TUT 1: Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python (joint session FM/TUT)

HyperSpy is a community-developed, open-source library providing a framework to facilitate interactive analyses of multidimensional datasets – in particular spectrum images – in an easy and reproducible fashion. It facilitates the application of analytical procedures operating on individual spectra/images to a multi-dimensional dataset and gives easy access to tools that exploit the multi-dimensionality of the dataset. Born out of the electron microscopy scientific community and building on the extensive scientific Python environment, HyperSpy provides tools to efficiently explore, manipulate, and visualize complex datasets of arbitrary dimensionality, including those larger than a system's memory. The HyperSpy ecosystem includes Python packages that provide dedicated routines for many electron microscopy-based measurement techniques, but also for luminescence spectroscopy and other fields. Through the library RosettaSciIO, the reading and writing of a large range of file formats is supported.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 01.03.2026 via a dedicated GitHub repository. Participants are encouraged to download them ahead of time, set-up Python on their computer following the instructions and run the jupyter notebooks presented during the tutorials on their laptops:

https://github.com/LumiSpy/DPG2026-Tutorial

Organized by Jonas Lähnemann (PDI Berlin), Benedikt Haas (HU Berlin), Aidan Campbell (PDI Berlin), Hannah C. Nerl (HU Berlin) and Magnus Nord (NTNU Trondheim).

Time: Sunday 16:00–18:15 Location: HSZ/0002

TUT 1.1 Sun 16:00 HSZ/0002

Introduction to HyperSpy — •Jonas Lähnemann[1], Aidan F. Campbell[1], Hannah C. Nerl[2], Magnus Nord[3], and Benedikt Haas[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Department of Physics, Humboldt Universität, Berlin, Germany — [3]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

The session begins with a brief introduction to HyperSpy that with its 2.0 release has grown to an ecosystem of Python packages that provide dedicated routines for electron microscopy-based measurement techniques such as EELS, EDX, 4DSTEM, holography, tomography and CL, but also for luminescence spectroscopy. In general, it can be useful for any measurement, where a signal is mapped over multiple dimensions (position, time, angle, ...).

Tutorial TUT 1.2 Sun 16:15 HSZ/0002

Hands-On Session 1: General usage HyperSpy/RosettaSciIO — •Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

In the initial tutorial, we will show how to easily read in data from a variety of formats and introduce the basic data structure of HyperSpy. General data operations, artefact removal and plotting functionalities as a basis of reproducible data analysis workflows will be covered as well.

Tutorial TUT 1.3 Sun 16:45 HSZ/0002

lumiSpy for luminescence spectroscopy — •Aidan Campbell — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

This session will focus on tools ideal for analysing data recorded with cathodoluminescence, photoluminescence or related spectroscopy techniques. We will demonstrate convenience functions for rapid spectroscopy data analysis, model fitting, and visualisation. Luminescence spectroscopy may also lead to more complicated data sets with spectral, spatial and time dimensions for which we showcase interactive tools for navigating and understanding this data.

Tutorial TUT 1.4 Sun 17:15 HSZ/0002

Hyperspy for Electron Energy-loss Spectroscopy — •Hannah Nerl — Humboldt Universität zu Berlin, Berlin, Germany

This hands-on session demonstrates a complete electron energy-loss spectroscopy (EELS) analysis workflow using HyperSpy and its exSpy extension. Participants will work through practical examples covering essential preprocessing steps including spectral alignment and drift correction, followed by quantitative analysis techniques such as model-based peak fitting and automated peak tracking across multidimensional datasets. The tutorial emphasizes reproducible analysis pipelines, showcasing how to leverage principal component analysis (PCA) for noise reduction in low-signal regimes. All examples use real EELS datasets and focus on practical workflows applicable to both core-loss and low-loss spectroscopy of 2D materials and nanostructures. Participants will gain hands-on experience with Jupyter notebooks that can be directly adapted to their own research data.

Tutorial TUT 1.5 Sun 17:45 HSZ/0002

Using pyXem for magnetic and structural analysis of 4D-STEM data — •Magnus Nord — Norwegian University of Science and Technology, Trondheim, Norway

pyXem is an extension of HyperSpy with a focus on data processing of 4D-STEM data: from crystallographic analysis using Scanning Precession Electron Microscopy (SPED), to magnetic imaging with Scanning Transmission Electron Microscopy - Differential Phase Contrast (STEM-DPC). In this tutorial, we will show how one can study the crystal structure and domain structure in a nanostructured magnetic material.

TUT 2: Tutorial des Fachverbands Didaktik der Physik (joint session DD/TUT)

Physics teaching at universities can be significantly enriched by moving beyond traditional lecture formats and embracing interactive, learner-centered approaches that foster deep and sustainable understanding. Drawing on successful practices from universities in Germany and abroad, this workshop highlights how insights from learning psychology and proven teaching innovations can be translated into effective physics education. It invites participants to explore how evidence-based, interactive methods can transform learning experiences and support lasting learning outcomes in everyday teaching practice.

Time: Sunday 16:00–18:15 Location: BEY/0137

Tutorial TUT 2.1 Sun 16:00 BEY/0137
Rethinking University Teaching: Creating interactive and sustainable learning environments in lectures — •Susanne Heinicke[1], Christian Kautz[2], Peter Riegler[3], Claudia Schäfle[4], Silke Stanzel[4], and Micol Alemani[5] — [1]Institute for Physics Education, University of Muenster — [2]Hamburg University of Technology — [3]Ostfalia University of Applied Sciences — [4]Technische Hochschule Rosenheim — [5]University of Potsdam

The workshop bridges current findings from learning psychology with experience and research findings on practical teaching formats to enhance effective learning in university physics education. We will give an overview of key principles from educational psychology concerning how we learn to provide a foundation for understanding learning effectiveness. Participants will explore and critically reflect on evidence-based interactive methods like peer instruction, interactive formats, and problem-based learning that can be transferred to their own teaching. The workshop concludes with a discussion on implementation strategies and evaluation approaches to support sustainable integration into everyday teaching practice.

TUT 3: Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)

Artificial intelligence (AI) tools are increasingly shaping research in materials science and physics by enabling advanced data analysis, modeling, and predictive capabilities.

This tutorial presents three practical use cases that demonstrate how machine learning methods can support materials science research.

Time: Sunday 16:00–18:15 Location: HSZ/0003

Tutorial TUT 3.1 Sun 16:00 HSZ/0003
Welcome Remarks Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz — DPG AKPIK and •Arash Rahimi-Iman — Deutsche Physikalische Gesellschaft e.V.

Inspired by last year's meeting program in Regensburg, March 2025, our interdisciplinary Working Group on Physics, Modern IT and Artificial Intelligence, the AKPIK, again offers a research-focused "AKPIK Day" on Tuesday during the upcoming conference. Together with the practical use cases of machine learning presented in this tutorial session, as well as the presentations and poster session planned for Thursday, we hope to encourage many conference attendees to engange scientifically in the areas of the AKPIK.

Tutorial TUT 3.2 Sun 16:05 HSZ/0003
A practical machine learning case study in materials science: Stumbling blocks, lucky breaks, and helpful colleagues — •Max Grossmann, •Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, German

Machine learning projects in materials science are often exciting at first, but quickly encounter practical challenges. In this tutorial, we present a hands-on case study from our group and walk through the entire process, from the initial idea to building a dataset to training a working model. Rather than focusing solely on technical details, we highlight the stumbling blocks, unexpected insights, helpful colleagues, and lucky coincidences that shaped the project. We discuss the most important aspects of starting a machine learning project in physics or materials science, such as choosing a meaningful target property, designing a reliable dataset, avoiding common pitfalls, and identifying situations where simple approaches are as effective as advanced ones. Our goal is to provide an honest, accessible, and experience-driven introduction and guidance to researchers considering venturing into machine learning for the first time – the kind of guidance we wish we had when we started.

5 min. break

Tutorial TUT 3.3 Sun 16:50 HSZ/0003
Machine Learning-based Analysis of Electron Microscopy Images: Preprocessing and Synthetic Data Generation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

In this tutorial session, participants will learn how to prepare electron microscopy (EM) images for machine learning (ML) analysis using a series of Jupyter Notebook demonstrations. The tutorial illustrates essential preprocessing steps such as denoising, normalization, and contrast enhancement using Python. The session then transitions to synthetic EM data generation, showing how classical augmentation and modern generative models can create controlled datasets that mimic real data. By observing these live examples, attendees will gain a conceptual understanding of how preprocessing pipelines and synthetic data strategies can be used for ML-based EM analysis.

5 min. break

Tutorial TUT 3.4 Sun 17:35 HSZ/0003
Machine Learning-based Analysis of Electron Microscopy Images: Segmentation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

The second session focuses on segmentation of EM images using modern deep-learning architectures. Through a step-by-step Jupyter Notebook demonstration, the tutorial walks through the training and evaluation of a U-Net style segmentation model. Participants will see real examples of common challenges in EM segmentation, such as low contrast, overlapping nanoscale structures, and label ambiguity. By the end of the session, attendees will have an implementation-oriented understanding of how segmentation pipelines are built and validated in practice.

TUT 4: Tutorium: Physics of Behavior (joint session SOE/TUT/DY)

The emerging field of the physics of behavior seeks to quantitatively characterize complex behavior in biological agents under naturalistic conditions, using tools from dynamical systems theory and statistical physics. Even in simple organisms, behavioral richness demands new methods of measurement and analysis, as well as new theoretical frameworks. In the absence of a first-principles theory, data-driven approaches are essential, and the many interacting degrees of freedom call for descriptions capable of handling high-dimensional systems.

This tutorial introduces how concepts from dynamical systems theory and statistical physics can be applied to quantify behavior across biological scales and to develop simple yet predictive models. It is intended for physicists at all levels, beginning with graduate students, who are interested in computational approaches to modeling animal behavior. The tutorial is accompanied by an openly accessible code repository to support hands-on exploration of selected topics.

Time: Sunday 16:00–18:15 Location: HSZ/0004

Tutorial TUT 4.1 Sun 16:00 HSZ/0004

Physics of Behavior — •Greg Stephens — Vrije Universiteit Amsterdam, Amsterdam NL — OIST Graduate University, Tancha, JP

In these tutorials we view behavior as a complex dynamical system and we incorporate insights from dynamical systems theory and statistical physics to quantitatively capture what animals do. Of course, such theory was not historically developed to understand animal behavior, and there are particular challenges associated with the modeling of living systems. Of these, the most important is a lack of first-principles theory necessitating a data-driven approach.

In the first half of our session we will introduce two primary concepts. (1) Posture Space Analysis via Dimensionality Reduction. We explore posture space analysis by demonstrating how to decompose high-dimensional postural data into a few meaningful eigenpostures using Principal Component Analysis (PCA). The dataset used comes from C. elegans posture tracking. (2) Posture Space Dynamics via State Space Reconstruction. We review the concepts of state space and chaotic systems through a toy model. We then introduce a modern data-driven technique for state space reconstruction.

15 min. break

Tutorial TUT 4.2 Sun 17:15 HSZ/0004

Physics of Behavior — •Antonio Carlos Costa — Paris Brain Institute, Paris, France

Animal behavior is inherently nonlinear and multiscale, spanning millisecond movements to hour-long strategies. In the second half of our session, we will complement first-principles approaches with data-driven methods to identify multiscale dynamics in behavioral data.

We will present three key techniques: (1) state space reconstruction combined with transfer operators to extract long-timescale modes from partial observations, (2) coarse-grained modeling to infer slowly-varying behavioral dynamics and explain heavy-tailed statistics, and (3) a multiscale distance metric for reconstructing behavioral phenotypes from dynamic observations.

We will review the theoretical foundations of slow mode identification using transfer operators (illustrated with stochastic and chaotic toy models), and then demonstrate their applicability to real-world data, including posture dynamics in C. elegans and zebrafish.

TUT 5: Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis (joint session MA/TUT)

The functionalities of many materials of contemporary interest are related to complex types of magnetic ordering. Accurate magnetic structure determination is thus crucial for understanding and optimizing such materials.

After an introduction into the subject, participants of the tutorial will gain hands-on experience on the methods for magnetic structure determination.

Time: Sunday 16:00–18:15 Location: TRE/PHYS

Invited Talk TUT 5.1 Sun 16:00 TRE/PHYS

Recent advances and challenges in magnetic structure determination — •Dmytro Inosov — Institut für Festkörper- und Materialphysik, TU Dresden, Germany

In this introductory tutorial talk, I will provide an overview of magnetic structure determination in the context of recent advances in magnetic materials. I will focus on the limitations and challenges of magnetic structure refinement, and explain why it is important to use the full range of complementary experimental methods alongside conventional diffraction in order to develop a consistent understanding of magnetic structures. This is particularly important when dealing with complex types of magnetic order, such as noncollinear and multi-Q spin textures, altermagnets, and systems with multiple magnetic sublattices or very weak and/or fluctuating magnetic moments.

Tutorial TUT 5.2 Sun 16:30 TRE/PHYS

Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis — •Matthias Frontzek — Oak Ridge National Laboratory, Neutron Scattering Division, One Bethel Valley Road, 37831 Oak Ridge, TN, USA

The determination of magnetic structures is a crucial aspect of materials science, particularly for understanding the magnetic properties of novel materials. Given the limited availability of neutrons with the closure of smaller sources, competitive access to beam time, and the high hurdles associated with software usage, there is an increasing need for training in the analysis of magnetic structures. This tutorial aims to provide participants with practical skills in magnetic structure determination using SARAh and Fullprof, two powerful tools frequently utilized in this field.

Participants will:

-Gain hands-on experience with the tools and techniques necessary for magnetic structure determination.

-Refine nuclear and magnetic structures using real data sets.

-Understand key concepts in diffraction techniques and steps involved in the magnetic structure determination process.

Important: for Hands-on participation, please bring a laptop with a working installation of Fullprof (https://www.ill.eu/sites/fullprof/).

For links to Fullprof, SARAh stand-alone and tutorial data visit: https://neutrons.ornl.gov/wand/users

TUT 6: Hands on tutorial: Linking large language models with digital workflows for materials science simulations (joint session MM/TUT)

Advanced computational simulations often require chaining several models and software packages together, a process that demands careful workflow management. In this tutorial you can gain hands-on experience with the Python based workflow environment pyiron (www.pyiron.org). Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: TRE/MATH

Tutorial TUT 6.1 Sun 16:00 TRE/MATH

Hands on tutorial: Linking large language models with digital workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]ICAMS, Ruhr Universität Bochum

Advanced computational simulations now reliably predict material properties, but they often require chaining several models and software packages together, a process that demands expert knowledge and careful workflow management. Efficient, reproducible research therefore hinges on automated workflow tools that can handle this complexity. In this tutorial we introduce pyiron (www.pyiron.org), a Python based workflow environment for building and executing fully automated simulation pipelines. We show how complex simulations workflows can be constructed programmatically via Python code as well as via a flow-based graphical user interface. We further introduce how large language models (LLMs) can be embedded to streamline the "human in the loop" tasks. After a brief overview of pyiron's core concepts, we construct workflows for computing ab initio thermodynamic bulk phase diagrams. The necessary steps, such as density functional theory calculations, training ACE-based machine learning potentials, and exploring phase stability using foundational models like GRACE, are all performed within pyiron workflows. Participants will learn how to develop and integrate such workflows into their own materials science simulations, thereby enabling faster, more transparent, and more reproducible research.