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.