



Community Workshop 2025: Materials Science with Advanced Data Management and Data Science Techniques

Wednesday, May 7, 2025

- 1:00 PM **Welcome, Prof. Matthias Müller, Director NHR4CES and Prof. Karsten Albe, TU Darmstadt**
- 1:15 PM **“Pyiron – Workflows for data-driven Materials Science“, Dr. Jan Janssen, Max Planck Institute for Sustainable Materials**
- 2:15 PM **”Combining high-performance computing, workflows and machine learning to get new insights in material sciences“, Dr. Michael Selzer, KIT Karlsruhe Institute of Technology**
- 3:15 PM **Break**
- 3.30 PM **“Data-driven approaches to atomistic modeling beyond interatomic potentials“, Dr. Chiheb Ben Mahmoud, University of Oxford**
- 4:30 PM **Panel Discussion, Moderation: Prof. Karsten Albe, TU Darmstadt**
- 5.30 PM **End of Day 1**

Thursday, May 8, 2025

- 09.00 AM **Welcome, Prof. Bai-Xiang Xu, TU Darmstadt**
- 09:15 AM **“Project: NFDI MatWerk“, Dr. Leonid Gerdt, Fraunhofer Institute Dresden and Ebrahim Norouzi, FIZ Karlsruhe**
- 10:10 AM **“Putting data into context: Metadata schemata and automated extraction of metadata“, Marcel Nellesen, RWTH Aachen University**
- 10:55 AM **Break**
- 11:10 AM **“AutoML Meets Materials Science: Automating Insights and Innovation“, Jonas Seng, TU Darmstadt**
- 12:05 AM **“Wrangling Tabular Data with LLMs: What’s Possible and What’s Not“, Jan Micha Bodensohn and Liane Vogel, TU Darmstadt**
- 01:00 PM **End of Day 2**