AKjDPG 1: Hacky Hour

Time: Thursday 9:30–11:30 Location: SCH/A101

AKjDPG 1.1 Thu 9:30 SCH/A101

Using NOMAD as an Electronic Laboratory Notebook — •Ahmed E. Mansour[1], Siamak Nakhaie[1], Claudia Draxl[1], Martin Aeschlimann[2], and The FAIRmat team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Kaiserslautern, Germany

NOMAD (nomad-lab.eu) [1, 2] is an open-source, web-based research data management (RDM) platform that allows researchers in condensed-matter physics and materials science to organize, analyze, share, and publish their data. It also enables them to explore and reuse data provided by others.

The electronic laboratory notebook (ELN) functionality in NOMAD supports the documentation of research workflows and the management of experiments by creating structured records of samples, processing steps, measurements, results, and analyses. These searchable records can be accessed from any device, and enhance data integration, collaboration, and long-term recordkeeping.

In this talk, I will demonstrate how to use NOMAD as an ELN through its built-in templates for different record types, which can be accessed directly via the graphical user interface (GUI). I will also demonstrate how users can create custom templates using YAML-based schema definitions or Python-based plugins.

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).
[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

AKjDPG 1.2 Thu 10:00 SCH/A101

Exploring and Publishing FAIR Research Data in NOMAD — •Siamak Nakhaie[1], Ahmed E. Mansour[1], Claudia Draxl[1], Martin Aeschlimann[2], and FAIRmat Team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Kaiserslautern, Germany

Are you looking for a platform where you can explore physics and materials-science data with rich and well-structured metadata? Would you like to organize your own research data in an environment specifically tailored to the needs of physicists and materials scientists and aligned with the FAIR principles? Are you preparing a manuscript and need a simple way to share your data with reviewers via a single link, while keeping the underlying data modifiable so you can still update it based on their feedback, and later publish the final version with a DOI to cite in your paper? If so, this Hacky Hour is for you. We will introduce NOMAD as a practical platform for publishing and exploring FAIR research data. First, we will explore 19 million+ existing NOMAD entries and answer example scientific questions using the advanced yet user-friendly metadata filters provided by NOMAD. Next, we will upload example raw data files, manage access control, and inspect how NOMAD automatically extracts and structures useful information from these files. Finally, we will create a dataset and simulate the publication process, including DOI assignment.

Join us in this relaxed Hacky Hour to get introduced to NOMAD as a practical platform for managing FAIR research data.

AKjDPG 1.3 Thu 10:30 SCH/A101

Controlling experiments and recording FAIR data with NOMAD CAMELS - FAIR Data Workflow — •Alexander Fuchs[1,2], Michael Krieger[1], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, Berlin, Germany

NOMAD CAMELS (Configurable Application for Measurements, Experiments and Laboratory Systems) [1, 2] is an open-source measurement orchestrator for easy control of lab instruments and recording of FAIR and fully self-describing measurement data directly from the experiment. CAMELS enables the definition of measurement protocols via a graphical user interface without requiring programming knowledge or deeper understanding of instrument communication. CAMELS provides the flexibility of controlling a large variety of measurement instruments in frequently changing experimental setups. Integrating the rich metadata of a measurement with a powerful ELN (e.g. NOMAD Oasis [3]) enables sophisticated research data management. This Hacky Hour contribution starts with a brief overview of CAMELS followed by a hands-on session on setting up CAMELS and performing measurements. To follow, bring your own laptop if possible. [1] A. Fuchs, J.A. F. Lehmeyer, H. Junkes, H.B. Weber, M. Krieger. NOMAD CAMELS: Configurable Application for Measurements, Experiments and Laboratory Systems. Journal of Open Source Software, 9(95), 6371 (2024), https://doi.org/10.21105/joss.06371 [2] NOMAD CAMELS documentation, https://fau-lap.github.io/NOMAD-CAMELS [3] Scheidgen et al., NOMAD: A distributed web-based platform for managing materials science research data. Journal of Open Source Software, 8(90), 5388 (2023), https://doi.org/10.21105/joss.05388

AKjDPG 1.4 Thu 11:00 SCH/A101

An exciting approach to electronic structure calculations — Hannah Kleine, •Kshitij Sinha, Martin Kuban, Marti Raya-Moreno, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

With more than 30,000 scientific papers published annually on electronic-structure theory, navigating the landscape of theoretical approximations, ranging from ground-state density functional theory to advanced excited-state methods can be overwhelming, especially for early-career researchers [1]. This hacky hour aims to lower the barrier to advanced excited-state simulations and foster informed, critical use of modern electronic-structure tools on the example of the `exciting` code, an all-electron full-potential, open-source DFT package which is known to achieve μ-Ha precision [2,3]. Participants will be guided through practical workflows implemented in interactive notebooks that span multiple levels of theory, starting from ground- state calculations and extending to excited-state approaches such as time-dependent DFT and the Bethe-Salpeter equation. This session is designed as an interactive hacking workspace: with representative systems, direct comparison of methods within a unified code base and user-friendly workflows. Please, find more information about `exciting` and our session at https://exciting-code.org/dpg-hacky-hour-2026

[1] A. Pribram-Jones, D. A. Gross, and K. Burke, Annu. Rev. Phys. Chem. 66, 283 (2015).
[2] A. Gulans et al, J. Phys.: Condens. Matter 26, 363202 (2014).
[3] A. Gulans et al, Phys.: Rev. B, 97, 161105 (2018).