FAIR Data Infrastructure for Condensed-Matter and Chemical Physics
Related Projects

- Aflow
- COD
- OQMD
- Materials Project
- NOMAD
- Jarvis
- Materials Cloud (Aiida)
- MatCloud
- OPTIMADE
- EMMO
- STREAM
- zenodo
- W3C: DCAT, ...
- HDF5
- EMME
- nexus
- OPTIMADE
- EMMO
- HIGH5
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- W3C: DCAT, ...
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- globus
- own cloud
- google
- EOSC
- DFN
- materials
- databases
- open databases
- large scale data infrastructures
- data transfer
- data publication
- lab automation
- instruments
- workflow engines
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DPG Condensed-Matter Section (SKM) and Chemical Physics of Solids

Interdisciplinarity within the field of research / consortium
- Extreme heterogeneity, very broad, full community on board
  - Researchers, working groups, research networks (CRCs, Clusters, ...), universities, research institutions, societies, ...

Embedded in the European and international landscape
- EOSC, GoFAIR, Research Data Alliance (RDA), FAIR-DI e.V.
- USA (e.g. NIST), China, Japan, Korea

Plenary and Invited talks, Publications, Organization of conferences
- International Conference on a FAIR Data Infrastructure for Materials Genomics
  - June 3-5, 2020, largest conference in the field (539 participants)
An *inclusive, user-driven* approach to develop easy-to-use tools and an infrastructure towards FAIR data processing, storage, curation, sharing, and *AI readiness* for future use of materials data.
Challenges & goals

Worldwide, synthesis recipes are collected for personal use of the scientists, often documented in handwritten lab notebooks. Log files created by the synthesis instruments, often not kept.

Goal 1: Establish metadata (standards), ontologies, and tools

Goal 2: Harmonize metadata schemes of synthesis and experimental characterization

Goal 3: Towards computer-aided development of synthesis recipes - interweaving experiment & theory
Challenges & goals

Goal 1: **Metadata and workflows for the extremely diverse** characterization methods used by the experimental condensed-matter community.

Goal 2: **Efficient and persistent linkage of data types** to be implemented by means of LIMS and ELN solutions.

Each experimental probe has its specific challenges concerning processing, curation, and storage, owing to differences in volume, velocity, data formats, etc.

ELN: Electronic Lab Notebook;
LIMS: Laboratory Information Management System
Challenges & goals

Goal 1: Integration of the NOMAD Laboratory into FAIRmat

Goal 2: Significant enhancement of its services

Goal 3: Much wider scope of methodologies

Huge variety of methods, e.g. sophisticated classical simulations (e.g. fluid dynamics), highly complex quantum-mechanical many-body techniques, and multi-scale modeling.
Challenges & goals

Different scientific methods require vastly different data handling (4V).
Large amounts of very heterogeneous data of various sources need to be integrated.
Long-term availability and data security.

Goal 1: Enabling individual scientists and research institutes to manage data following common principles, with compatible technologies and a shared interface

Goal 2: Creation of a FAIR data exploration and sharing platform

Goal 3: Become role model of data security

![Diagram](https://example.com/diagram.png)
Challenges & goals

Goal 1: Test and demonstrate the functionality of the FAIRmat data infrastructure and identify weaknesses to be improved.

Goal 2: Show how the developed DI tools will significantly support the research of the various sub-communities.

Goal 3: Demonstrate the interfaces to and hand-shakes with other NFDI consortia.

Can we have tools that not only get us organized but really enable us to enhance science in daily life?
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What is NOMAD
NOMAD makes materials science data FAIR

More than 12 million of simulations from over 400 authors world-wide

→ Free publication and sharing data of data
→ Extracts rich metadata for more than 40 codes
→ All data in a raw and a common machine readable from
→ Use integrated tools to explore, visualize, and analyze
NOMAD: A FAIR-data sharing platform for materials science
NOMAD to assist research processes

- upload
- private local data
- NOMAD Oasis
- analyse
- explore
- published data
- central NOMAD
- publish
- data on your hard-drive
NOMAD (Oasis) for all of materials science (i.e. the FAIRmat project)

Manage materials science research data

FAIRmat builds on a federated infrastructure of local repositories

→ Organise research data through its whole life-cycle
→ Inclusion of data handling for experiments
→ Adaptable to your workflows and data-types
→ A first step to connect with in the FAIRmat network
→ Oasis is being developed and you can shape its future

VISIT NOMAD OASIS WEB-SITE SOON
To be done?

FAIRmat

- Builds on extensive experience
- Provides easy-to-use tools and infrastructure for FAIR data processing, storage, curation, sharing, and AI
- Emphasizes education and training
Basic organizational principles of FAIRmat

Design infrastructure and measures bottom-up
Advance basic science of condensed-matter and materials physics
Help the active researchers, and don’t create burden
Lead by example, not by rules

Join the FAIRmat activities
https://www.fair-di.eu/fairmat/
Tell us your needs and worries

Integrating synthesis, experiment, theory, computations, and applications, FAIRmat will further the basic physical sciences in condensed-matter physics and chemical physics.
o Support der Nutzer:innen

o Lösungen für die “last mile”, die auf Fachgebiete und Nutzungsgewohnheiten zugeschnitten sind

o Allgemein niedrige Eintrittsbarrieren