FAIR Data Infrastructure for Condensed-Matter and Chemical Physics
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.

“Findable and AI ready”
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
Goal 1: Integration of the NOMAD Laboratory into FAIRmat

Goal 2: Significant enhancement of its services

Goal 3: Much wider scope of methodologies

Challenges & goals

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 showing data tiers with Centralized metadata, local data with PID, local data and data at different tiers.](image)
Challenges & goals

Can we have tools that not only get us organized but really enable us to enhance science in daily life?

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.
Challenges & goals

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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

SEARCH NOMAD  LEARN MORE
**NOMAD:** A FAIR-data sharing platform for materials science
NOMAD to assist research processes

1. Data on your hard-drive
2. Upload
3. Explore
4. Analyze
5. Private local data
6. NOMAD Oasis
7. Published data
8. Central NOMAD
9. Publish
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
- 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.

Claudia Draxl
○ Support der Nutzer:innen

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

○ Allgemein niedrige Eintrittsbarrieren