

Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

jointly organised by
 the Surface Science Division (O),
 the Biological Physics Division (BP),
 the Metal and Material Physics Division (MM),
 the Environmental Physics Division (UP),
 the Working Group "Young DPG" (AKjDPG), and
 the Working Group on Physics, Modern IT and Artificial Intelligence (AKPIK)

Jörg Neugebauer
 MPI für Nachhaltige Materialien
 Max-Planck-Straße 1
 40237 Düsseldorf
 neugebauer@mpi-susmat.de

Karsten Reuter
 Fritz-Haber-Institut der MPG
 Faradayweg 4-6
 14195 Berlin
 reuter@fhi.mpg.de

So-called Self-driving Laboratories (SDLs) or Materials Acceleration Platforms (MAPs) represent a cutting-edge convergence of artificial intelligence (AI) and machine learning (ML) with lab automation and robotics. SDLs are designed to automate and accelerate experimental processes, addressing inefficiencies and enhancing the precision and safety of lab operations. SDLs operate in active learning loops, in which an ML algorithm selects and plans experiments that are subsequently executed by increasingly automated (robotic) modules. Data from these experiments are fed back into the ML model, refining it and guiding subsequent experiments. This iterative process enhances the efficiency and effectiveness of experimental exploration, and it is the adaptive quality to directly exploit the information gained through the experiments in the past loops that distinguishes modern SDLs from classic approaches in high-throughput experimentation or combinatorial chemistry.

With SDLs emerging in a wide range of application fields from heterogeneous catalysis over optoelectronics to batteries, advances in experiment automation and robotization are obvious drivers for improved throughputs. Complementary to this are, however, multiple IT- and AI/ML-related aspects of SDLs, not least comprising data pipelines and management, workflows, AI-agent platforms, featurization of the experimental data or experiment planning (especially using noisy and multi-fidelity data). This symposium will survey the present state-of-the-art of these aspects and discuss current frontiers.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	Data and Experimental Foundations for Reliable Self-Driving Laboratories — •DR. MARCUS TZE-KIAT NG
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	Digital Catalysis - AI for Experiment Planning and Control — •CHRISTOPH SCHEURER
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron — •JAN JANSEN, JOERG NEUGEBAUER
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	Machine Learning for Autonomous Optimization and Discovery of Materials — •PASCAL FRIEDERICH
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	Transforming Our View on Transformers in the Sciences — •KEVIN MAIK JABLONKA

Sessions

SYAI 1.1–1.5	Thu	9:30–12:15	HSZ/AUDI	AI and Data Challenges behind Emerging Self-Driving Laboratories
--------------	-----	------------	----------	---