

Seventh FAIRmat Users Meeting

November 20, 2025

Center for the Science of Materials Berlin (CSMB)

Humboldt-Universität zu Berlin, Germany



Schedule Overview

Thursday, November 20
FAIRmat Talk <i>9:00–9:25; Room: 2.049</i>
User Talks <i>9:25–10:15; Room: 2.049</i>
Coffee Break <i>10:15–10:45; Foyer</i>
User Talks <i>10:45–12:00; Room: 2.049</i>
Lunch <i>12:00–13:00; Foyer</i>
Hands-on Workshop I <i>13:00–14:30; Room: 2.049</i>
Coffee Break <i>14:30–15:00; Room: Foyer</i>
Hands-on Workshop II <i>15:00–16:30; Room: 2.049</i>
Users-Meet-Developers Exhibit <i>16:30–18:00; Room: Foyer</i>
Dinner <i>19:00; Il Porto Restaurant</i>

The detailed program can be found below and on the [webpage](#).

FAIRmat Talk



FAIRmat and NOMAD: Recent Updates and Emerging Use Cases

José A. Márquez Prieto

This talk will provide an overview of recent developments in FAIRmat and the NOMAD platform, highlighting advances in research data infrastructure for materials science. I will present features and updates to the NOMAD ecosystem focused on enhancing data sharing, interoperability, and analysis, and illustrate their application through selected experimental and computational use cases. The talk will also introduce our ongoing efforts to support user communities and integrate FAIR principles across diverse research domains.

Time: 9:00–9:25

Users Talks



NOMAD Data Management Workflow for Multidimensional Time-Resolved Photoemission Data

Laurenz Rettig

Recent integration of NeXus metadata search extends NOMAD's advanced data management capabilities to a wealth of experimental techniques based on standardized NeXus metadata schema. I will give insight into our workflows for metadata collection, data conversion and NeXus standardization for time- and angle-resolved photoemission data. These are based on the NXmpes definition, and utilize comprehensive and flexible tools for NeXus standardization developed within FAIRmat. In addition, I will showcase data management within NOMAD Oasis, as well as online data analytics workflows enabled by comprehensive NORTH toolboxes.

Time: 9:25–9:50



NOMAD Oasis for the Solid-State NMR Community

Sathya Sai Seetharaman

The talk outlines how a NOMAD Oasis has been adapted to support the data management needs of the UK's solid-state NMR community. The speaker shares their experience of adapting to NOMAD's plugins and apps to extend the NMR schema, advance the parsing capabilities to accommodate domain-specific quantities while maintaining alignment with FAIR data principles. The presentation will reflect on lessons learned from integrating community-specific requirements within the framework, and how this experience can hopefully inform future developments for other materials data domains.

Time: 9:50–10:15



FAIR Data Management for Fabrication Processes. A Plugin as Implemented at CNR-IFN@TN

Matteo Bontorno

The talk will focus on the development of a FAIR-by-design data environment for fabrication processes at the Trento facilities of CNR-IFN (Consiglio Nazionale delle Ricerche - Istituto di Fotonica e Nanotecnologie) and FBK (Fondazione Bruno Kessler). After presenting the starting point of the work, e.g. the management system and workflow used in Trento at the beginning of last year, we will discuss the solution created to exchange and share data in a FAIR-compliant way. We will introduce an initial trial of an interoperable taxonomy for fabrication, developed in collaboration with ISMN (Istituto per lo studio dei materiali nanostrutturati) in Bologna. In the second part, we will focus on the solution implemented to extend the metainfo capabilities of the NOMAD platform. We will demonstrate how this extension is being used in a local instance of NOMAD running on the Trento servers and present the first steps toward including characterization techniques in the workflow. This feature could also support laboratories that are not yet able to produce NeXus data, helping them convert raw experimental data into more broadly compatible data formats.

Time: 10:45–11:10



Extending NOMAD with Plugin and Metadata Support for EPR, NMR, and EFG

Cecilia Zagni

The talk outlines the activities and development of a NOMAD Oasis plugin for the parsing of QE-GIPAW NMR, EPR, and EFG data. The speaker will present the FAIRY-MAGIC project and the reasons why NOMAD Oasis was chosen as the development framework. The speaker will then share their experience in the development of the parser for NMR, EPR, and EFG, and the effort in the definition of an EPR schema, which has been integrated into the existing NMR metadata schema to ensure a unified representation of spectroscopic tensor quantities.

Time: 11:10–11:35



Seamless Data to Discovery: Digitalizing Electrocatalysis with NOMAD

Carla Terboven and Marcel Risch

Catalysis research increasingly relies on digital tools to enhance efficiency, reproducibility, and collaboration. This presentation demonstrates how digitalization can transform catalysis research by integrating data science, experimentation, and advanced research data management. Using the example of the Investigator Group Oxygen Evolution Mechanism Engineering, we present a laboratory-scale approach to digital catalysis that leverages the NOMAD (Oasis) infrastructure to manage, analyze, and share research data.

The first part introduces the scientific use case in electrocatalysis, capturing parts of a typical workflow of measuring physical properties of the sample, performing electrochemical measurements, checking the validity of those measurements and guiding the selection of further electrochemical measurement parameters by Bayesian optimization. Examples are shown and discussed for analysis of the electronic structure by X-ray absorption spectroscopy, benchmarking activity of electrodes performing oxygen evolution by water oxidation, statistical analysis of the potential reference in

electrochemical cells and optimization of deposition parameters to improve electrochemical performance.

The second part focuses on the technical implementation within the NOMAD Chemical Energy Oasis at HZB, where experimental conditions and results are seamlessly converted into machine-readable, FAIR data. By utilizing NORTH tools and combining multiple NOMAD entries, this approach enables systematic evaluation of electrocatalytic performance via a dedicated NOMAD Explore app. This example illustrates how seamless, user-oriented digital workflows emerge from the combined expertise of laboratory scientists and data stewards.

Time: 11:35–12:00

Hands-on Workshop I: Getting Started with NOMAD for Materials-Science Research Data Management



Siamak Nakhaie

In this hands-on workshop, you will learn how to efficiently search, filter, and explore data in NOMAD. We will guide you through managing, uploading, and sharing your research data, as well as steps to publish datasets with DOIs to guarantee accessibility and reusability. You will also gain practical experience using NOMAD's ELN functionality to document your research. Please bring your laptop to participate in the interactive exercises.

Time: 13:00–14:30

Hands-on Workshop II: Role-Based NOMAD Usage and Development



Joseph F. Rudzinski

NOMAD now provides a broad ecosystem of data infrastructure software and tools, enabling robust data management at the individual, research group, and institutional levels. To navigate this ecosystem effectively, it is helpful to identify your role and intended use. In this tutorial, we will help you get started on the right path, whether you are an experienced user or completely new to NOMAD.

The tutorial is organized into several modules, allowing participants to choose and follow the topics at their own pace. Our trainers will be available throughout the session to provide individual support and guidance. The modules cover different aspects of the NOMAD ecosystem, from data organization and sharing to customization, automation, and local deployment.

Time: 15:00–16:30

Users-Meet-Developers Exhibit



This open forum will offer participants the opportunity to showcase their work, exchange ideas, and interact directly with NOMAD developers and FAIRmat experts. Users will present and discuss their RDM workflows with NOMAD, uploaded datasets, developed plugins, custom schemas, data analysis tools, or other related solutions.

Time: 16:30–18:00

Venue

Center for the Science of Materials Berlin (CSMB)

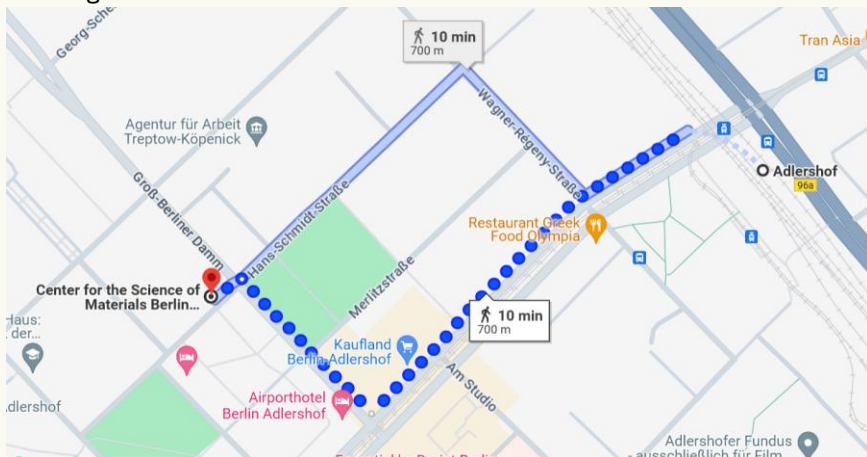
Humboldt-Universität zu Berlin

Zum Großen Windkanal 2,

12489 Berlin, Germany

Public transport: S Adlershof (Lines: S8, S85, S9, S45, S46)

Walking from S Adlershof:



Stay in Touch

General organizational questions:

- Natalia Slepenco: natalia.slepenco@physik.hu-berlin.de

