MACHINE LEARNING

IN MATERIALS SCIENCE & CRYSTAL GROWTH

JANUARY 23 - 25, 2023 | BERLIN, GERMANY

IKZ-FAIRmat Winter School | Machine Learning in Materials Science & Crystal Growth

Machine Learning (ML) opened up completely new opportunities in Material Science. Together with advances in research data management and software tools ML got more and more accessible.

The IKZ Berlin and FAIRmat joint Winter School invited internationally renowned lecturers to address ML in Material Science and Crystal Growth for any scientist new to the field.

The lectures cover fundamentals of ML and AI and explores data management for ML. It clarifies how to use ML to automatically extract data from experiments and to help making decisions. Challenges of ML with small data sets and possible solutions will be discussed, as well as the question: What can be simulated now with the help of ML which was not possible before?

The lectures are accompanied by a hands-on tutorial based on our NOMAD AI toolkit.

Organization

The Leibniz-Institut für Kristallzüchtung (IKZ) is a research institution that is unique in Europe. It explores the scientific and technological fundamentals of crystal growth, from basic research to pre-industrial development and provides scientific services for research institutions and industry.
This includes, in particular, the growth of specific crystals for research purposes, the characterization of crystalline materials or industry-oriented technology development.

FAIRmat is funded as a consortium of the German Research-Data Infrastructure NFDI and represents a broad community of researchers from universities and other leading institutions in Germany.
Scientific data are a significant raw material of the 21st century. To really exploit their value, data must be Findable, Accessible, Interoperable and Re-purposable. To really exploit their value, data must be Findable, Accessible, Interoperable and Re-purposable. FAIRmat is making this happen for the field of condensed-matter physics and the chemical physics of solids.

Venue
Erwin-Schrödinger-Zentrum - Humboldt-Universität Berlin
Rudower Chaussee 26, 12489 Berlin, Germany
COVID-19 Info:
There is no test or mask requirement at the venue. If if you test positive or have symptoms, please participate via Zoom.

Organization | Contact
Lucia Alessandra Rotheray
winter.school@ikz-berlin.de

Arrival by public transport
In public transport it is mandatory to wear an FFP2 mask.
S-Bahn: *S45, S46, S85, S9 to Adlershof station + 10 min walk*
Tram: *27, 61, 63, 67 to Magnusstraße*
Bus: *162, 163, 164 to Magnusstraße*

Route planner and timetable information
https://www.bvg.de/en/connections/connection-search
BVG Fahrinfo-App: **Apple App Store** | **Google Playstore**

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Join the Zoom meeting:	https://hu-berlin.zoom.us/j/61829474831?pwd=dm53R1J4bzN2K0FSL0tIYzNzU0NOZz09
	**Meeting-ID: 618 2947 4831	Passwort: 682575**
	Winter school details on: www.ikz-berlin.de/4-ikz-winterschool

Monday, January 23

11:45am – 12:30pm .... Registration & Welcome by the Organizers

12:30pm – 2:00pm .... *Introduction to artificial intelligence and its application to materials science*
Live talk　　　　　　　Dr. Luca Ghiringhelli
　　　　　　　　　　　　The NOMAD Laboratory at Humboldt-Universität zu Berlin

2:00pm – 3:45pm........... *NOMAD – managing and accessing FAIR research data*
Live talk　　　　　　　Dr. Markus Scheidgen
　　　　　　　　　　　　The NOMAD Laboratory at Humboldt-Universität zu Berlin

3:45pm – 4:15pm .... Coffee break

4:15pm – 6:00pm .... *Introduction to ML and FAIR research data management*
Live tutorial　　　　　Dr. Markus Scheidgen & Dr. Luca Ghiringhelli

Tuesday, January 24

9:00am – 10:30am .... *Machine learning - Acceleration of global optimization*
Live talk　　　　　　　Prof. Bjork Hammer
　　　　　　　　　　　　Center for Interstellar Catalysis, Department of Physics and Astronomy, Aarhus University

10:30am – 11:00am .... Coffee break

11:00am – 12:00pm .... *Acceleration of global optimization*
Live tutorial　　　　　Prof. Bjork Hammer

12:00pm – 1:00pm .... Lunch break

1:00pm – 4:00pm .... *Automated experiments - Workflow design*
Remote talk + tutorial　Prof. Sergei Kalinin
　　　　　　　　　　　　Department of Materials Science and Engineering, The University of Tennessee, Knoxville

4:00pm – 4:30pm .... Coffee break

4:30pm – 6:00pm .... *Machine learning for interatomic potentials*
Remote talk + tutorial　Dr. Daniel Schwalbe Koda
　　　　　　　　　　　　Lawrence Livermore National Laboratory

7:00pm – .... Dinner | If you wish to attend the dinner, please sign up at the registration desk on Monday, January 23.

Wednesday, January 25

9:00am – 10:30am .... *Bayesian optimization*
Live talk　　　　　　　Dr. Kentaro Kutsukake
　　　　　　　　　　　　Center for Advanced Intelligence Project, RIKEN, Ujihara Laboratory, Nagoya University
　　　　　　　　　　　　Japan Center for Advanced Intelligence Project, Tokyo

10:30am – 11:00am .... Coffee break

11:00m – 12:00pm .... *Bayesian optimization*
Live tutorial　　　　　Dr. Kentaro Kutsukake

12:00pm – 12:30pm .... Lunch break

12:30m – 2:00pm .... *Materials property prediction from limited and multi-fidelity datasets*
Live talk + tutorial　　Prof. Gian-Marco Ringanese
　　　　　　　　　　　　MODL, Chemin des Étoiles, Louvain-la-Neuve, Belgium

2:00pm – 2:30pm .... Coffee break

2:30pm – 5:30pm .... *Title TBA*
Remote talk + live tutorial　Prof. Volker Deringer
　　　　　　　　　　　　Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, UK