FAIRmat for Materials Science to follow FAIR principles

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FAIRmat @ NFDI

- NFDI – German National Research Data Infrastructure
  9 projects started in 2020
  10 projects starts in 2021
  …

- **FAIRmat project**
  5 years
  9 institutes
  52 research groups
  20 M€

FAIR Data Infrastructure
for Condensed-Matter Physics
and the Chemical Physics of Solids

7 project Area

- A – Synthesis
- B – Experiments
- C – Theory and Computation
- D – Digital Infrastructure
- E – Use-case Demonstrators
- F – User Support, Training, and Outreach
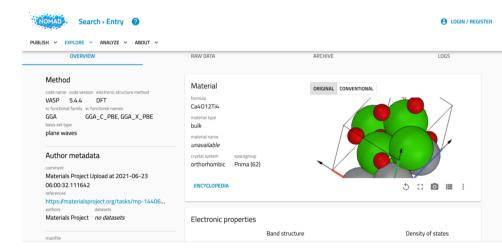- G – Administration and Coordination

Novel Materials Discovery

- Biggest database in Materials Science
  more than 100 million high-quality calculations

- Ecylopedia

- Atrificial Intelligence Toolkit

- Data Center @ MPCDF

- Local OASIS deployments

- Modern Technology
  - Backend with **Python** Flask and Fastapi, MongoDB, Elasticsearch
  - Workflows with Celery, RabbitMQ
  - Frontend with **Javascript**: React, MaterialUI
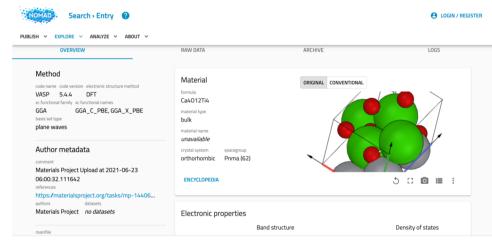 - Docker, Kubernetes, Keycloak

Novel Materials Discovery

- **NOMAD HUB (*NOMAD Data Center at HU Berlin*)**
  - connecting Sysnthesis – Experiments – Calculations
  - Integrate experimental data (e.g. NEXUS)
  - NEXUS application definitions for
    - Electron Microscopy
    - Angle Resolved Photoemission
    - Core-level Spectroscopy
    - Optical Spectorscopy
    - Atom-probe Tomography

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https://nomad-lab.eu/career/