



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

The screenshot displays the NOMAD web application interface. At the top, there is a navigation bar with the NOMAD logo, a search bar, and links for 'Search > Entry', 'PUBLISH', 'EXPLORE', 'ANALYZE', and 'ABOUT'. A 'LOGIN / REGISTER' link is also present. The main content area is divided into several sections:

- Method**: A table showing calculation parameters: code name (VASP), code version (5.4.4), electronic structure method (DFT), xc functional family (GGA), xc functional names (GGA_C_PBE, GGA_X_PBE), basis set type (plane waves), and material type (bulk).
- Author metadata**: A section containing a comment, upload date (2021-06-23), a unique identifier (06:00:32.111642), a reference link to the Materials Project, and author information (Materials Project, no datasets).
- Material**: A section displaying the formula (Ca4O12Ti4), material type (bulk), material name (unavailable), crystal system (orthorhombic), and space group (Pnma (62)).
- Electronic properties**: A section with tabs for 'Band structure' and 'Density of states'.

On the right side of the 'Material' section, there is a 3D visualization of the crystal structure, showing green spheres (likely Ti) and red spheres (likely O) arranged in a lattice. The visualization includes a coordinate system and a 'CONVENTIONAL' label.



Novel Materials Discovery



- **NOMAD HUB (*NOMAD Data Center at HU Berlin*)**

- connecting Synthesis – Experiments – Calculations
- Integrate experimental data (e.g. NEXUS)
- NEXUS application definitions for
 - Electron Microscopy
 - Angle Resolved Photoemission
 - Core-level Spectroscopy
 - Optical Spectroscopy
 - Atom-probe Tomography

- **Modern Technology**

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The screenshot displays the NOMAD HUB web interface. At the top, there is a navigation bar with 'NOMAD' logo, 'Search > Entry', and 'LOGIN / REGISTER'. Below the navigation bar, there are tabs for 'PUBLISH', 'EXPLORE', 'ANALYZE', and 'ABOUT'. The main content area is divided into two columns. The left column, titled 'OVERVIEW', contains sections for 'Method' (listing code name 'VASP', code version '5.4.4', and electronic structure method 'DFT'), 'Author metadata' (comment: 'Materials Project Upload at 2021-06-23 06:00:32.111642', references: 'https://materialsproject.org/tasks/mp-14406...'), and 'mainfile'. The right column, titled 'RAW DATA', contains a 'Material' section with fields for 'formula' (Ca4O12Ti4), 'material type' (bulk), 'material name' (unavailable), 'crystal system' (orthorhombic), and 'spacegroup' (Pnma (62)). To the right of the material information is a 3D visualization of the crystal structure, showing green spheres (atoms) and red spheres (atoms) in a 3D arrangement. Below the 3D visualization is a 'Band structure' plot and a 'Density of states' plot. The bottom of the interface has a 'Electronic properties' section with 'Band structure' and 'Density of states' plots.



Novel Materials Discovery



- **NOMAD HUB (*NOMAD Data*)**

- connecting Synthesis – Experiment
- Integrate experimental data
- NEXUS application definition
 - Electron Microscopy
 - Angle Resolved Photoemission Spectroscopy
 - Core-level Spectroscopy
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<https://nomad-lab.eu/career/>

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