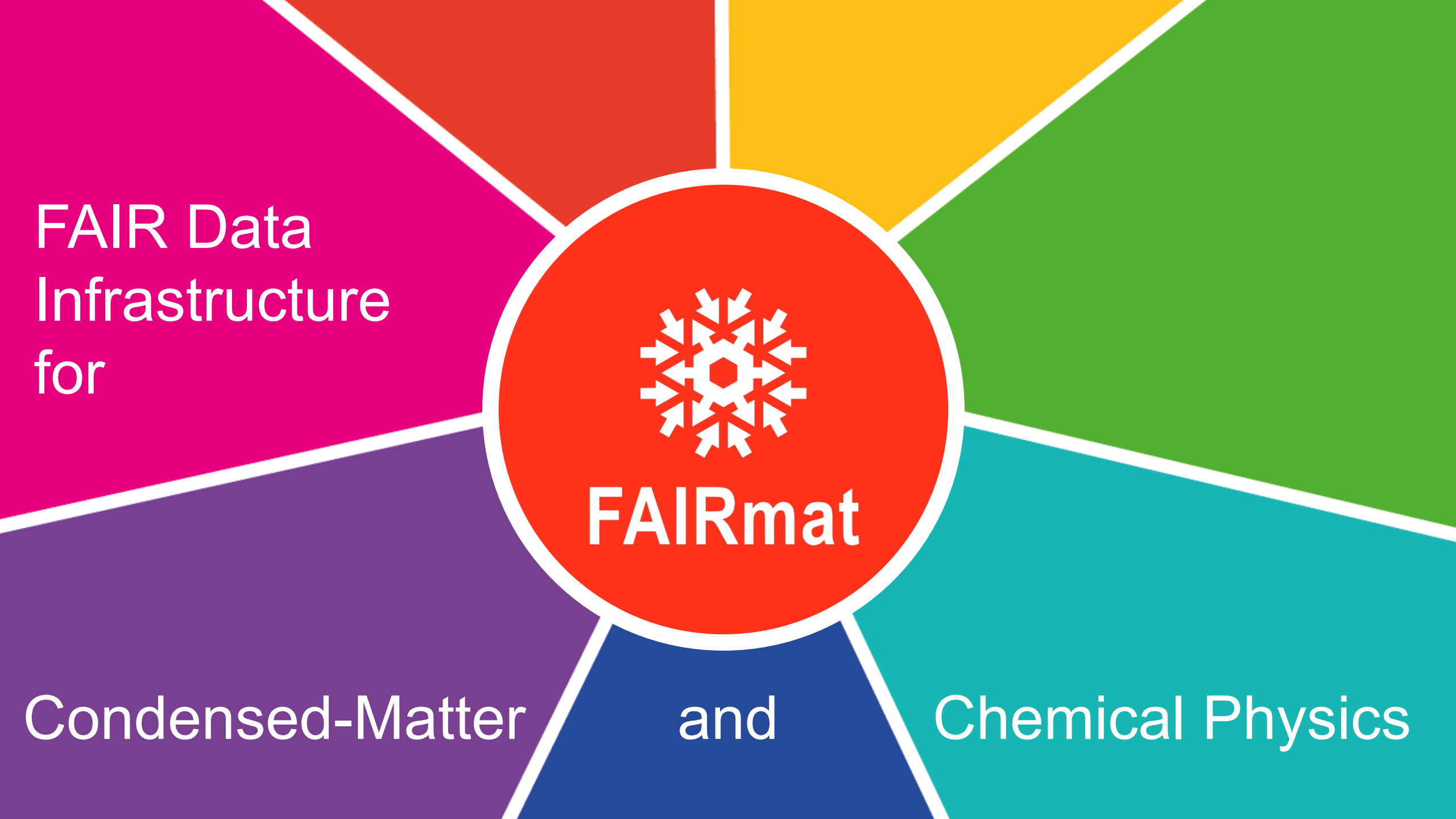
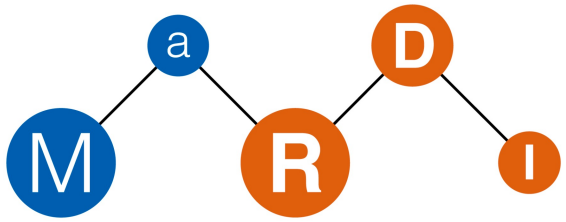
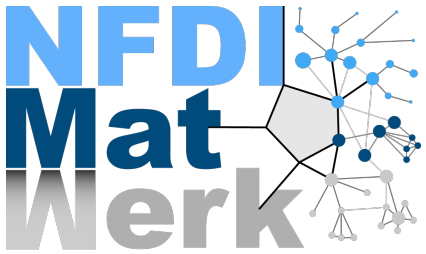
FAIR Data Infrastructure for



Condensed-Matter and Chemical Physics

FAIRmat NFDI Context





Related Projects

HDF5

formats

nexus

EMMO

ontologies

schemas

COD

OQMD

(closed) databases

Aflow

OPTIMADE

W3C:
DCAT, ...

Materials
Project

Jarvis

STREAM

VASP

codes

open databases

large scale data infrastructures

EOSC

DFN

lammps

NOMAD

FAIRmat

nfdi Nationale Forschungsdaten Infrastruktur

MatCloud

phonopy

Materials
Cloud (Aiida)

data publication

zenodo

fireworks

workflow engines

ase

eLabFTW

globus

data transfer

pymatgen

lab automation

instruments

own cloud

google

Community and Cooperations

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

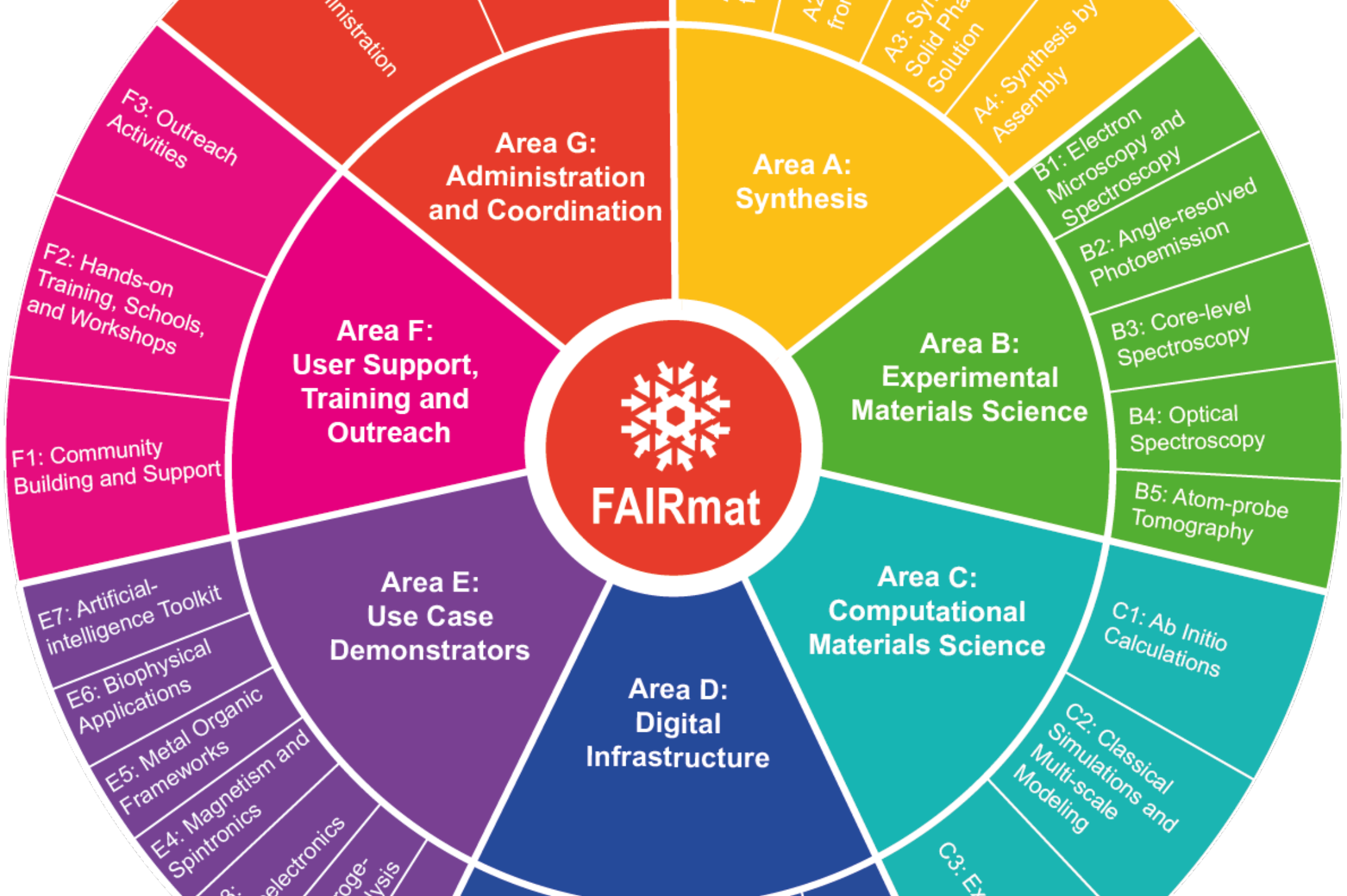
June 3-5, 2020, largest conference in the field (539 participants)

FAIRmat

“Findable and AI ready”

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

Task Areas



FAIRmat

A: Synthesis

Challenges & goals

M. Albrecht

C. Felser

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

FAIRmat

Area B: Experiment

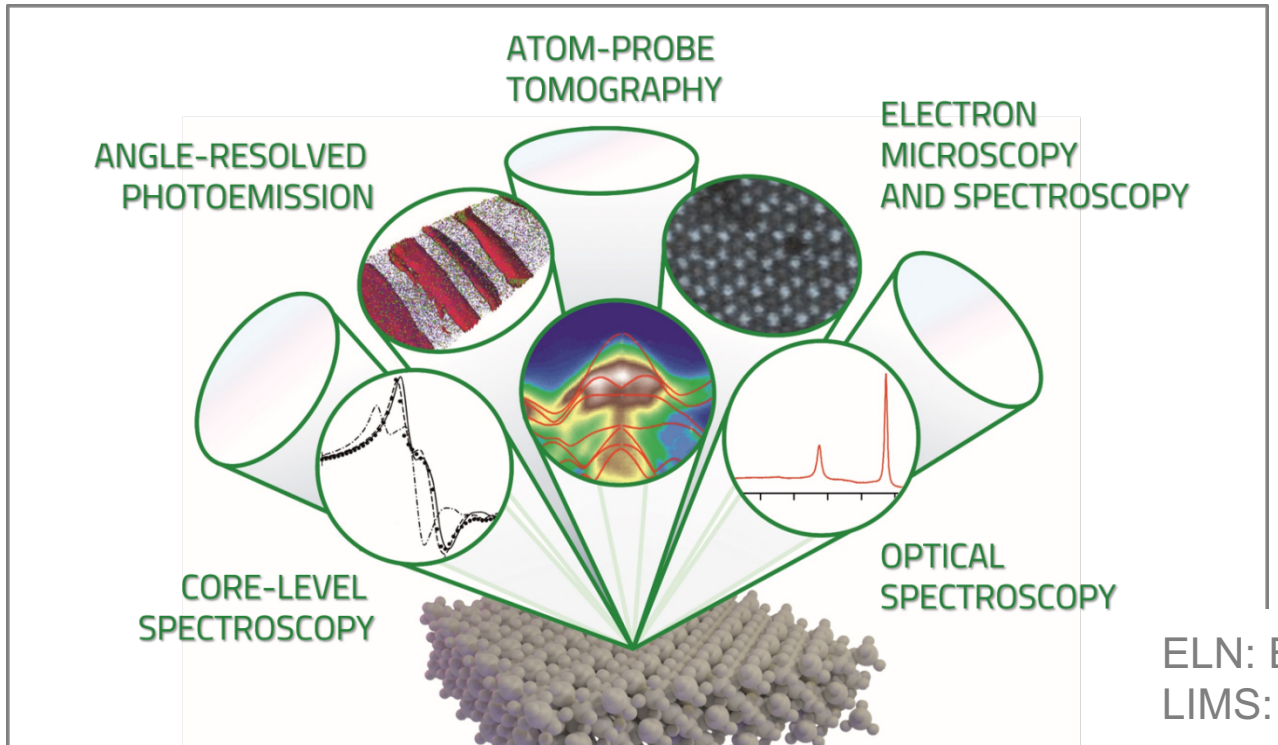
FAIRmat

Challenges & goals

M. Greiner C. Koch

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

Area C: Computations

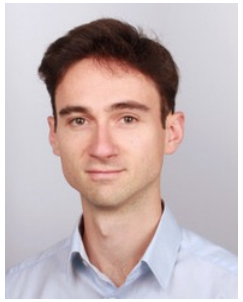
FAIRmat

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.


S. Botti

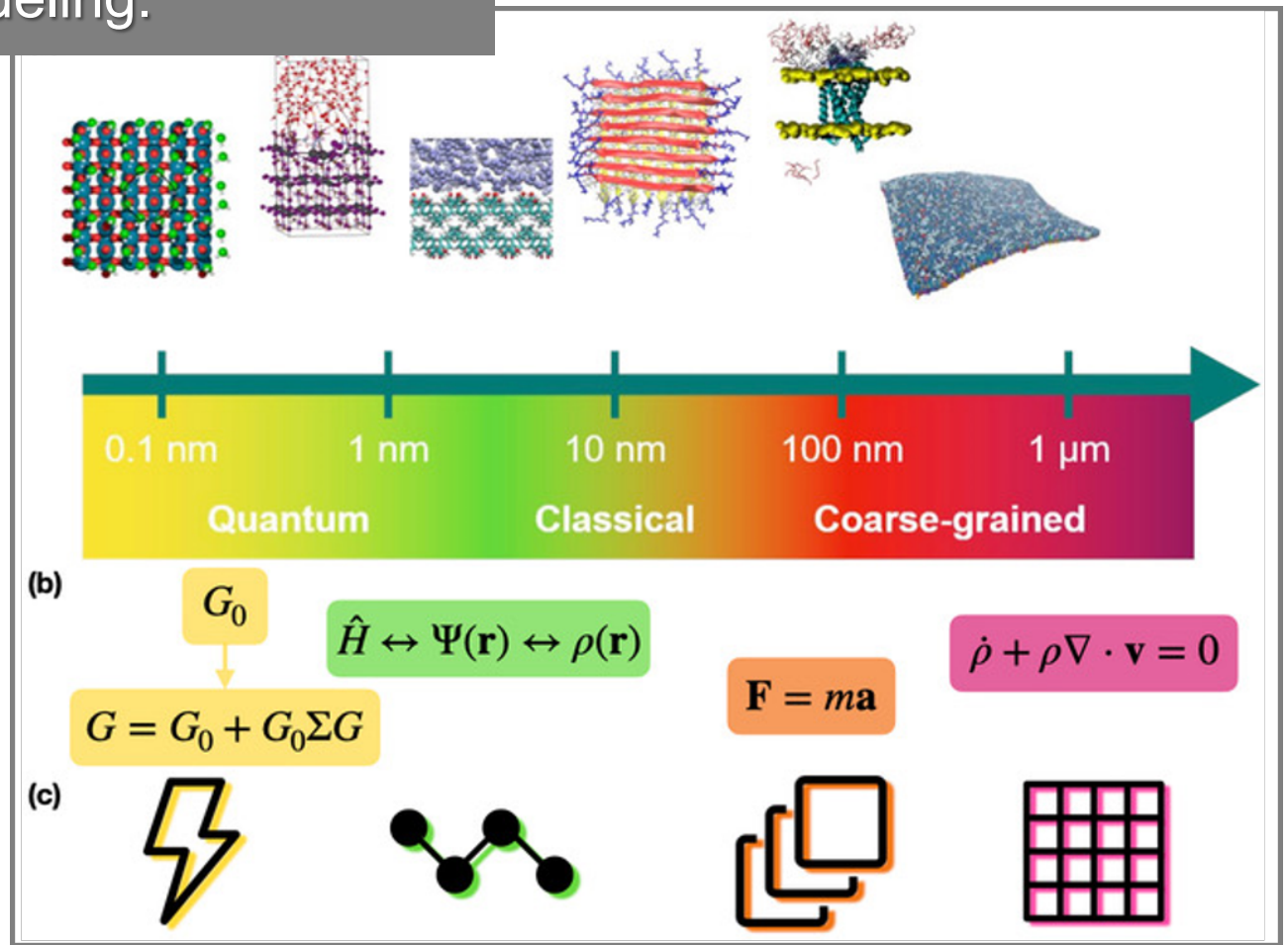

K. Kremer


T. Bereau

Goal 1: Integration of the NOMAD Laboratory into FAIRmat

Goal 2: Significant enhancement of its services

Goal 3: Much wider scope of methodologies



Area D: Infrastructure

FAIRmat

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.

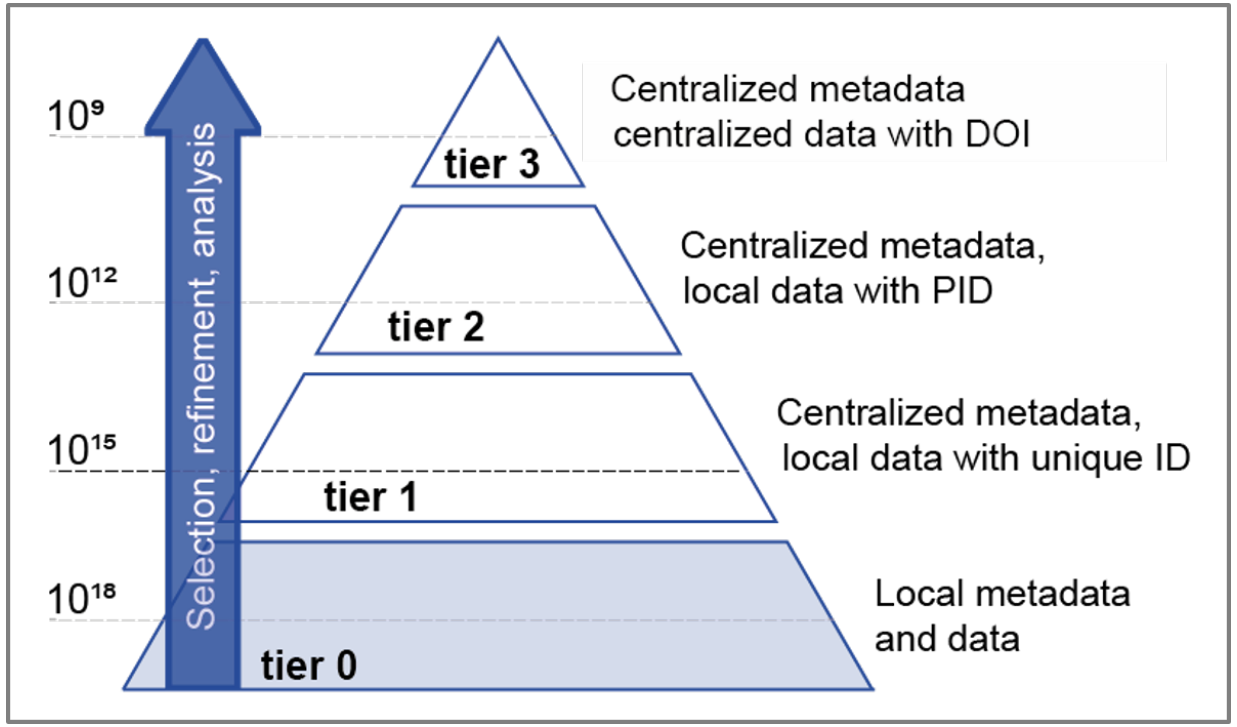
H. Bungartz

W. Nagel

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



Area E: Use Cases

FAIRmat

Challenges & goals

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

C.Wöll

A. Groß

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.

Area D: Infrastructure

FAIRmat

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.

H. Bungartz

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NOMAD

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

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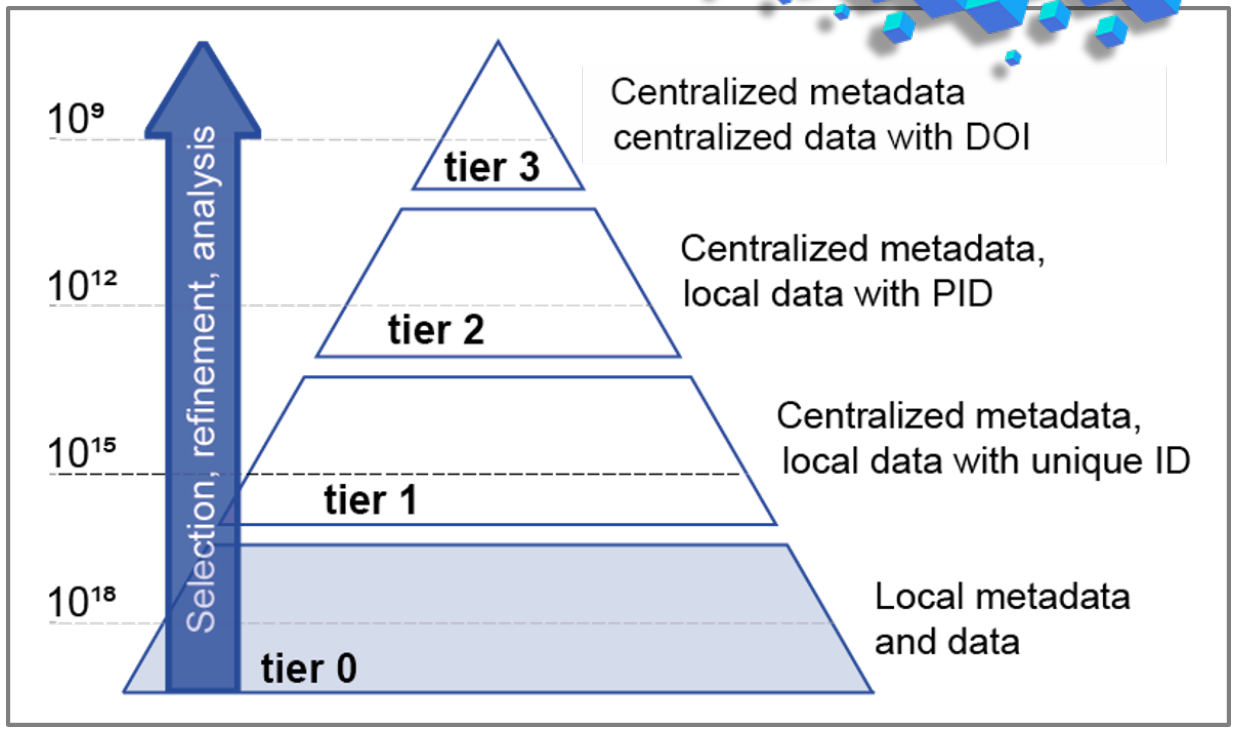
Goal 3: Become role model of data security



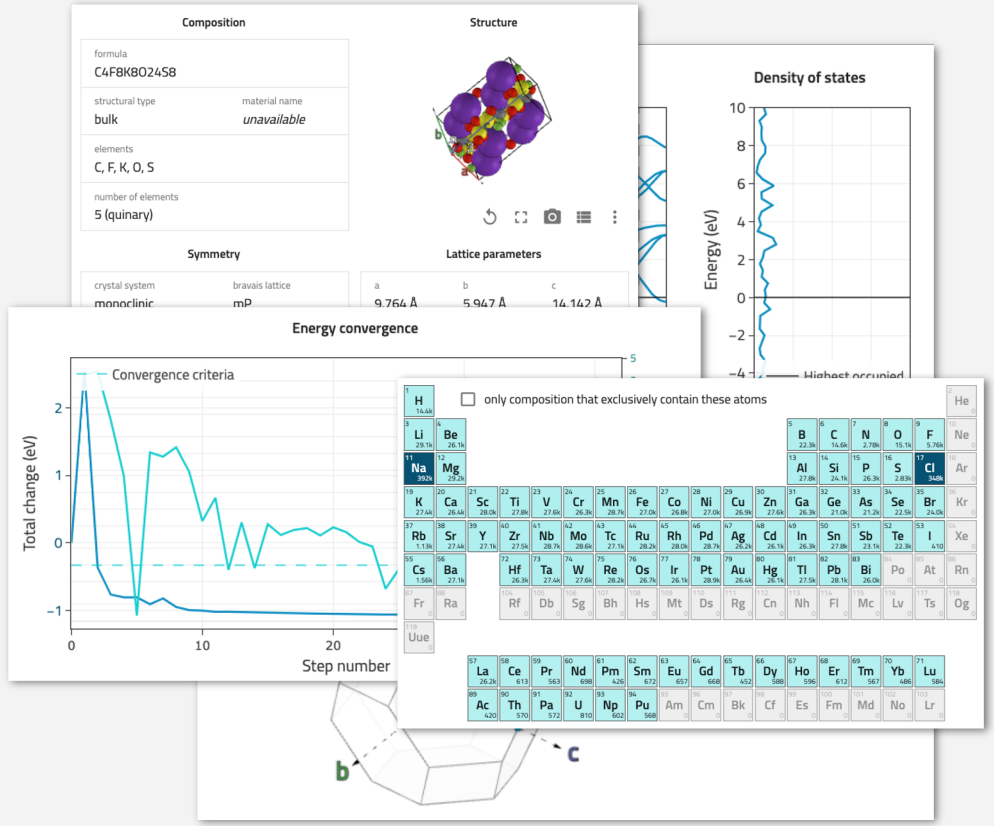
What is NOMAD

NOMAD makes materials science data FAIR

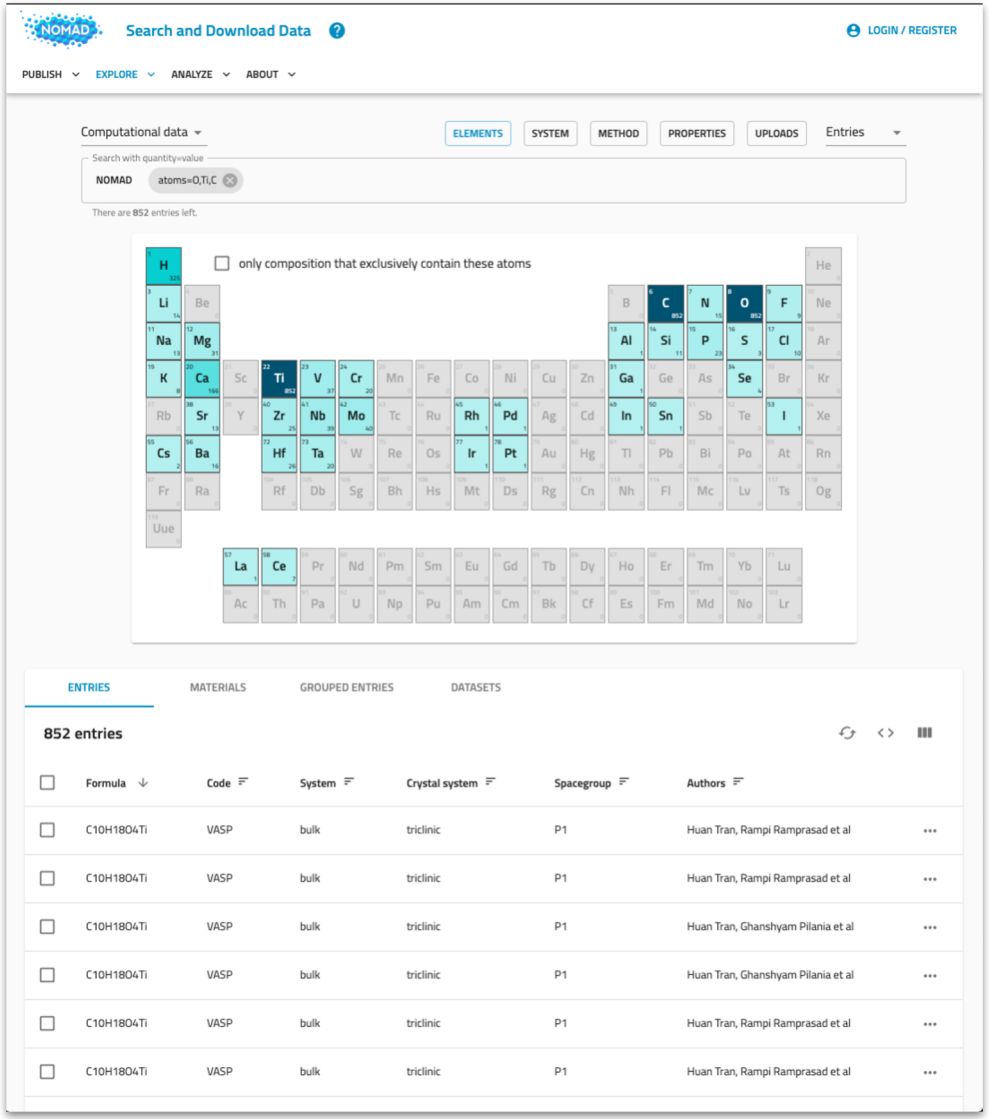
More than 12 million of simulations from over 400 authors world-wide

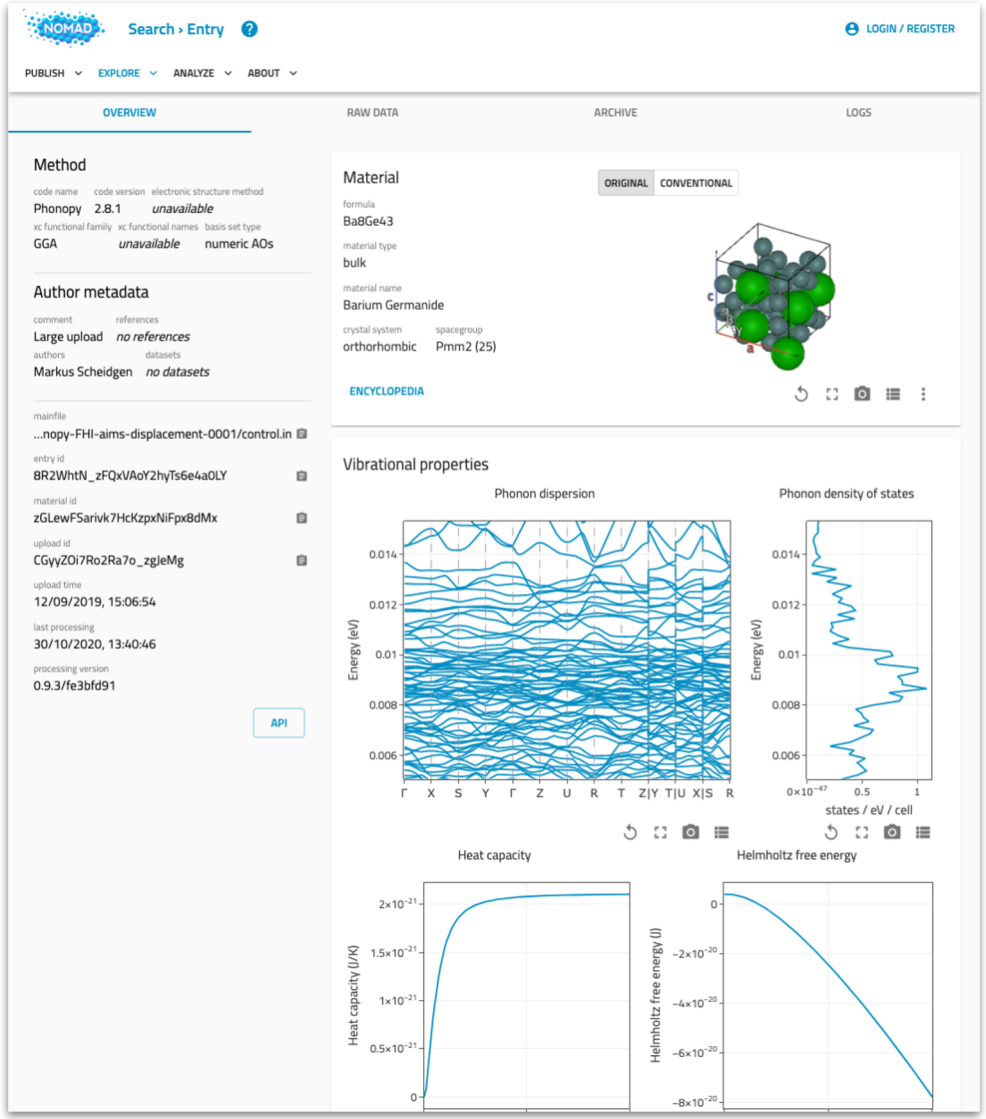
- ➔ Free publication and sharing data of data
- ➔ Extracts **rich metadata** for more than **40 codes**
- ➔ All data in a **raw** and a common **machine readable** from
- ➔ Use integrated tools to **explore**, **visualize**, and **analyze**

SEARCH NOMAD **LEARN MORE**

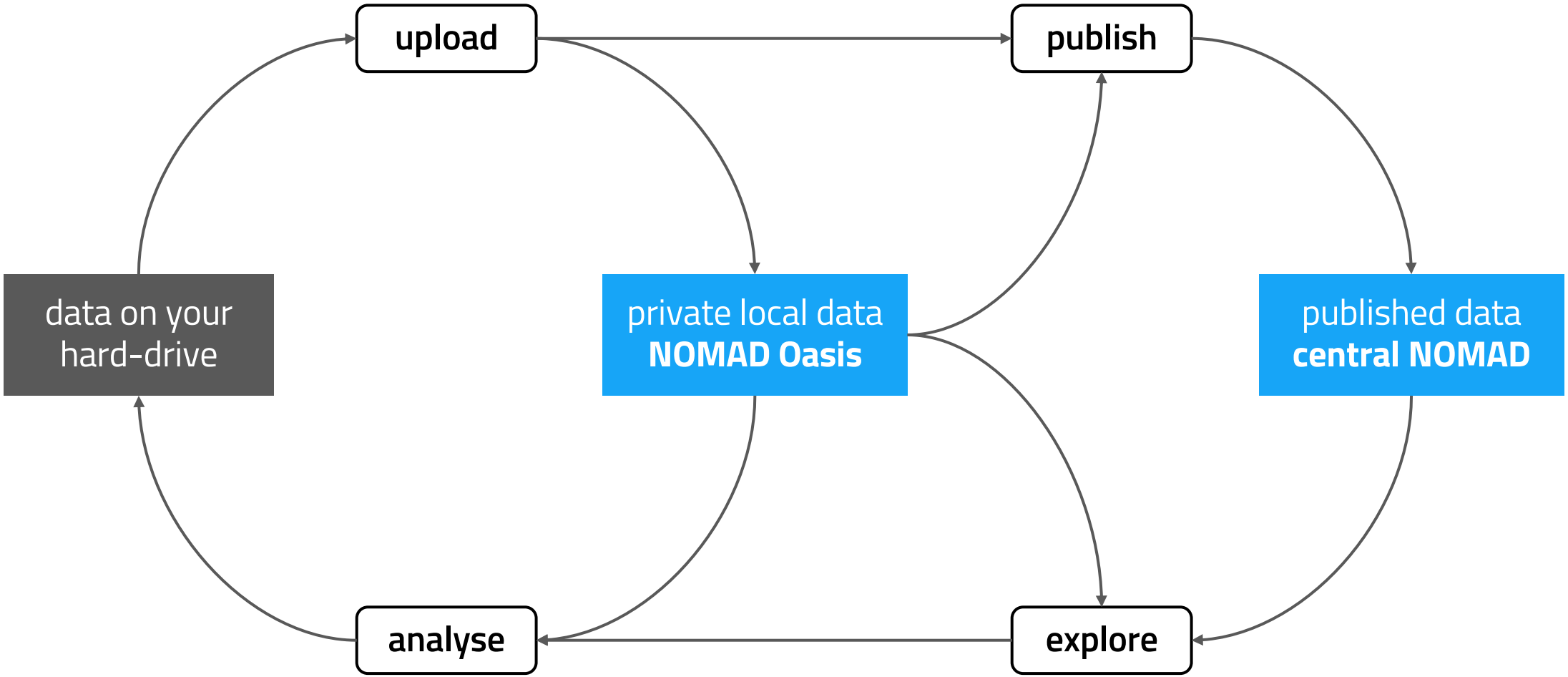


NOMAD: A FAIR-data sharing platform for materials science





NOMAD to assist research processes

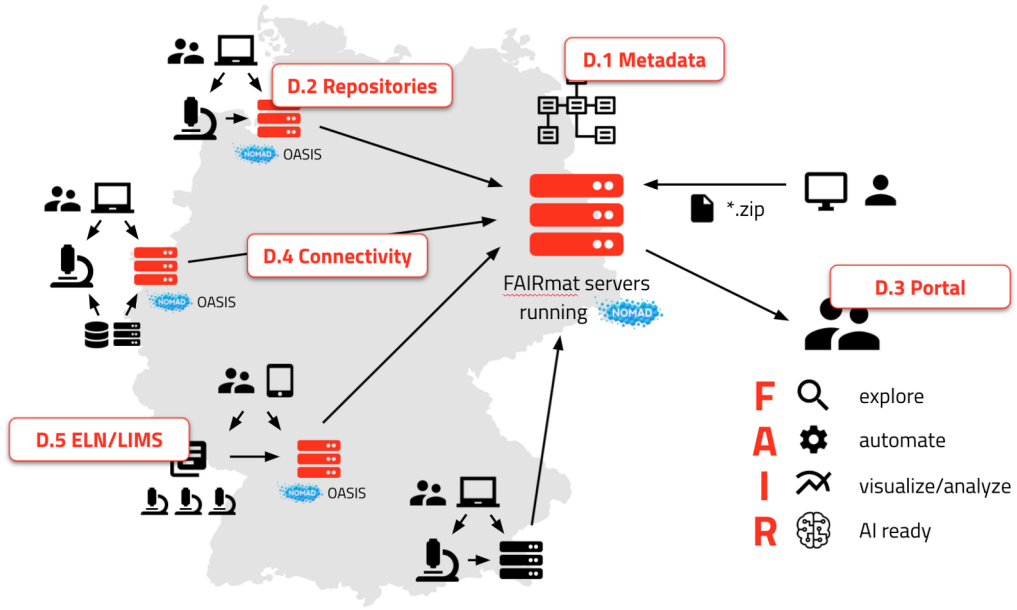


Manage materials science research data

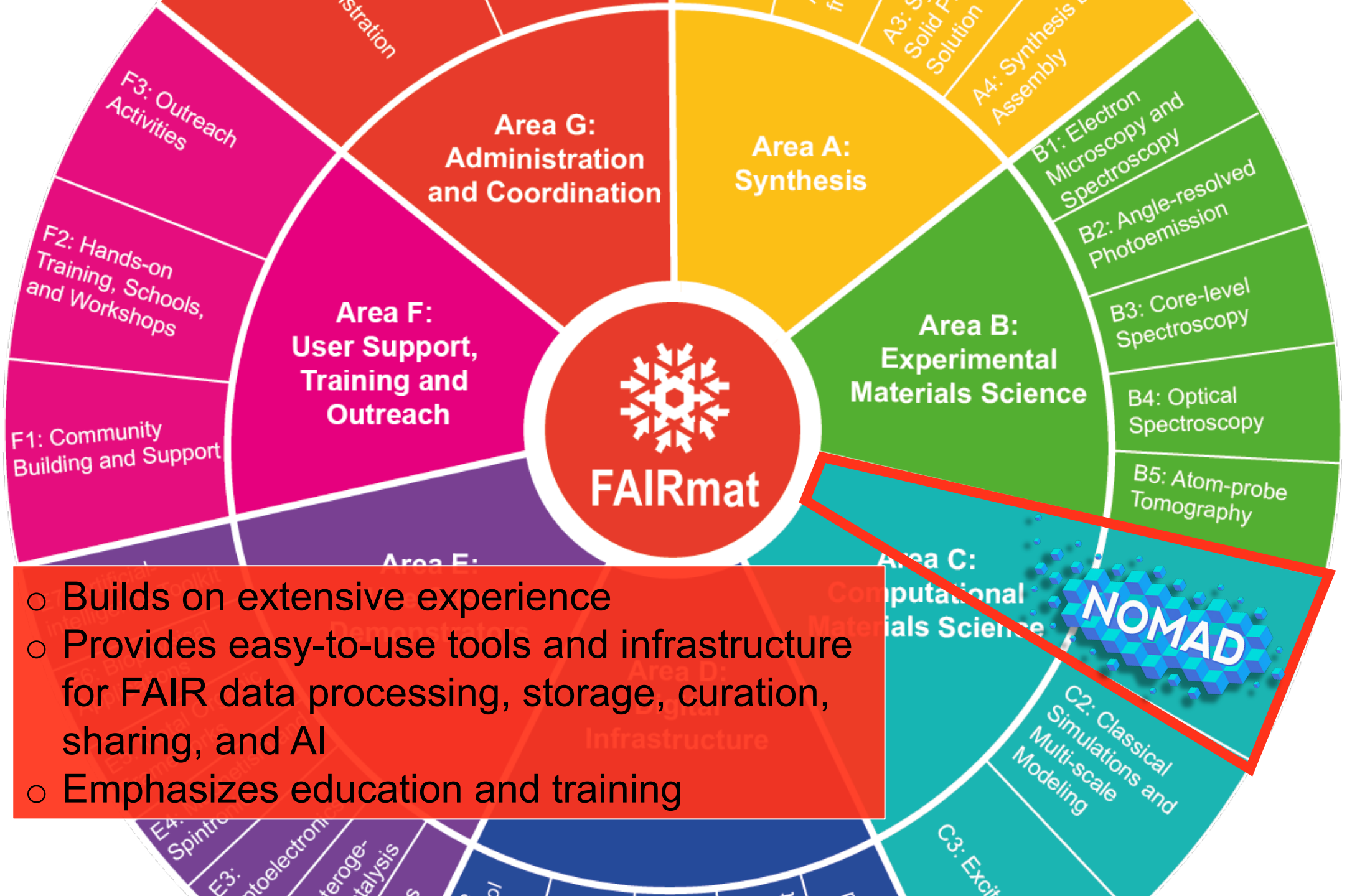
FAIRmat builds on a federated infrastructure of local repositories

- ➔ 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?



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

FAIRmat

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

FAIRmat

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.

FAIRmat

- Support der Nutzer:innen
- Lösungen für die “last mile”, die auf Fachgebiete und Nutzungsgewohnheiten zugeschnitten sind
- Allgemein niedrige Eintrittsbarrieren

FAIRmat