SYAI 1: AI and Data Challenges behind Emerging Self-Driving Laboratories

Time: Thursday 9:30–12:15 Location: HSZ/AUDI

Invited Talk SYAI 1.1 Thu 9:30 HSZ/AUDI

Data and Experimental Foundations for Reliable Self-Driving Laboratories — •Dr. Marcus Tze-Kiat Ng — Magnusstr. 11, 12489 Berlin

Self-driving laboratories are increasingly guided by machine learning, yet progress is constrained by the quality, structure, and consistency of experimental data. In this work, autonomous experimental platforms are presented in which high-throughput synthesis, electrochemical testing, and multi-modal characterisation are carried out with high reproducibility. Through these systems, challenges that are rarely captured in benchmark datasets are revealed, including drift, batch effects, measurement noise, and incomplete metadata. Physics-informed representations, uncertainty-aware models, and active-learning strategies are shown to be effective when applied to such real-world data. Case studies in catalyst optimisation and discovery are used to demonstrate how large chemical spaces can be explored once the experimental feedback loop is closed. The experimental and data foundations required for reliable AI-driven materials discovery will be outlined.

Invited Talk SYAI 1.2 Thu 10:00 HSZ/AUDI

Digital Catalysis - AI for Experiment Planning and Control — •Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Self-driving laboratories (SDLs) epitomize a cutting-edge integration of machine learning with laboratory automation. Operating in active learning loops, SDLs use machine learning algorithms to plan experiments that are then executed by increasingly automated (robotic) modules. Here, I will present our perspective on emerging SDLs for accelerated discovery and process optimization in heterogeneous catalysis. Drawing on recent work in catalyst discovery, kinetic modelling, and catalyst degradation studies, I will argue against the paradigm of full automation and the objective of keeping the human out of the loop. Analysis of the associated workflows indicates that crucial advances will stem from establishing fast proxy experiments, re-engineering existing apparatuses and measurement protocols, and developing modelling approaches with real-time capabilities. Industrially relevant use cases will also require humans to remain in the loop for continuous decision-making, mandating explainable AI. In turn, active learning algorithms must be advanced to flexibly accommodate adaptations of the design space and variations in information content and noise in the acquired data.

Invited Talk SYAI 1.3 Thu 10:30 HSZ/AUDI

Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron — •Jan Janssen and Joerg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The hierarchical nature of materials – spanning electronic, atomistic, microstructural, and macroscopic scales – necessitates an integrated multiscale strategy for accelerating materials discovery. Realizing such a strategy requires close coordination across chemistry, materials science, and physics, and an equally tight coupling of simulation and experiment. Materials Acceleration Platforms (MAPs) address this need by embedding both theoretical and experimental data streams into a unified active-learning loop. A central challenge is ensuring that information can be meaningfully transferred across scales. We approach this by propagating uncertainties throughout the entire multiscale workflow, enabling quantitative comparison from ab-initio predictions to experimental measurements. This uncertainty-aware integration makes it possible to reduce the number of required experiments by several orders of magnitude. The resulting hierarchy of simulations is powered by machine-learning models – including ML interatomic potentials, Bayesian optimization, and large-language-model (LLM) agents – each contributing to decision-making within the MAP. The pyiron workflow framework provides the digital backbone for this integration. By encoding domain expertise into modular, machine-actionable workflows, pyiron enables simulation specialists to formalize their methods in a way that is both reproducible and interoperable.

15 min. break

Invited Talk SYAI 1.4 Thu 11:15 HSZ/AUDI

Machine Learning for Autonomous Optimization and Discovery of Materials — •Pascal Friederich — Karlsruhe Institute of Technology, Karlsruhe, Germany

Machine learning can accelerate the screening, design, and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on the use of machine learning for automated data analysis and autonomous decision-making in self-driving labs [1,2]. I will discuss extensions of Bayesian optimization to extend the autonomous decision-making process to more complex experimental and computational self-driving labs, as well as possibilities to include machine learning based recommendations already in the process of designing the experiments [3].

[1] Wu et al., Science 386, 6727 (2024), Inverse design workflow discovers hole-transport materials tailored for perovskite solar cells

[2] Marwitz et al., arXiv:2506.16824 (2025), Predicting New Research Directions in Materials Science using Large Language Models and Concept Graphs

[3] Jenewein et al., J. Mater. Chem. A 12, 3072-3083 (2024), Navigating the unknown with AI: multiobjective Bayesian optimization of non-noble acidic OER catalysts

Invited Talk SYAI 1.5 Thu 11:45 HSZ/AUDI

Transforming Our View on Transformers in the Sciences — •Kevin Maik Jablonka — Friedrich-Schiller Universität Jena, Jena, Germany — HPOLE Jena, Jena, Germany

The sciences face a fundamental challenge: much of the data we need for building models is not currently reported or usable in any structured form. Large language models (LLMs) have shown promise in addressing this through text-to-data conversion and direct predictive capabilities, attracting tremendous attention across scientific applications. In my contribution, I will present a roadmap based on comprehensive benchmarks of language models, multimodal models, and autonomous agents in chemistry and beyond. We have developed specialized evaluation benchmarks to assess scientific knowledge, reasoning abilities, and autonomous tool use across frontier models. Our results reveal a striking paradox: these models can exceed the performance of experts with decades of experience on certain tasks, while simultaneously failing worse than novices on other seemingly basic problems. I will discuss what these benchmark findings mean for the future of LLMs in scientific research, which applications are ready for deployment, where critical gaps remain, and how the field should prioritize development efforts. Finally, I will present the advances in models, systems, and infrastructure we have developed to enable practical impact across the sciences.