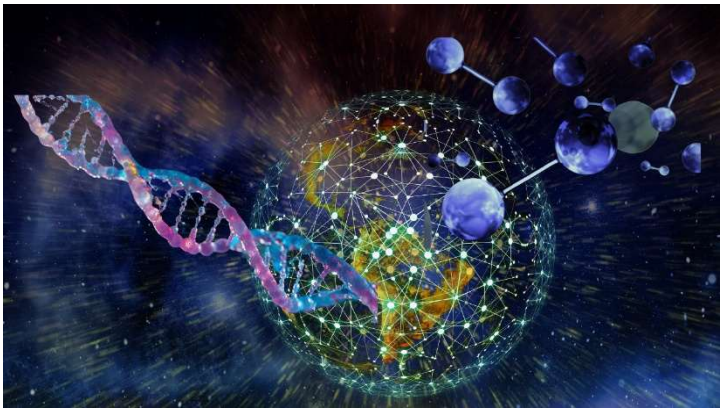
2ND BERLIN-BIOTECH SYMPOSIUM

AUTONOMOUS DISCOVERY IN BIO- & CHEMICAL ENGINEERING



November 27-28, 2025

Versuchs- und Lehranstalt für Brauerei in Berlin (VLB)
Seestraße 13, 13353 Berlin, Germany

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Program Day 1 Thursday 27.11.2025

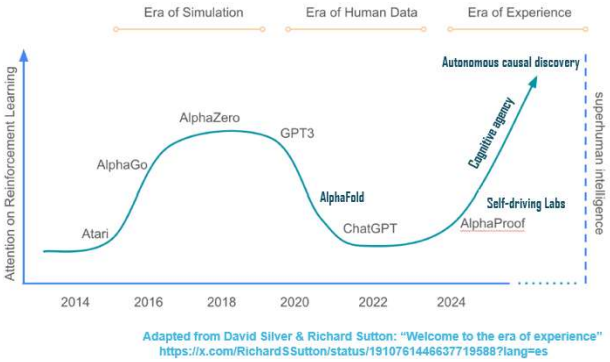
09:00	Lab Tour (for registered people only) - Chair of Bioprocess Engineering, Ackerstraße 76, 13355, Berlin	
11:00	Travel from Ackerstraße to VLB, Seestraße (self-organized)	
12:00	Registration & lunch	
13:00	Welcome	Nicolas Cruz, Ernesto Martinez, Peter Neubauer, *TU Berlin, DE*
13:30	Automated Scientific Discovery: From Equation Discovery to Autonomous Discovery Systems	Stefan Kramer, *Johannes Gutenberg - Universität Mainz, DE*
14:15	Democratizing the journey to smart manufacturing: Accelerating in-silico process optimization across the product lifecycle fueled by operational data Today	Alessandro Butté, *DataHow AG, CH*
14:45	Advancing Small-Data Modelling in Process Engineering from Prediction to Discovery	Dongda Zhang, *University of Manchester, UK*
15:15	*Coffee Break*	
16:00	Agentes Q and Gráfico: Autonomous agents for quantum chemistry	Jiaru Bai, *University of Toronto, CA*
16:45	From Automated Tasks to Autonomous Bioprocessing	Annina Kemmer, *TU Berlin, DE*
17:15	Hybrid bioprocess models integrating metabolic network constraints	Mathias Gotsmy, *ETH Zürich, CH*
18:00	*Pilot brewery tour (for registered people only) and get-together until 21:00*	

Program Day 2 Friday 28.11.2025

09:00	Learning, Dynamics, and Uncertainty: Foundations for Autonomous Discovery in Chemical and Biochemical Processes	Sergio Lucia, *TU Dortmund, DE*
09:45	Using synthetic biology and automated cytometry to optimize bioproduction	Gregory Batt, *Inria and Institut Pasteur, FR*
10:15	Integrating Sustainability Assessment with Process Development Workflow in Biotechnology	Sumesh Sukumara, *The Novo Nordisk Foundation Center for Biosustainability, DK*
10:45	*Coffee Break*	
11:30	FAIR data analysis workflows with Snakemake	Johannes Köster, *University of Duisbug-Essen, DE*
12:15	From Bayesian optimization to reinforcement learning for bioprocess optimization and control	Antonio del Rio Chanona, *Imperial College London, UK*
12:45	Lessons Learned from the Application of Bayesian Optimization in (Bio-) Chemical Process Optimization	Lukas Hebing, *Bayer AG, DE*
13:15	Closing remarks	Nicolas Cruz, *TU Berlin, DE*
13:30	*Lunch*	
14:00	Round table, ending 15:30	Ernesto Martinez, Nicolas Cruz, *TU Berlin, DE*

In the emerging era of AI-driven science, the ability of artificial intelligence to autonomously generate informative data is transforming the landscape of bio- and chemical engineering.

At the heart of this transformation lies the concept of Cognitive Self-driving Laboratories: automated experimental platforms capable of 1. Designing experiments, 2. Executing and monitoring the experimental plan, 3. Analyzing the experimental results, 4. Learning using evaluative feedback from the observations with minimal human intervention and 5. Infer new knowledge based on counterfactual reasoning. These labs are being extended to become engines of autonomous discovery, enabling AI systems to propose, test, and refine hypotheses, thereby accelerating scientific breakthroughs and uncovering complex causal relationships.



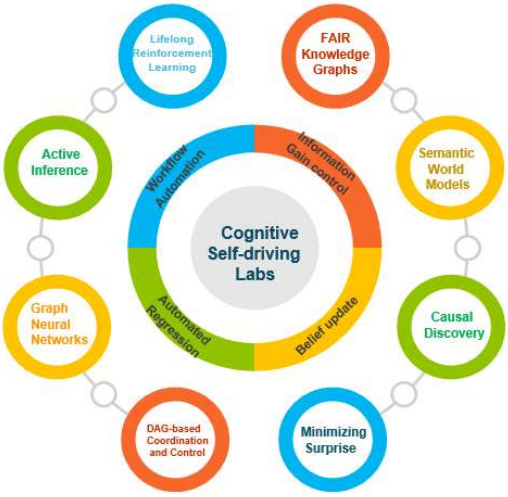
Adapted from David Silver & Richard Sutton: "Welcome to the era of experience" https://x.com/RichardSSutton/status/1910761446637719588?lang=es

This symposium brings together leading researchers from diverse yet complementary fields to explore the foundational building blocks of autonomous discovery to speed up innovation and foster a new era of experimentation and modeling in bioprocess and chemical engineering.

- **Data/Information/Knowledge - Jiaru Bai, Johanes Köster, Stefan Kramer**

The existing and the autonomously generated data needs to be transformed into interoperable and machine actionable knowledge. AI has shown the potential of a thorough management of information but there is still a long path to go before standards and procedures are mature enough to ensure FAIR-by-design generation of experimental results.

- **ML for bio- & chemical engineering - Antonio del Rio Chanona, Sergio Lucia, Dongda Zhang**



Process dynamics, plant-wide optimization, and large-scale difficulties all pose very specific challenges that significantly differ from standard AI applications. While the use of several tools has shown great performance, several issues still remain unsolved. The control of a dynamic process, for example, is still an open challenge for existing AI tools.

- **Handling biologocial complexity - Gregory Batt, Mathias Gotsmy, Annina Kemmer**

Biology offers systems with incredible complexity. AI can help to handle and analyse the huge number of species and inter- as well as intracellular interactions. Yet, computing a complete cell with molecular dynamics (MD) today would require 20 times the energy the whole earth can generate today. Autonomous systems need to leverage the interaction between experimentation and computation to boost research and achieve truly disruptive discoveries.

- **Tackling real societal and industrial challenges - Alessandro Butté, Lukas Hebing, Sumesh Sukumara**

Both society and industry have come to realize the immense potential of autonomous systems. Recently, ChatGPT, delivering a user-friendly interface with powerful LLMs has also brought non-experts closer to the technologies. It is hence essential to understand the real necessities and opportunities in these fields to enable autonomous systems to discover the knowledge necessary to address the major challenges that threaten humanity and its very existence.

Together with these experts, we will chart a path to address the challenges of cognitive self-driving labs and explore the potential of **autonomous discovery** in shaping the next generation AI for bio- & chemical engineering. Join us to tackle all our challenges from different points of view, research philosophies, and cultural processes.

Our speakers

Jiaru Bai is a Schmidt AI in Science Postdoc Fellow in the Matter Lab at the University of Toronto. His research focuses on pushing forward dynamic knowledge graphs, developing cognitive operating systems for self-driving labs that support adaptive, heterogeneous workflows and robust decision-making under uncertainty.

Gregory Batt is a senior research scientist at Inria. After a postdoctoral stay at Boston University, he joined Inria in 2007. Since 2017, he leads the InBio team, an Inria/Institut Pasteur joint research group. His work focuses on deciphering complex biological systems, contributing to the development of AI models that can interpret fragmented biological data.

Alessandro Butté is the CEO of DataHow, a company dedicated to the biopharmaceutical industry's digital transformation using advanced technologies, including AI and machine learning, to support biopharma companies' implementation and the democratization of data-driven solutions to solve their greatest process development challenges.

Mathias Gotsmy is a postdoctoral researcher in the SUPERlab at the ETH Zürich (Switzerland). He is an expert in bioprocess model design, parameterization, and optimization. Currently, he develops hybrid bioprocess models that combine metabolic network constraints, kinetic knowledge, and machine learning.

Lukas Hebing is a scientist in the Data Science organization at Bayer. His projects span machine learning, statistics, or Bayesian optimization, together with organizational topics such as digitalization strategies, and change management. Lukas applies these approaches across chemical and biotechnological research and development as well as production.

Annina Kemmer is currently a postdoctoral researcher in the KIWI-biolab and serves as coordinator of the high-throughput laboratory. Her work is focused on the automation and model-based execution of complex multidevice high throughput experiments for bioprocess development.

Johannes Köster research is focused on reproducibility in three ways: 1. author of the popular workflow management system Snakemake and the founder of the Bioconda, 2. author of the Rust-Bio library, enabling the use of the Rust programming language for bioinformatics, and 3. he is working in the field of Bayesian statistics (e.g., for variant calling and single cell transcriptomics).

Stefan Kramer is Professor of Data Mining and Machine Learning at Johannes Gutenberg-Universität Mainz. His work focuses on the role of knowledge in machine learning, neuro-symbolic AI, scientific discovery, and applications mostly in the life sciences. In 2025, Hannu Toivonen and Stefan Kramer published the popular science book "Was ist künstliche Intelligenz: 100 Fragen und Antworten".

Sergio Lucia is the head of the Chair of process automation systems at TU Dortmund. His work focuses on model predictive and distributed control to explore how machine learning can enhance decision-making under uncertainty—critical for ensuring reliable and autonomous lab operations in highly nonlinear dynamic systems.

Antonio Del Rio Chanona is the head of the Optimisation and Machine Learning for Process Systems Engineering group at Imperial College London. His work focuses on the integration of reinforcement learning into process systems engineering for adaptive decisions in bioprocess control and optimization.

Sumesh Sukumara is a tenured Senior Researcher and Independent Team Leader at DTU Biosustain. His work critically examines the notion of biotechnology's inherent sustainability, promoting a data-driven approach to avoid greenwashing and ensure genuine impact.

Dongda Zhang is a lecturer at the Department of Chemical Engineering in the University of Manchester. His group develops methodologies and practical applications for mathematical modelling and data analytics to understand, optimise, and upscale complex chemical and biochemical processes.