities ▾

Project Registration **Project Browser** Collection Registration **Object Registration**

Object Type: ENTRY ▾

Code: * ENTRY1

Collection:

Project: Choose project... ▾

Space: * Choose Space... ▾

Parents: List of Object (codes or identifiers) separated by commas (",") or one Object per line. (0)

Tags: List of tag names separated by commas (",") or one tag name per line. If a tag does not exist, it will be created. (0)

General info

Name: ⓘ

Show in project overview: ⓘ

Document: ⓘ

ELN – electronic laboratory notebook(s)

Kadi4Mat

- Developed at Institute for Applied Materials in Karlsruhe, Germany
- Youngest member of the team – still in early development
- Simply extensible, very easy to use
- Missing some important advanced features or functions
- Integrated with CIDS through KadiAI – framework for statistics and ML
- <https://kadi.iam-cms.kit.edu/>

ELN – electronic laboratory notebook(s)

Kadi4Mat

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Kadi4Mat is the Karlsruhe Data Infrastructure for Materials Science, an open source software for managing research data.

The goal of this project is to combine the ability to manage and exchange data, the *repository*, with the possibility to analyze, visualize and transform said data, the *electronic lab notebook (ELN)*.

[Demo instance](#)

[Documentation](#)

About

Kadi4Mat supports a close cooperation between experimenters, theorists and simulators, especially in materials science, to enable the acquisition of new knowledge and the development of novel materials. This is made possible by employing a modular and generic architecture, which allows to cover the specific needs of different scientists, each utilizing unique workflows. At the same time, this covers up the

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Kadi4Mat

The screenshot displays the Kadi4Mat web interface for creating a new record. The top navigation bar includes the Kadi4Mat logo and menu items: Records, Collections, Templates, Users, Groups, and Workflows. A search bar is located on the right. The main content area is titled 'Records / New record' and features a dropdown menu for selecting a record template, currently showing 'No record template selected.' Below this is the 'Metadata' section with the following fields:

- Title***: A text input field.
- Identifier***: A text input field with a yellow tooltip that reads 'Unique identifier of this record.'
- Type**: A dropdown menu with the placeholder text 'Enter or search for a record type' and a tooltip that reads 'Optional type of this record, e.g. dataset, experimental device, etc.'
- Description**: A rich text editor with a toolbar containing icons for bold (H), italic (I), strikethrough (ABC), subscript (x₂), superscript (x²), code (</>), square root (√), bulleted list, numbered list, indent, link, and unlink. It also includes undo, redo, and refresh icons. A note at the bottom of the editor states: 'This editor supports Markdown, including math written in LaTeX syntax rendered with KaTeX. Note that HTML tags and external images are not supported.'
- License**: A dropdown menu with the placeholder text 'Search for a license'.
- Visibility**: A dropdown menu with the selected option 'Private'.

At the bottom of the form, there is a small text note: 'Public visibility automatically grants EVERY logged-in user read permissions for this record.'

ELN – electronic laboratory notebook(s)

NOMAD (Oasis)

- Quickly developed lately but still grant funded
- Focused on material science
- Either central hosted or own instance (Oasis) possible
- JupyterLab integration – useful for Python/R calculations
- <https://nomad-lab.eu/>



Join our team
and apply now!

NOMAD Laboratory

enables FAIR sharing and use of materials science data

Jun 2, 2021 [NOMAD Data Center at HU Berlin: Open Positions!](#)

Publish

- Publish your data with our without embargo, get a DOI, and share data with others.
- We support input and output files of most electronic-structure codes.
- Watch our [video tutorial](#) on how to upload and publish data.

UPLOAD

Explore

- Search for [materials](#) (Encyclopedia) or [calculations](#) (Repository).
- All raw and processed data can be downloaded and used under the [CC BY 4.0](#).
- Watch our [video tutorials](#) on how to use the Encyclopedia and Repository.

MATERIALS

CALCULATIONS

Analyze

- Analyze data with [Jupyter notebooks](#) directly on NOMAD servers (Artificial Intelligence (AI) Toolkit).
- Access all data programmatically via [NOMAD API](#) or [OPTIMADE API](#).
- Watch our [video tutorial](#) on how to use the NOMAD API.

AI TOOLKIT TUTORIALS

ELN – electronic laboratory notebook(s)

NOMAD (Oasis)

The screenshot displays the NOMAD web interface. At the top, there is a navigation bar with the NOMAD logo, a menu (PUBLISH, EXPLORE, ANALYZE, ABOUT), and user information (Welcome Jakob Zach, LOGOUT, UNITS). Below the navigation bar, the page title is "Your uploads / Upload". The main content area is titled "OVERVIEW" and shows a list of uploads. The first upload is titled "My first upload on NOMAD" with an upload ID of "dE05K0R-57yE73vYBVDPz2Q". A "SAVE" button and several icons are visible next to the upload ID. Below the upload list, there are four numbered steps: 1. Prepare and upload your files, 2. Process data, 3. Edit author metadata, and 4. Publish. Step 1 is currently active and expanded. It contains instructions on how to prepare data (using zip or tar), a list of supported atomic codes (ABACUS, ABINIT, AMS, ASAP, Amber, BigDFT, CASTEP, CHARMM, CP2K, CPMD, CRYSTAL, DFTB+, DL_POLY, DMol3, Elk, FHI-aims, FLEUR, FPLO, GAMESS, GPAW, GROMACS, GROMOS, GULP, Gaussian, LAMMPS, MOPAC, Molcas, NAMD, NWChem, ONETEP, ORCA, Octopus, OpenMX, Psi4, Qbox, QuantumATK, QuantumESPRESSO, SIESTA, TURBOMOLE, Tinker, VASP, WIEN2k, Wannier90, YAMBO, exciting, libAtoms, w2dynamics), workflow managers (AFLOW, ASR, Atomate, ElaStic, FHI-vibes, LOBSTER, MOFStructures, QuantumEspressoPhonon, QuantumEspressoEPW, phonopy), and database managers (EELSDb, NeXus, OpenKIM). Below the instructions is a "CLICK OR DROP FILES" button, a file input field containing "> /", and a section for manual entry with a table for "name" and "schema" (PerovskiteSolarCell) and an "ADD" button. The interface is clean and modern, with a light gray background and blue accents.

ELN – electronic laboratory notebook(s)

And now some practical demonstration

ELNs comparison

ELN and their features

	ENG/CZE	Own instance needed	MATECH group support	Honours FAIR principles	Maturity (yrs)	Repository integration	Big data linking	Open source	Web UI	University login	Fill your tax return
OpenBIS	YES/NO	YES	YES	YES	10+	Zenodo	YES	YES	YES	YES	NO
Kadi4Mat	YES/NO	YES	YES	YES	1+	Zenodo	NO*	YES	YES	NO*	NO
NOMAD	YES/NO	NO	NO	YES	3+	NOMAD	NO	YES	YES	YES	NO

*in process

DATA STEWARD role and counsell @ CXI

What is role/purpose of Data Steward?

- He/she is your bridge between your research and world of digitized data
- Can help you with issues that require deeper data-related knowledge
- Should be able to communicate and explain data concepts to non-technical researchers (or people in general)
- Data Steward always knows what are we trying to achieve – goals, objectives

OMI (Department of Process Modelling and Artificial Intelligence) **is able to help you with:**

1. Data Management Plan
2. Any Open Science issues
3. Data FAIRification
4. Project documentation
5. ...and of course anything related to ELN

Data security at CXI and in DDR project

- Right now there are no general rules at CXI on data security
- Although within DDR project data sharing will have strict rules with explicit exceptions
- No need to upload data if NDA does not approve
- Systematic approach should be set

FAQs (1)

- **How do I log into an ELN?**
- **Can I collect other data?
E.g.: data for audits, machine
tunning/calibration**
- **Is it possible to add own
metadata to the measurement
(or any other entry to an ELN)?**
- Each ELN has its user management. We plan to implement university login in the chosen ELN.
- Yes. Everything that you want you can save in the associated record.
- Yes. You are free to write and save anything through ELN. (It is highly recommended to add as much [valid] metadata as possible.)

FAQs (2)

- **What happens if I haven't got any PC connected to instrument?**
- **How can I share work on one sample with my group?**
- **Do I have to have some programming skills to use ELN?**
- You can use ELN from any device that is connected to the internet.
- Linking data of a single sample between researchers is one of the key elements in ELN.
- No. You just need to learn how to work with ELN via user interface.

FAQs (3)

- **Can I use ELN with my smartphone or tablet?**
- **Is it possible to digitize my previous handwritten notes?**
- **I would like to set user interface to different colours. May I?**
- Kadi4Mat for sure, others do not have responsive UI.
- Yes, it is possible to transform handwritten text to digital form (but the result may not be useful)
- Well – we cannot promise, but we'll do our best.



Thanks for your attention