MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Report
2023–2024

+ **Antonio Sorrentino** (left) and **Monisha Sivasankaran** (right) are researchers in the Electrochemical Energy Conversion group.

Young scientists Antonio Sorrentino and Monisha Sivasankaran are exploring the potential to control the selectivity of electrochemical reactions through optimal dynamic inputs. Discover how their groundbreaking work is paving the way for advancements in sustainable energy conversion and chemical processes. Read more on pages 64-65 in this issue of our MPI Report.

Report 2023–2024

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FREQUENTLY USED ABBREVIATIONS

Research Groups headed by MPI Directors

BPE	Bioprocess Engineering
CSC	Computational Methods in Systems and Control Theory
PCF	Physical and Chemical Foundations of Process Engineering
PSE	Process Systems Engineering

Research Groups headed by External Scientific Members

PSD	Process Synthesis and Dynamics

Research Groups headed by Senior Scientists

ARB	Analysis and Redesign of Biological Networks
DMP	Data-driven Modeling of Complex Physical Systems
EEC	Electrochemical Energy Conversion
MSD	Molecular Simulations and Design

Max Planck Fellow Group

OML	Mathematical Optimization and Machine Learning

Others

ATP	Adenosine triphosphate, organic compound that provides energy to drive many processes in living cells
BMBF	German Federal Ministry of Education and Research
BMWK	German Federal Ministry for Economic Affairs and Climate Action
CDS	Center for Dynamic Systems
CORE	European project: Continuous Resolution and Deracemization of Chiral Compounds by Crystallization
COST	European Cooperation in Science and Technology
CPTS	Chemistry, Physics and Technology Section of MPG
DAAD	German Academic Exchange Service
DARPA	Defense Advanced Research Projects Agency (United States)
DECHEMA	Expert Network for Chemical Engineering and Biotechnology in Germany (Gesellschaft für Chemische Technik und Biotechnologie e.V.)
ERC	European Research Council
ERDF	European Regional Development Fund (Europäischer Fonds für regionale Entwicklung, EFRE)
EXIST	University-Based Business Start-Ups (support programme of the BMWK)
DFG	German Science Foundation (Deutsche Forschungsgemeinschaft)
FOR	Research Unit funded by the DFG (DFG finanzierte Forschungsgruppe)
FVST	Faculty of Process and Systems Engineering at OVGU Magdeburg
GAMM	International Association of Applied Mathematics and Mechanics (Gesellschaft für Angewandte Mathematik und Mechanik)
IMPRS	International Max Planck Research School
IMPD4Cat	Multistep Catalytic Production Systems for Fine Chemistry by Integrated Molecular, Material and Process Design
LIKAT	Leibniz Institute for Catalysis e.V., Rostock
LSA	German Federal State of Saxony-Anhalt
MaRDI	Mathematical Research Data Initiative in Germany
MLU	Martin Luther University Halle-Wittenberg
MPG	Max Planck Society (Max-Planck-Gesellschaft)
MPI	Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
NFDI	Nationale Forschungsdateninfrastruktur (Network on research data management in Germany)
NFDI4Cat	NFDI for Catalysis-Related Sciences
Omics	Various disciplines in biology whose names end in the suffix -omics, such as genomics, proteomics, metabolomics and glycomics
OVGU	Otto von Guericke University Magdeburg
SAB	Scientific Advisory Board
SFB	DFG-funded Collaborative Research Center (Sonderforschungsbereich)
SIAM	Society for Industrial and Applied Mathematics
SmartProSys	Research Cluster Smart Process Systems for a Green Carbon-based Chemical Production in a Sustainable Society
SPP	Priority Programme (Schwerpunktprogramm)
TH	University of Applied Sciences (Technische Hochschule)
TU	Technical University (Technische Universität)

+ Research Groups

Introduction

Research Groups

Directors

External Scientific Members and Max Planck Fellows

+ Download as PDF: www.mpi-magdeburg.mpg.de/mpi_annual_report

Senior Scientists

Future-oriented Cooperation in Highly Relevant Research Areas at the Science Location Magdeburg

There are many reasons for the successful development of the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg over the past 25 years to become one of the world's leading institutions. Outstanding scientists, interdisciplinary approaches in basic research with a focus on applications for relevant topics of our time, fantastic laboratory facilities and diverse collaborations are key success factors. The Otto von Guericke University (OVGU) has been a key partner at the site since the institute was founded. Many of the MPI scientists have an affiliation with the university, and we work closely together on recruitment. In order to plan joint activities in the long term and largely independently of personnel changes or financial conditions, such cooperation requires an institutional form. This was created in 2007 with the Centre for Dynamic Systems (CDS). The scientists can utilise state funding largely autonomously in a targeted manner and in line with their respective strategies. Together with the International Max Planck Research School, we have been laying the foundations for scientific excellence for many years, particularly in the training of young scientists.

In the midterm, this will also enable successful participation in larger joint projects of the German Research Foundation and has led to the consistent development of the application for the SmartProSys Cluster of Excellence over the last four years. It fills me with pride that the university and MPI have succeeded in inspiring 22 Principal Investigators at the site to work towards the goal of restructuring the carbon cycles of the chemical industry in a sustainable society. The benefits will not only be seen at the chemicals sites in the south of Saxony-Anhalt, which are undergoing a far-reaching transformation process, but also for Germany as an industrial location as a whole.

In times of limited state budgets, science will have to emphasise its high relevance even more in the future. At the Magdeburg site, the Max Planck Institute and OVGU will certainly succeed in doing this.

Prof. Dr.-Ing. Jens Strackeljan
Rector of
Otto von Guericke University Magdeburg

+ **Intro**duction

+ **Figure 1:**
The directors and heads of research groups, the head of the administration department and the research coordinator of the MPI Magdeburg. From left to right: Prof. Andreas Seidel-Morgenstern, Dr. Steffen Klamt, Dr. Kai-Friederike Oelbermann, Dr. Feliks Nüske, Dr. Bettina Heise, Prof. Peter Benner, Prof. Kai Sundmacher, Prof. Udo Reichl, Dr. Tanja Vidaković-Koch, Prof. Sebastian Sager, Prof. Achim Kienle, Prof. Matthias Stein

+ **Figure 2:**
On 31 January 2023, the President-elect of the Max Planck Society, Prof. Patrick Cramer, visited the Max Planck Institute Magdeburg together with the Secretary General of the Max Planck Society, Dr. Simone Schwanitz. from left to right: Prof. Andreas Seidel-Morgenstern, Dr. Bettina Heise, Dr. Britta Peschel, Prof. Udo Reichl, Prof. Kai Sundmacher, Prof. Patrick Cramer, Dr. Simone Schwanitz, Prof. Peter Benner.

+ **Figure 3:**
In 2023, our MPI looked back on 25 years of research in Magdeburg. The symposium on "Dynamics of Complex Technical Systems: Current Status and Future Prospects" on 29 June 2023 at the Festung Mark in Magdeburg reunited many people who have accompanied our institute over the past 25 years and continue to do so. (also see p. 8)

+ **Figure 4:**
1,273 guests visited our open labs, the pilot scale hall and computer cluster during the 17th Science Night on June 3, 2023. Mayor Simone Borris was very complimentary of LN8MD and she found the MPI particularly interesting as part of the guided VIP tour.

The Max Planck Institute in Magdeburg: Retrospective of 2023–2024

+ Looking back on my time as Managing Director of our MPI in Magdeburg from January 2023 to December 2024, I am proud of what we have achieved together and feel really confident about the future of our institute.

In 2023, our MPI celebrated its 25th anniversary. We marked this milestone with various events and a special edition of our MPI Report, which looks back on the scientific work and development of the institute in the 25 years since its founding in Magdeburg in 1998. We celebrated the anniversary together with guests of honor from politics and academic institutions, as well as alumni of our institute and our employees. We highlighted significant scientific achievements and visions for the future at a symposium on "Dynamics of Complex Technical Systems: Current Status and Future Perspectives" on June 29, 2023, at the Festung Mark in Magdeburg. It was a great honor to welcome Prof. Claire Adjiman (Imperial College London) and Prof. Dr. Marco Mazzotti (ETH Zurich) as keynote speakers for this occasion. Their presentations on "Engineering Molecules for Sustainability" and "The Journey of a Purpose-Driven CO_2 Scientist: From Molecules to Systems - from Switzerland to Iceland" provided the 300 attendees with valuable inspiration. I would like to take this opportunity to once again express my sincere thanks to the organizing team for their excellent preparation of a thoroughly successful event.

In an extremely competitive scientific environment, we have the task of constantly breaking new ground in research with innovative topics and achieving high international visibility in the process. To ensure this, we have not only launched new research projects over the past two years (for example, see the research unit FOR 5538 IMPD4Cat on pages 20–21) but also pushed ahead with the renewal of the institute's staff at various levels and used various instruments to network internationally with outstanding scientists. In December 2023, we presented the newly created Ernst Dieter Gilles Lecture Award to Prof. Martha Grover, Georgia Institute of Technology (Atlanta, USA). This award recognizes her outstanding methodological contributions to the dynamics and control of complex chemical processes and biological systems and expresses our hope for fruitful and intensive scientific collaboration with Martha Grover and her home university in the coming years. In a first joint project, a novel process is currently being investigated in which fine chemicals can be obtained with maximum efficiency by integrating a biocatalytic reaction with the crystallization of the product.

Another international collaboration has been established through the creation of a new Max Planck Partner Group led by Dr.-Ing. Teng Zhou, an alumnus of our institute and now assistant professor at Hong Kong University of Science & Technology (HKUST) in Guangzhou (China). Several doctoral theses have been and are being supervised jointly with this partner group. Our collaboration focuses on the development of advanced computational methods for the design of materials and processes for highly efficient CO_2 capture. The partner group's research encompasses process and energy systems engineering, computer-aided molecular and process design, and the application of machine learning methods for the discovery of functional materials. The group is also working on the integration of hybrid modeling approaches and artificial intelligence to enable the simultaneous design of novel materials and process concepts for efficient CO_2 capture.

Furthermore, in September 2023, at the request of the institute, Prof. Dr. Sebastian Sager, Professor of Mathematical Optimization at Otto von Guericke University Magdeburg, was appointed Max Planck Fellow at our MPI. His research group focuses on the application-oriented development of optimization methods, the close connection to machine learning methods, and the efficient implementation of optimization algorithms on computers. His main research areas include nonlinear and mixed-integer optimization, as well as optimal control and optimal design of experiments. A particular focus is on numerical algorithms for mixed-integer optimization with differential equations. The necessary mathematical models originate from various applications in (bio)chemical process engineering, which are developed jointly with the other research groups at the MPI.

Prof. Sager's appointment as Max Planck Fellow is part of our overall strategy to not only maintain our long-standing close and trusting collaboration with Otto von Guericke University Magdeburg, but also to align it with new ambitious goals and develop it further. The central element of this future strategy is the focus on the research topic "Smart Process Systems for a Green Carbon-based Chemical Production in a Sustainable Society." To this end, our institute, together with colleagues from Otto

+ Figure 5:
The mathematician Prof. Dr. rer. nat. habil. Sebastian Sager (right) has been appointed Max Planck Fellow. He heads the Mathematical Optimization and Machine Learning research group since October 1, 2023. Here he is pictured with Prof. Dr.-Ing. Kai Sundmacher (left).

+ Figure 6:
Meeting of the Board of Trustees of the MPI Magdeburg in April 2024: from left to right: Dr. Andreas Neubert, Hon.-Prof. Dr. Mirko Peglow, Dr. Eva E. Wille, Dr. Wilhelm Otten, Prof. Kurt Wagemann, Simone Borris, Prof. Andreas Schuppert, Prof. Jens Strackeljan, Thomas Wünsch (State Secretary, representative of Minister Prof. Armin Willingmann)

+ Figure 7:
On occasion of MPI's 25th anniversary, the author and actor Steffen Schroeder took us back to the life and times of Max Planck with his vivid descriptions and his exciting, emotional reading from his book. 110 members of the audience showed their interest on 14 November 2023 at the MPI.

+ Figure 8:
A team from our institute, led by the chemical engineer Ronny Tobias Zimmermann, received one of the 2023 Environmental Awards from the state capital of Magdeburg, taking first place in the "Research" category for the invention of easy-to-manufacture core-shell catalysts. From left to right: Prof. Dr. Kai Sundmacher, Markus Ikert, Bianka Stein, Dr. Ronny Tobias Zimmermann, Prof. Dr. Jens Bremer.

+ Figure 9:
Tomorrow Labs is Magdeburg's new festival. On 8 June 2024, science and future issues met music and culture at the Science Port. The research institutions and universities presented themselves in experiments, talks and shows. We held good conversations with interested visitors at our stand, our exhibits, quizzes and puzzles being a good introduction into our research topics.

+ Figure 10:
The Scientific Advisory Board meets every three years for regular evaluation of the institute's scientific achievements. Their last meeting was held from 25 to 27 November 2024. The current members of the board: front row: Prof. Matthias Wessling, Prof. Claire Adjiman, 2nd row: Prof. Sabine Flitsch, Prof. Diethard Mattanovich, Prof. Daniele Marchisio, 3rd row: Prof. Omar Ghattas, Prof. Lars Nielsen, Prof. Barbara Kaltenbacher, Dr. Samuel De Visser

von Guericke University Magdeburg, the Leibniz Institute for Catalysis in Rostock, and Brandenburg University of Technology in Cottbus-Senftenberg, prepared a proposal for a Cluster of Excellence "SmartProSys" to the German Research Foundation (DFG) in 2023. We were delighted that our draft proposal was selected for the final round of the competition. The cluster concept has a strong interdisciplinary focus and has inspired many new collaborations between the MPI and its partner institutions, in particular with the OVGU. Regardless of the final outcome of the Cluster of Excellence application, the topics of circular carbon economy and sustainable production of chemicals will continue to be key areas of research at the MPI in the future.

In line with this focus, we submitted an application in July 2024 to establish the new International Max Planck Research School of Systems and Process Engineering for a Sustainable Chemical Production (IMPRS SysProSus), which was approved by the Max Planck Society in November 2024. At the same time, the Center for Dynamics Systems (CDS), which has been jointly supported by OVGU and the MPI since 2007, was also aligned with this topic and successfully submitted a funding application. Following a positive review, the center will be financed by ERDF funding from the state of Saxony-Anhalt until the end of 2027. The aim of the new CDS concept is to conduct application-oriented research in pre-competitive cooperation with companies in the chemical industry based in Saxony-Anhalt, focusing on the use of renewable raw materials and renewable energy, making new products, and pushing the digitalization of chemical production processes in a future circular economy. We are very grateful to the state of Saxony-Anhalt for this funding as it enables us to establish Magdeburg as a nationally and internationally visible science location in the field of sustainable chemical production – a topic that is of utmost importance for the economic future of our federal state.

The most important aspect of the personnel changes mentioned above was finding a successor for Prof. Dr.-Ing. Andreas Seidel-Morgenstern, who retired as Director of the Department of Physical & Chemical Fundamentals of Process Engineering in August 2024. We are very grateful to him for his many years of countless and highly successful research activities at our MPI. In particular, we are very proud that Andreas Seidel-Morgenstern was newly inducted into the National Academy of Engineering of the United States of America in February 2023 for his contributions to adsorption, preparative chromatography, crystallization, and to process development as well as theory for resolving enantiomeric mixtures. The search for a successor, which we started in October 2020, proved to be challenging and lengthy overall. We were therefore all the more delighted when, at a colloquium held at the beginning of April 2024, we could finally succeed in identifying an outstanding scientist, whom we proposed to the Chemistry-Physics-Technology Section (CPTS) of the Max Planck Society (MPG) for appointment as a new director of our MPI in October 2024. We are pleased to announce that the CPTS approved the appointment in February 2025, paving the way for negotiations with the President of the MPG, Prof. Patrick Cramer. We are very optimistic that the appointment will be accepted in the course of 2025, so that we can welcome our new Scientific Member of the MPG at our institute. We are very much looking forward to it!

These are all developments that can be viewed as very positive for the MPI and for Magdeburg as a science location. And the list of positive developments and visible successes (awards, appointments, improved sustainability, equality opportunity plan, and so on) could be significantly expanded. However, at the end of this short review of 2023–2024, I must unfortunately also mention an event whose possible consequences continue to cause me great concern. 2024 ended with a shock for all of us: the terrible attack on the Magdeburg Christmas market on December 20, which left six people dead and over 300 injured. This was and remains a traumatic event for the city and for all of us. Our deepest sympathy and solidarity go out to all our fellow citizens who lost loved ones in the attack and to those who suffered serious physical and psychological injuries. Some of our employees and their families witnessed the attack firsthand and are still suffering from severe psychological trauma. Foreign students at OVGU, some of whom are taught by MPI employees, were also physically affected by this heinous act. As the mayor, Simone Borris, who is also a member of the MPI Board of Trustees, clearly stated at a memorial service in Magdeburg Cathedral, our society must not allow itself to be divided by this terrible event. Hatred and exclusion of foreign fellow citizens must not be the result. Tolerance, cosmopolitanism, liberal thinking, and equality for all people are core values without which science cannot exist and flourish. To sum it up in a sentence from our MPG President, Prof. Patrick Cramer: "We need an open society!"

Magdeburg, April 2025

Prof. Dr.-Ing. Kai Sundmacher
Managing Director of MPI DCTS, 2023–2024

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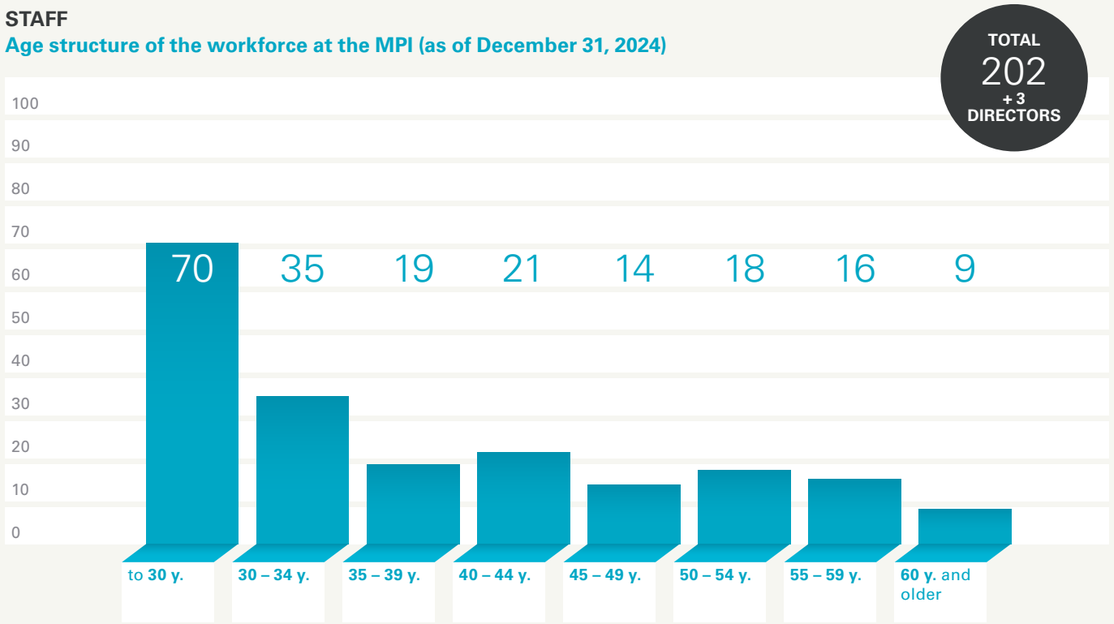
Facts and Figures

STAFF

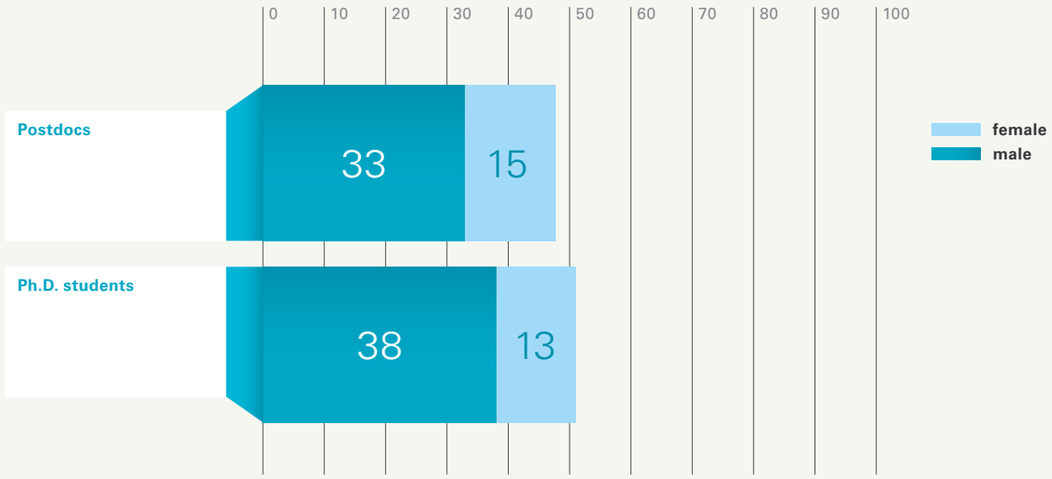
Age structure of the workforce at the MPI (as of December 31, 2024)



STAFF

Distribution of scientists by gender

Female employees: 15% Postdocs and 13% Ph.D. students

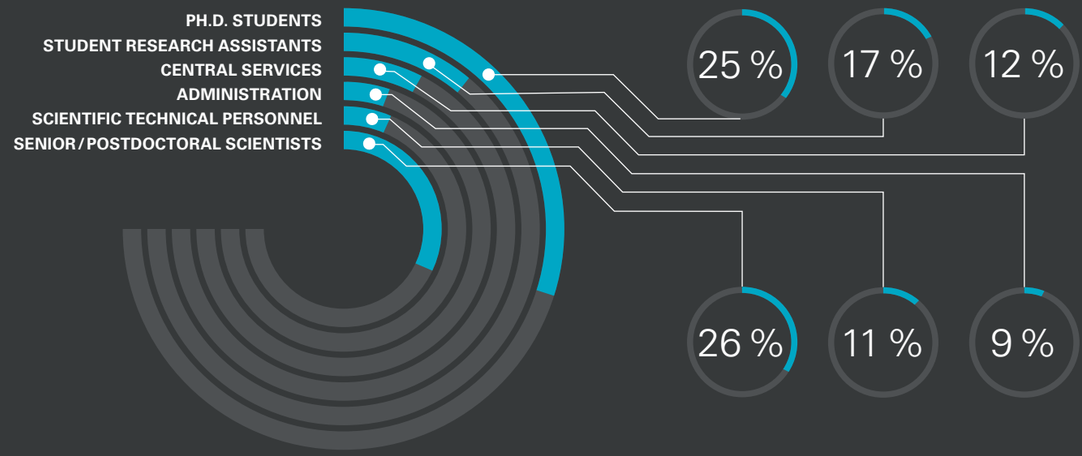


The two graphs above show the age structure and the gender balance among the institute's scientists on the Postdoc and Ph.D. levels, respectively. As Max Planck Institutes are run with very few permanent scientists, the average age of employees is quite low as the majority of scientists consists of Ph.D. students and young Postdocs.

STAFF

December 31, 2024: 202 Employees

99 Scientists: 48 Postdocs, 51 Ph.D. students



At the end of 2024, the MPI employed 202 persons. The majority are scientists and student researchers as illustrated by the pie chart above. As can be seen, the institute is run by a lean administration, while operating the labs and technical facilities accounts for the rest of the employees.

EXPENDITURE PATTERN IN 2024

Total Expenses in Fiscal Year 2024: 15,65 million Euro

The total budget of the MPI in the fiscal year 2024 was 15.65 million Euro. The pie chart above shows how this was distributed to the major budget categories. As can be seen, nearly 70 % of the budget was used for salaries.

MPI-GENERAL BUDGET 2024

Total Revenue: 15.65 million Euro

Third-party funds: 2.93 million Euro

This pie chart related to the budget shows the distribution of the budget sources. As usual for Max Planck Institutes, the main source is institutional funding provided by the Max Planck Society.

Selected Events 2023 – 2024

+ Group photo showing the participants of the inaugural NFDI@MPG Workshop at the Ringberg Castle, 19-22 April 2023

GlycoBioTec 2023 – 3rd International GlycoBioTec Symposium

The third edition of the conference had to be rescheduled due to the COVID19 pandemic und finally took place from 17 to 19 January 2023 at the Harnack House in Berlin, the conference venue of the Max Planck Society.

The conference was an interactive forum for discussing cutting-edge research on the frontiers of Glycobiotechnology, spanning fundamental theory to method & technology developments relevant to Biopharma, health, medicine and functional food areas.

Topics of GlycoBioTec2023 were Glycosylation & Protein Function, Synthesis of Glycoconjugates, Glycans and Nucleotide Sugars, Cell-Based and Cell-Free Glycoengineering, Synthesis and Function of Human Milk Oligosaccharides, Biopharmaceuticals: Control on Glycosylation Quality Attributes, High-Throughput Glycoanalytics for In-Process Control, Novel Technologies & Methods for Glycoanalytics, Glycoimmunology, Glycobioinformatics, Glycosylation & Biomarkers.

On the 2 ½ days, 180 participants gathered together, attending to five invited keynote lectures and 20 short talks, to an evening poster session and a conference dinner as well as networking successfully at various discussion tables. Due to the success of the format, the next GlycoBioTec Symposium is scheduled to take place in February 2025.
| Dr. Thomas Rexer

NFDI@MPG Ringberg Workshop

The German National Research Data Infrastructure (NFDI) is part of a nationwide effort to promote science and research through a data infrastructure that establishes minimal standards for research data, provides data repositories and services, brings forward education and fosters a new data culture. The NFDI now consists of 27 consortia, with Max Planck Institutes (MPIs) strongly represented across various disciplines. A 3-day workshop organized by MPI Magdeburg and the Max Planck Computing and Data Facility (MPCDF) took place at the Ringberg Castle from 19th to 22nd April 2023, bringing together 30 senior and early-stage scientists from 14 MPIs to discuss the current challenges in research data management (RDM). Fifteen talks covered various aspects of RDM, with discussions on common issues, expectations, and solutions. With domain-specific viewpoints, all talks addressed key cross-cutting aspects of research data management while highlighting the tools and services developed across the MPIs. In addition, during the workshop, shared challenges were collaboratively explored in dedicated open sessions on the final day for thorough evaluation. Electronic Lab Notebooks (ELNs) were a key topic of discussion. While a common ELN for interdisciplinary use was not developed, open-source solutions like ELN-Finder and LabFolder were suggested. A highlight was the presentation of geospatial data, which, due to its large volume, requires advanced interfaces and data structures. Going forward, all participants agreed on the need for a strategic roadmap for promoting RDM awareness among MPI researchers, and organizing frequent workshops on research data management within the MPG.
| Dr. Pavan Laxmipathy Veluvali

2nd Symposium “Smart Process Systems Engineering: Towards Sustainable & Circular Production Processes”

On April 21st 2023, the SmartProSys research initiative hosted their 2nd symposium on “Smart Process Systems Engineering: Towards Sustainable & Circular Production Processes”. The symposium was held in person in Lecture Hall 6 in Building 44 of Otto von Guericke University in order to facilitate networking and exchange among project members and to compensate for the online format required in previous years due to the COVID 19 pandemic. A total of 121 participants have attended the symposium.

The Secretary of State for Science in Saxony-Anhalt, Thomas Wünsch, and the Rector of the Otto-von-Guericke University, Prof. Jens Strackeljan, honored us by attending our symposium and giving opening speeches. Scientific presentations were given at four different levels of the project structure: Process Level, Molecular Level, Systems Level, Computational Methods & Algorithms. After the opening speech by the SmartProSys Spokesperson Prof. Dr.-Ing. Kai Sundmacher, the Process Level was presented by Prof. Dr.-Ing. Achim Kienle and the Molecular Level by Prof. Dr.-Ing. Christof Hamel, both focusing on efficiently transforming plastic and biogenic waste into valuable molecules for new products. Prof. Dr. Ellen Matthies talked about the aims of the research area Systems Level, using social science methods to investigate the role that psychological, sociological, and political aspects play in this process. Finally, Prof. Dr. Sebastian Sager talked about Efficient Algorithms for Complex Recurrent Processes.

The symposium concluded with a reception and poster session, where the young scientists had the opportunity to present their research results to the other project members and to engage in fruitful discussions to enable joint research projects. **| Dr. Esra Boz**

6th Workshop on Virus Dynamics in Nagoya

On July 4–6, 2023, the Interdisciplinary Biology Laboratory (iBLab) hosted the Workshop on Virus Dynamics at Noyori Memorial Hall, Nagoya University, Japan. It marked the 6th iteration of this international conference with around 90 participants. The event showcased cutting-edge research on virus infection dynamics, including insights into new coronaviruses influenced by the COVID-19 pandemic.

The timing of the conference was ideal, bringing together researchers from different countries and backgrounds for open discussions on viral dynamics. Unlike the 2021 online conference, the event in 2023 was held in person for the first time in four years, fostering a lively exchange among participants.

+ Impressions of the SmartProSys Symposium 2023. Dr. Hans-Gerhard Husung (Head of the OVGU Board of Trustees), Thomas Wünsch (State Secretary at MWU), Prof. Achim Kienle, Prof. Kai Sundmacher, Prof. Ellen Matthies (Spokespersons), Prof. Jens Strackeljan (President of OVGU).

+ Prof. Kai Sundmacher hands over the *Ernst Dieter Gilles Lecture Award* to Prof. Martha Grover on 14 December 2023 at the MPI.

+ The participants of the 5th Indo-German Workshop on "Advances in Materials, Reactions and Separation Processes"

A cultural highlight was the reception at *Tokugawa-en,* the former residence of the Owari Tokugawa family. This Japanese garden, with its circular courtyard and pond, provided a serene atmosphere for networking. Attendees enjoyed a traditional "barrel sake" performance, experiencing sake aged in cedar or cypress barrels for a unique taste of Japanese culture.

Conference sessions were designed to maximize engagement and collaboration through keynote presentations, poster sessions, and informal discussions. This format allowed participants to explore the latest research and collaborative opportunities, emphasizing interdisciplinary approaches to understanding viral dynamics and the role of international collaboration in advancing scientific knowledge.

| Dr.-Ing. Daniel Rüdiger

1st Ernst Dieter Gilles Lecture given by Prof. Martha Grover

"I have never met Professor Ernst Dieter Gilles personally, but it feels like I did. However, I did get to know many people from his circle, including here at the MPI Magdeburg.", said Professor Martha Grover on the occasion of the 1st *Ernst Dieter Gilles Lecture* on 14 December 2023 at the Max Planck Institute Magdeburg. Martha Grover gave the lecture on the topic "Continuous biocatalytic crystallization to address beta-lactam supply challenges".

The Max Planck Institute Magdeburg has selected US chemical engineer Prof. Martha Grover as the first prize winner of the *Ernst Dieter Gilles Lecture Award*. She has made outstanding methodological contributions to the process dynamics and process control of complex process engineering and biological systems. Martha Grover is a Professor in the School of Chemical & Biomolecular Engineering at Georgia Tech, and Associate Chair for Graduate Studies. She holds a joint appointment with Savannah River National Laboratory, Jackson, USA. Her research considers molecular self assembly and the emergence of biological functions.

With the *Ernst Dieter Gilles Lecture Award,* the MPI Magdeburg honors outstanding scientific achievements in the field of systems theory, system dynamics, control engineering and systems biology commemorating the pioneering scientific work of Prof. Dr.-Ing. Dr. h.c. mult. Ernst Dieter Gilles and his unparalleled influence in the world of System Dynamics and Control.

| Gabriele Ebel

5th Indo-German Workshop on "Advances in Materials, Reactions and Separation Processes"

A series of Indo-German Workshops on "Advances in Materials, Reaction and Separation Processes" was started at the Indian Institute of Technology (IIT) in Madras in 2008 followed by consecutive events in Bad Herrenalb (2012), at the IIT Guwahati (2016) and Berlin (2020). The aim is to strengthen collaborative research activities between Indian and German colleagues and to introduce doctoral students to current research activities.

The meetings supported exchanges of students, visits by scientists from one country to the other and working in cooperation projects. The success of the collaboration can be gauged from numerous publications in internationally reputed journals which have been co-authored by scientists from both countries.

The 5th Indo-German Workshop, organized by Prof. Rabibrata Mukherjee, was successfully held from February 19 to 21, 2024 at the Indian Institute of Technology in Kharagpur. It was attended by more than 60 scientists, among them 15 from Germany.

Topics covered in particular processes to purify biomolecules and enantiomers, novel concepts in reaction engineering, process systems engineering and control and innovations in material science. The German participants were impressed by the tremendous progress made by their Indian colleagues in the last years.

The excellently organized workshop took place in a very enjoyable and relaxing atmosphere and was supported by many highly motivated students. The informal character supported a quick and intensive contact between the young generations of Indian and German scientists and provided insight into the specific research structures and activities of the two countries. The preparation of a 6th workshop in Germany is already underway.

| Prof. Dr.-Ing. Andreas Seidel-Morgenstern

94th GAMM Annual Meeting

The 94th annual meeting of the GAMM, the International Association for Applied Mathematics and Mechanics, was held for the first time in its history of more than 100 years at the Otto von Guericke University from 14 to 18 March 2024 and attracted about 1,000 participants from more than 30 countries to Magdeburg.

The success of this conference was made possible through the close cooperation of the colleagues from OVGU and MPI Magdeburg. The main organizing team consisting of Prof. Dr. Peter Benner, Prof. Dr.-Ing. Daniel Juhre, Prof. Dr. Thomas Richter and Prof. Dr.-Ing. Elmar Woschke spans not only from the OVGU to the Max Planck Institute, but also across the disciplines defining GAMM - Applied Mathematics and Mechanics.

The conference was opened by Prof. Dr. Karsten Urban, the current president of GAMM, and Prof. Dr. Peter Benner as representative of the local organizers. Welcome addresses were given by the rector of the OVGU, Prof. Dr. Jens Strackeljan, and by the prime minister of Saxony-Anhalt, Dr. Reiner Haseloff, via video message.

The program committee carefully selected the plenary lecturers and managed to establish a scientific program of outstanding quality comprising almost 800 talks and lectures, including minisymposia and poster sessions as well as offering an open marketplace for ideas and exchange in particular for young scientists, including activities of the GAMM Juniors and the GAMM Student Chapters

| Prof. Dr. Peter Benner

+ A notable highlight of the GAMM Annual Meeting was the public lecture by Peter Streitenberger, Otto von Guericke Society in Magdeburg, titled "Vacuum and Air Pressure - Otto von Guericke and the Scientific Revolution in the 17th Century," featuring experiments demonstrating Otto von Guericke's historical relevance.

+ Prof. Peter Benner welcomes the participants during the opening of the 94th Annual Meeting of the GAMM Association on 14 March 2024 at the Lecture Hall 1 on the campus of Otto von Guericke Universiy.

+ The Workshop on Uncertainty Quantification in Molecular Simulation brought together researchers from various disciplines like applied mathematics, physics and chemistry on August 29–30, 2024, at the MPI.

Workshop on Uncertainty Quantification in Molecular Simulation

On August 29–30, 2024, MPI hosted a workshop on *Uncertainty Quantification in Molecular Simulation*. The goal of this meeting was to bring together researchers in applied mathematics, physics, chemistry, and related disciplines to discuss the state of the art in modelling and evaluating uncertainties in computer simulations of matter at the molecular scale.

Computer simulations have become one of the most powerful tools for making predictions about the behaviour of complex systems at the molecular scale, with scales ranging from the microscopic world of atoms and small molecules all the way up to the macroscopic world of our lived experience. Prominent models used at different scales include methods for electronic structure such as density functional theory (DFT), classical molecular dynamics (MD), coarse-grained MD, reaction-diffusion models, continuum fluid mechanics, and many others. These simulations are subject to uncertainties stemming from multiple sources, for instance, due to the use of stochastic algorithms in the process of simulation, or inherent uncertainties with respect to model inputs and parameters. Correctly assessing these uncertainties is often challenging due to the presence of high-dimensional, multi-modal distributions associated with parameters of the model.

At the workshop, we heard from researchers investigating this topic both from a theoretical and from a practical angle. Our plenary speakers Sebastian Krumscheid (KIT, Germany), Gabriel Stoltz (CERMICS, France), and Thomas D. Swinburne (CNRS, France) covered the mathematical theory, the sources of uncertainties in simulation, and numerical approaches to evaluating uncertainties in simulation.

| Dr. Feliks Nüske

Managing Research Data: 2nd MaRDI Workshop on Scientific Computing

Findability, Accessibility, Interoperability and Reusability of research data (FAIR principles) are key factors for further scientific progress. Representatives of the University of Münster and the MPI Magdeburg hosted a workshop with 40 participants of the *Mathematical Research Data Initiative* (MaRDI) within the *National Research Data Infrastructure* (NFDI) of Germany from October 16 to 18, 2024.

With this second “MaRDI Workshop on Scientific Computing”, they brought together researchers from the Scientific Computing community and related disciplines, who are interested in the FAIRness of their research data. Their aim is to ensure data that are Findable, Accessible, Interoperable, and Reusable (FAIR). Apart from presentations on the current MaRDI projects and selected keynote talks with speakers from the University of Stuttgart, Otto von Guericke University Magdeburg, Dassault Systèmes Deutschland GmbH, University of Cambridge, Durham University and the MPI for Biogeochemistry, the workshop left generous room for discussions.

The participants presented their work in progress, open problems, or reported on personal experiences on topics like knowledge graphs and ontologies, research software (engineering/interfaces/management), benchmarks, formal workflow descriptions, reproduction of numerical experiments, research data management.

| Organizing Committee

+ Research Groups

IMPD4Cat
FOR5538

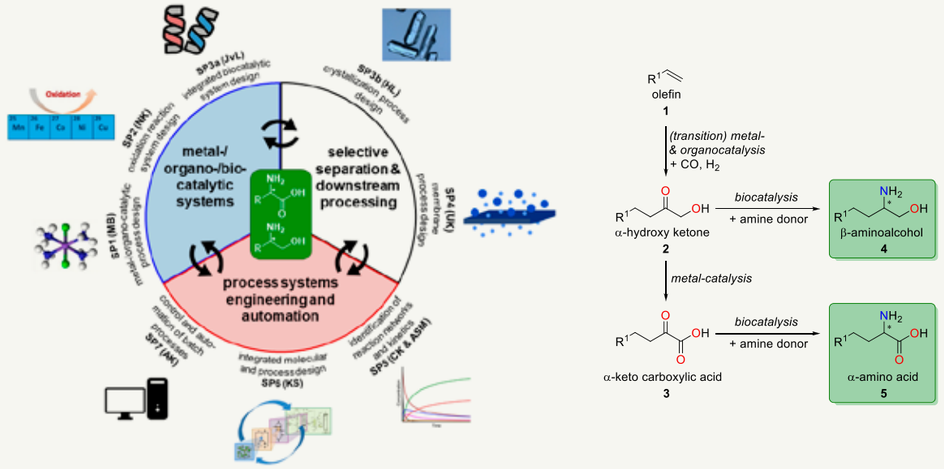


Figure 1:
Left: The research unit FOR 5538 is composed of seven subprojects (SP), grouped in three research areas. **Right:** Synthetic route for the preparation of valuable α-amino alcohols (4) and β-amino acids (5).

RESEARCH UNIT FOR 5538: MULTI-STEP CATALYTIC PRODUCTION SYSTEMS FOR FINE CHEMISTRY BY INTEGRATED MOLECULAR, MATERIAL AND PROCESS DESIGN (IMPD4CAT)

Green process engineering for a waste-free production of fine chemicals started in September 2023: Interdisciplinary research unit involving the MPI Magdeburg received 3.7 million euros for the development of sustainable chemical production processes.

Scientists of the Max Planck Institute in Magdeburg are working closely together with researchers at Otto von Guericke University Magdeburg, Potsdam University, Rostock University and the Leibniz Institute for Catalysis (LIKAT) in Rostock on the development of sustainable and resource-efficient chemical production processes for fine chemicals. Fine chemicals are the basis for the production of active pharmaceutical ingredients, cosmetics or detergent additives. The aim of the research unit, which was approved by the German Research Foundation (DFG) in August 2023, is to closely link experiments in miniaturized chemical plants (“mini-plants”) with computer-aided simulation and optimization in order to identify new process designs for a waste-free production.

Such new methodological approaches could also help to prevent future bottlenecks in the supply of medication in Germany. These bottlenecks have been caused by the fact that the production of important fine chemicals has largely been outsourced abroad in the past. If we want to manufacture pharmaceutically relevant substances in Germany and Europe again, we need a new generation of chemical production processes that are more cost-effective and environmentally friendly than before. This is precisely the central motivation of the research unit FOR 5538.

The research unit “Multistage Catalytic Production Systems for Fine Chemistry through Integrated Design of Molecules, Materials and Processes” aims at developing the foundations for new production systems that run stably, and in which all stages of the manufacturing process are optimally coordinated. The key idea is that all decisions to be taken regarding raw materials, catalysts, solvents, additives, separating materials, types of devices or operating conditions are integrated in a cross-scale design approach.

Up to now, process development has involved chemists first selecting the substances, solvents and catalysts involved, and then process engineers designing the technical process for carrying out the chemical synthesis and purifying the product. This sequential approach does not usually lead to the best result because the range of possible material-process combinations is severely limited. As a result, we see, for example, processes in which the chemical reaction runs very well, but the separation of the product is only possible with a high energy input. The research unit FOR 5538 therefore takes an approach that considers all the important variables in the process at the same time: the molecular variables of the substances involved and the process-related variables, such as the pressure and temperature of the process steps involved. We call this a simultaneous cross-scale design concept.

To this end, our scientists combine computer-aided modeling and optimization methods with experimental investigations in miniaturized chemical plants. The participating working groups initially set up the so-called miniplant modules individually and later connect them to an entire plant in Magdeburg. This enables the simulation of a complete production process, for example for the production of amino acids from olefins. Amino acids are important building blocks for pharmaceutical agents, among other things.

The task ahead of the research team is very complex because a large number of decision variables have to be taken into account at the same time. There are a multitude of interactions between these variables, some of which are unknown. To manage this complexity, our team wants to make systematic use of data-driven methods and machine learning for process design and process control. If we succeed in finding the best combination of catalysts, solvents, reaction conditions, apparatus types and operating modes in the huge search space of possible solutions, then it would be possible to realize chemical production processes that are not only economically attractive but also environmentally friendly.

In 2024, special experimental devices for studying specific reaction and separation process steps were set up and put into operation in Magdeburg, Rostock and Potsdam. At the same time, first computer-aided calculations were already carried out to determine the first possible candidates for catalysts, solvents and nanofiltration membranes. The researchers started to experimentally evaluate the molecules and materials that were predicted by means of computer simulations using the experimental devices. The aim is to identify an optimal combination of molecules, materials and process stages for selected pharmaceutically relevant target substances by the end of the first funding period in 2027.

More information on the Research Unit FOR 5538, can be found on the following website: https://impd4cat.de

Prof. Dr.-Ing. Kai Sundmacher

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Kai Sundmacher studied mechanical and process engineering at the University of Hannover and the TU Clausthal. After his doctorate, he worked as a postdoctoral researcher at the University of Newcastle, U.K., and completed his habilitation at TU Clausthal. In 1999, he was appointed to the professorship of Process Systems Engineering at Otto von Guericke University Magdeburg and since 2001, Kai Sundmacher has been Director at the Max Planck Institute in Magdeburg and Scientific Member of the Max Planck Society. Since 2023, Kai Sundmacher acts as spokesperson of the DFG-funded research unit FOR 5538 IMPD4Cat.

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BPE | BIOPROCESS ENGINEERING

+ Bioprocess engineer Sven Göbel takes a sample from a bioreactor for analyzing the virus yield. Read more on his research on oncolytic viruses for cancer therapy on the following pages.

PROF. DR.-ING. UDO REICHL | DIRECTOR

+ Bioprocess engineering involves the use of microorganisms in the production of bulk industrial products, food, and biopharmaceuticals. In addition, bioprocess engineering plays an important role in the production of biogas and biofuels, wastewater treatment, and solid waste treatment. From both an engineering and a biological perspective, the design and optimization of bioprocesses requires an integrated view of complex biological systems, a deep understanding of (bio) chemical reactions, specialized equipment, and modeling tools. A wide range of assays for process monitoring and a comprehensive set of analytical and "omics" technologies should be utilized.

In the context of biopharmaceutical production, the **Bioprocess Engineering group**, led by Professor Udo Reichl, investigates key aspects of the cell culture-based production of viral particles, viral vectors, and other biologicals. Virus production processes are currently experiencing a very strong increase in market share due to the emergence of new diseases and a steady rise in general demand. This was particularly true with regard to the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) pandemic. Currently, avian influenza, mpox, foot-and-mouth disease, and swine fever are challenging our health systems and economies. In addition, the growing use of viral vectors in gene therapy and promising options for viral therapy to cure certain types of cancers or autoimmune diseases require significant efforts.

The Bioprocessing Engineering group combines the expertise of five teams covering different aspects of biologics production, process analytics, and modeling. The **Upstream Processing team** (Apl. Prof. Yvonne Genzel) focuses on virus and viral vector production processes. The propagation of mainly enveloped viruses such as influenza virus, Zika virus, chimeric yellow fever virus, recombinant vesicular stomatitis virus, and modified vaccinia Ankara virus in adherent and suspension cell lines is characterized. Studies include the design and optimization of processes performed in stirred and orbital shaken bioreactors, hollow fiber-based systems, and disposable units. In addition, advanced cultivation strategies using online sensors and cell retention devices are being evaluated to intensify and streamline overall process development to improve readiness for viral diseases and the upcoming demand for viral therapies. Details of virus-host cell interactions are being studied by the **Molecular Biology team** (Dr.-Ing. Sascha Kupke) to identify bottlenecks in virus replication and to develop new strategies for antiviral treatment. Virus dynamics are investigated on the single cell and cell population level using a combination of classical virus quantification assays and state-of-the-art methods such as quantitative real-time PCR and imaging cytometry. The experimental data obtained by both groups are used by the **Mathematical Modeling team** (Prof. Udo Reichl) to elucidate the fundamentals of cell growth, metabolism, and virus replication. Multiscale models are established to simulate the spread of infections and the accumulation of viruses in bioreactors starting from the single cell level. With a focus on proteomics, glycomics, and glycoproteomics, the **Bio/Process Analytics team** (Dr. Erdmann Rapp) is developing and applying a comprehensive set of cutting-edge bioanalytical tools for the in-depth analysis of proteins and their posttranslational modifications. Finally, the **Synthetic Biotechnology team** (Dr. Thomas Rexer) is developing enzyme-based process platforms for efficient *in vitro* glycosylation of proteins and peptides and establishing technologies for the synthesis of nucleotide sugars and human milk oligosaccharides.

Over the past few years, the Upstream Processing team, together with many academic and industrial partners, has continued its efforts towards process intensification and process integration by optimizing perfusion strategies for high cell density cultures. New viral constructs have been added to the existing portfolio to cover a wider range of process options and to better handle the intrinsic variations due to the specificities of virus-host cell interactions. Including new sensors, the introduction of tangential flow depth filtration devices for virus harvesting, cell line screening for host selection, and design of experiment approaches involving high-throughput, automated micro-bioreactor systems have proven essential for increasing process yields. While the latter approaches have been used for many years in the production of cell-based recombinant proteins, the feasibility of screening approaches in virus production has been questionable and few groups have addressed the challenges involved.

A unique reverse genetics workflow to engineer and reconstitute new DIP constructs was developed by the Molecular Biology team. It enables the high-yield production of conventional defective interfering particles (cDIPs) and OP7 without the need to complement missing functions by adding an infectious wild-type virus. This eliminates the need for UV inactivation of DIP preparations and helps address safety concerns regarding the use of DIPs as a new and potent class of antivirals. In a collaboration with Prof. Dunja Bruder (Head of Infection Immunology Research Group, Institute of Medical Microbiology and Hospital Hygiene, OVGU, Magdeburg) and supported by a "Lighthouse Project" of the Max Planck Society (MPG), animal studies in mice were performed which showed very promising properties. In addition, a master cell and virus bank has been produced under good manufacturing practice (GMP) conditions by the Fraunhofer ITEM (Prof. Holger Ziehr and Dr. Claudius Seitz, Fraunhofer Institute for Toxicology and Experimental Medicine, Department of Pharmaceutical Biotechnology, Braunschweig) as a next step towards the clinical studies required for DIPs for human use. Also in 2024, a follow-up "Lighthouse Project" DIP-Vac "A novel class of mucosal broad-spectrum antivirals and live intranasal influenza vaccines – in-depth biological characterization and first steps towards clinical trials" was granted funding by the MPG. Validated preclinical data may encourage investors to license this technology and proceed with clinical trials.

Covered by a strong patent portfolio of the Synthetic Biotechnology team, the spin-off eversyn GmbH (https://www.eversyn.de/) was founded in early 2024 to commercialize its technology for the efficient and scalable production of activated sugars for the production of complex human milk oligosaccharides and for the tailor-made glycosylation of therapeutic proteins. Finally, the Bio/Process Analytics team successfully applied for a European grant in the highly competitive EIC Pathfinder Challenges program – MENTORING "Addressing malnutrition and metabolic health in non-communicable diseases through precision nutrition: impact in quality of life and prognosis of lung cancer patients."

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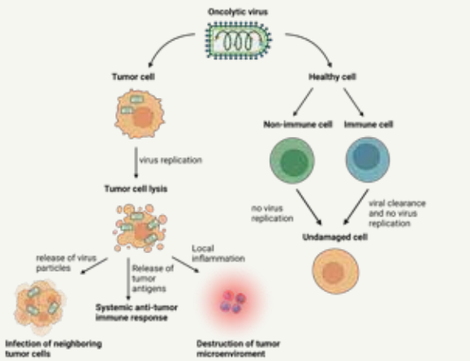

Figure 1: Mechanism of action of OVs in tumor cells. While OVs have the ability to infect both normal and tumor cells, the intrinsic dysfunctions in cancer cells confer a selective advantage for viral replication. In healthy cells (immune and non-immune cell types), OVs do not replicate due to the presence of antiviral type I interferon (IFN) signaling and other regulatory mechanisms. However, after infection of tumor cells, OVs can replicate, causing tumor cell lysis and the release of new viruses that can subsequently infect adjacent tumor cells. Secondary immune and antiviral responses are enhanced by the release of various signaling molecules. Figure adapted from[6]. Created with BioRender.com.

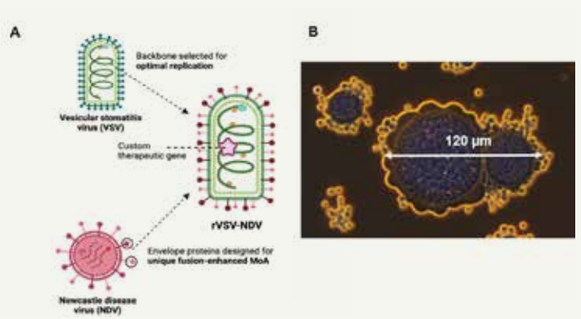

Figure 2:
Construction of the hybrid rVSV-NDV virus and syncytia formation of suspension cells used in perfusion culture. A) A full-length genome of recombinant vesicular stomatitis virus (rVSV) and a full-length Newcastle disease virus (rNDV/F3aa(L289A)) are combined to construct the chimeric rVSV-NDV virus. **B)** Syncytia formed after infection of BHK-21 cells in a 1 L bioreactor.[3]

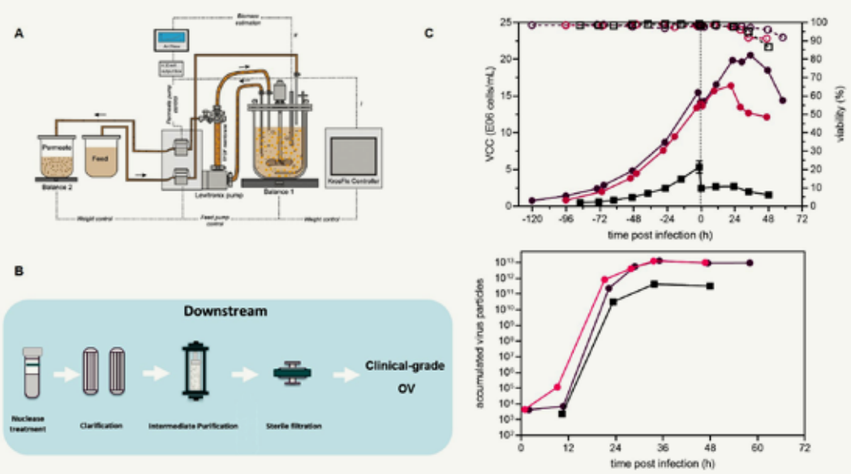

Figure 3: rVSV-NDV production in perfusion and batch mode. A) Schematic of a setup for cell retention in perfusion culture. **B)** Schematic of a GMP-compliant downstream purification process. **C)** Concentration (full symbol) and viability (empty symbol) of BHK-21 cells screened for rVSV-NDV production in perfusion mode (circles) and batch mode (squares).

Oncolytic Viruses: A New Approach to Cancer Therapy

Oncolytic viruses (OVs) are promising tools in the fight against cancer. They work using a dual mechanism: directly killing tumor cells while simultaneously activating the immune system to target the cancer (Figure 1). By expressing specific proteins, OVs can spread efficiently within tumors, causing infected cells to fuse into large structures called syncytia, where they rapidly die (Figure 2).

To achieve therapeutic effects, very high doses of viruses (up to 10^{11} infectious particles per injection) are required. Producing such quantities is challenging, as the host cells used to grow the viruses often die too quickly, limiting the yield.

Challenges in Manufacturing Oncolytic Viruses

Although significant progress has been made in the development of OVs, early research often focuses on designing viral constructs and testing their therapeutic potential, leaving production aspects underdeveloped until later stages. Many current manufacturing platforms rely on anchorage-dependent cell cultures, which have historically been used for vaccine production. However, these systems have limited scalability, yield, and only reach relatively low maximum cell concentrations. This renders them unsuitable for large-scale OV production.

Suspension cell lines offer a more scalable alternative because they can grow freely in bioreactors. However, few of these cell lines meet the stringent quality standards required for medical use (GMP). Additionally, the purification of viral harvests presents unique challenges. Oncolytic viruses are large and structurally complex, making them difficult to handle in traditional purification processes. For example, clarification steps to remove cell debris can damage the delicate virus particles, and the viruses' sensitivity to physical and chemical stress complicates subsequent downstream processing steps.

A Collaborative Solution

To overcome these hurdles, our project brought together five industrial and three academic partners to develop an integrated production process for a novel type of OV. This process includes:

1. Identification of suspension cell lines that grow rapidly and produce high virus yields.
2. Development of scalable batch and perfusion bioreactor systems for virus production.
3. Design of a downstream purification process based on anion exchange chromatography that meets medical manufacturing standards. An example of a perfusion culture system including a purification process is shown in Figure 3.

As a proof of concept, we focused on a hyper-fusogenic hybrid virus (rVSV-NDV) that combines features of vesicular stomatitis virus and Newcastle disease virus. In small-scale experiments, we optimized key cultivation parameters, such as temperature, pH, and the ratio of viruses to cells used for infection. These conditions were then scaled up to larger bioreactors, increasing virus yields 100-fold compared to traditional anchorage-dependent cell culture methods.[1,2]

To further improve efficiency, we tested advanced perfusion processes that maintain high cell concentrations by continuously removing waste while retaining cells in the bioreactor. By switching to innovative filtration systems, we were able to continuously remove the viruses without damaging their structure, despite the formation of large syncytia. Depending on the cell substrate, concentrations up to 15.0-45.9x10^6 cells/mL and rVSV-NDV yields of up to 7.1x10^9 infectious units/mL (>1,000-fold increase compared to baseline) were achieved without loss of oncolytic potency.[3,4] Cell-specific virus yields obtained in these high cell density cultivations were up to 2-fold higher than previous batch cultivations, resulting in space-time yield increases of >460% and comparable volumetric virus productivities.

In a final step, downstream processing (DSP) was optimized to ensure efficient purification and concentration of the virus. We developed a process involving DNA digestion, clarification, anion exchange chromatography, and sterile filtration that achieved an overall recovery rate of ~64%.[5] This high yield was critical to producing sufficient quantities of virus particles while maintaining their oncolytic potency and structural integrity.

Preparing for Clinical Trials

For the first time, we have successfully produced a fusogenic OV virus in therapeutic doses. This achievement lays the foundation for a Phase I clinical trial in cancer patients. In collaboration with academic partners in Portugal and Germany (iBET and Technical University of Munich), we have established a fully integrated production process that combines high-yield virus production with continuous purification steps. The next milestone is to transfer this process to a pre-GMP manufacturing facility in Portugal to prepare for large-scale production under clinical standards.

Dr.-Ing. Sven Göbel

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Author **Dr.-Ing. Sven Göbel**

Sven Göbel holds a Bachelor (B.Sc.) and Master's degree (M.Sc.) from the University of Stuttgart, Germany. After graduating, he transitioned to the Max Planck Institute in Magdeburg, Germany to complete a PhD in bioprocess engineering. During this time, his main focus was on the characterization, optimization, and intensification of processes to produce viral vectors, recombinant subunit vaccines, and oncolytic viruses in bioreactors, in cooperation with several academic and industrial partners. Currently, Sven works as a Post-Doc where he continues the development and scale-up of an integrated production processes for clinical-grade oncolytic virus production.

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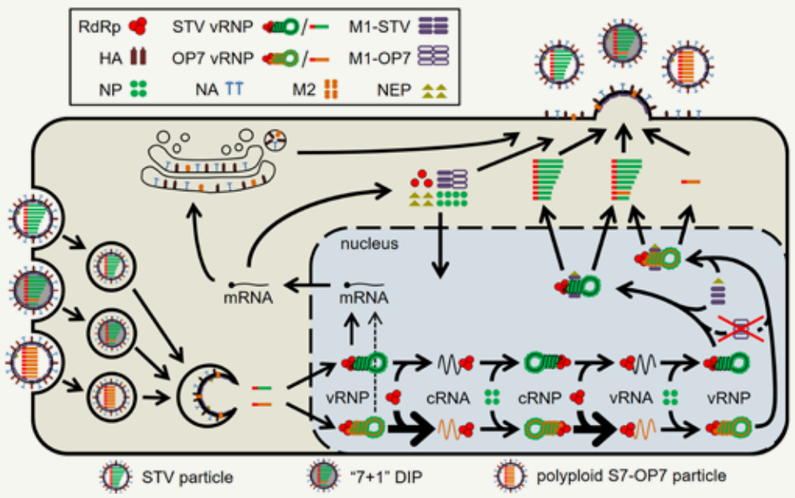
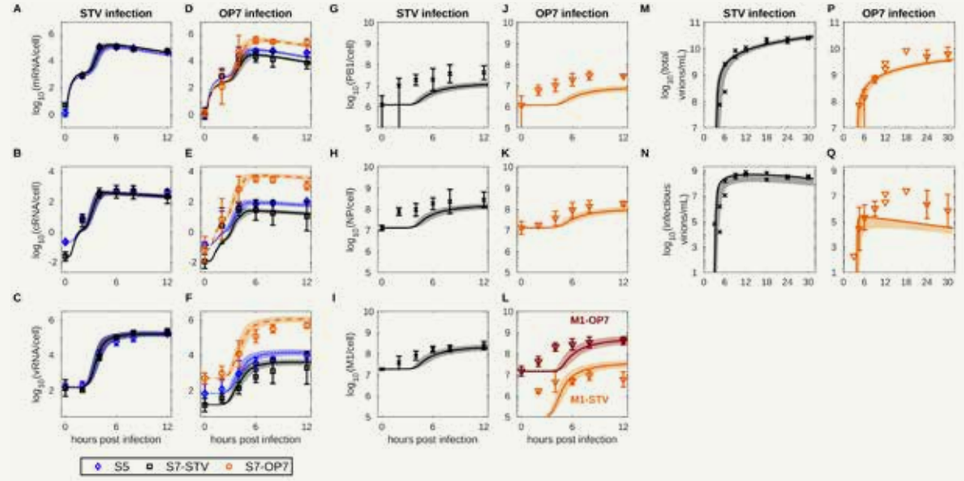


+ Figure 1:
Virus entry, nuclear import, viral RNA and protein synthesis, nuclear export, virion assembly and progeny virus particle release during OP7/STV co-infection.



+ Figure 2:
Simulations of the final OP7/STV co-infection model fitted to experimental data and 95% prediction bands. (A–F) Cell-specific viral RNAs, (G-L) cell-specific viral proteins and (M N, P-Q) extracellular virus titers for MDCK cells infected with STV seed or OP7 seed virus.

Modeling the Effects of Mutations in Defective Interfering Particles

+ Viral infections cause millions of deaths each year and pose significant global socio-economic challenges. Although vaccination is the preferred approach for disease prevention, antiviral therapy plays a critical role in the treatment of acute infections to save lives and reduce the spread of viruses. However, the efficacy of existing antivirals can be compromised by the emergence of resistant strains, such as those observed for influenza A virus (IAV). Therefore, the development of broad-spectrum and readily available antiviral agents is vital for pandemic preparedness. Recently, promising animal studies have been conducted with antivirals based on virus-derived defective interfering particles (DIPs).[1, 2]

DIPs are mutated, replication-incompetent virus particles that can inhibit their standard virus (STV) counterpart by depriving it of viral resources to enhance their own replication. In conventional IAV DIPs, this defect is caused by large internal deletions. Previous research has demonstrated the efficacy of IAV-derived DIPs against various viral species, such as influenza B virus, respiratory syncytial virus, and SARS-CoV-2, in both cell culture and animal studies, supporting their potential as broad-spectrum antiviral agents. OP7, a newly identified influenza DIP with 37 nucleotide changes in its segment 7 (S7) vRNA, has been shown to be more effective at suppressing STV replication than conventional DIPs.[1, 2, 3, 4] However, the effect of these mutations on OP7 replication and its mechanism of interference with the STV remained unclear.

To facilitate the identification of the impact of these mutations, we followed an interdisciplinary approach combining experimental and mathematical modeling techniques. As a first step, our Molecular Biology team studied the virus dynamics during OP7 replication. To this end, influenza STV infections and coinfections of OP7 and STV were performed in animal cell culture.[3] In these experiments, viral titers were determined by HA assay, the infection dynamics of viral RNAs were monitored by real-time reverse transcription qPCR, and viral protein levels were assessed by an innovative mass spectrometry-based method. These *in vitro* coinfection experiments showed that S7 of OP7 (S7-OP7) outcompetes all STV genome segments, including S7 of the STV (S7-STV), and accumulates to high levels in infected cells and progeny virions. Additionally, viral protein levels were reduced compared to a STV infection. M1 derived from S7-STV showed a one log decrease during coinfection while M1 derived from S7-OP7 (M1-OP7) accumulated to significantly higher levels than all other proteins.

Based on these experimental data and the previous work of our Mathematical Modeling team, we developed a model to simulate the coinfection of OP7 and STV (Figure 1).[5] Initially, we calibrated this model to the STV infection dynamics to obtain a baseline parameter set. However, this model could not describe the dynamics during a coinfection of OP7 and STV. Therefore, we tested several hypotheses regarding the effect of the mutations in the genome sequence of OP7 RNA on its replication. The main properties we investigated were: (1) the replication of OP7 viral genomic RNA (vRNA), (2) the functionality of the protein M1-OP7, and (3) the transcription of OP7 mRNA.

First, we focused on the replication of S7-OP7 vRNA because two of the mutations found in the S7 OP7 genome sequence (G3A/C8U) have been described to carry a superpromoter, which induces higher vRNA synthesis. By considering an increased replication for S7-OP7 vRNA, we were able to induce the large differences between the levels of the different vRNAs (Figure 2F). Second, we tested whether a loss of function for M1-OP7 could improve the description of the experimental data. M1 is a multi-functional protein that (1) binds to viral genomes in the nucleus to initiate their export to the cytoplasm and (2) is involved in the formation of progeny virions. After disabling the binding of M1-OP7 to viral genomes in the model, the resulting simulations could closely describe the trajectories of viral RNAs in Figure 2. Implementing these two changes still led to an overprediction of S7-OP7 mRNA, so we hypothesized that its transcription might be reduced due to the mutations. This was later confirmed experimentally, supporting the predictive power of the model.

Overall, our model simulations suggest that the mutations in the genome sequence of OP7 induce a strongly increased rate of vRNA replication and a significant decrease in S7 OP7 mRNA transcription. Furthermore, we propose that the M1 protein produced from S7-OP7 mRNA is likely defective and unable to bind to viral genomes in the nucleus.

In summary, we have developed a coinfection model for STV and OP7 that closely describes the virus dynamics of the mutated genomic S7 OP7. This model allowed us to infer the effects of the mutations within its sequence. It can be further extended to simulate *in vivo* infections in tissues or be modulated with a description of the innate immune response, which is considered crucial for the antiviral action of DIPs. Ultimately, this model is finely tuned to predict IAV infections subject to OP7 interference, providing a strong basis for evaluating strategies to prevent or treat viral infections using OP7.

| Dr.-Ing. Daniel Rüdiger

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Daniel Rüdiger studied Biosystems Engineering at Otto von Guericke University in Magdeburg. In 2015, he received his degree (Dipl.-Ing.) and joined the Bioprocess Engineering Group at the Max Planck Institute. There, he worked on the mathematical modeling of infectious diseases. He finished his Ph.D. in 2022 and currently works as a postdoctoral researcher in the BPE group focusing on modeling approaches to support the establishment of new antiviral agents.

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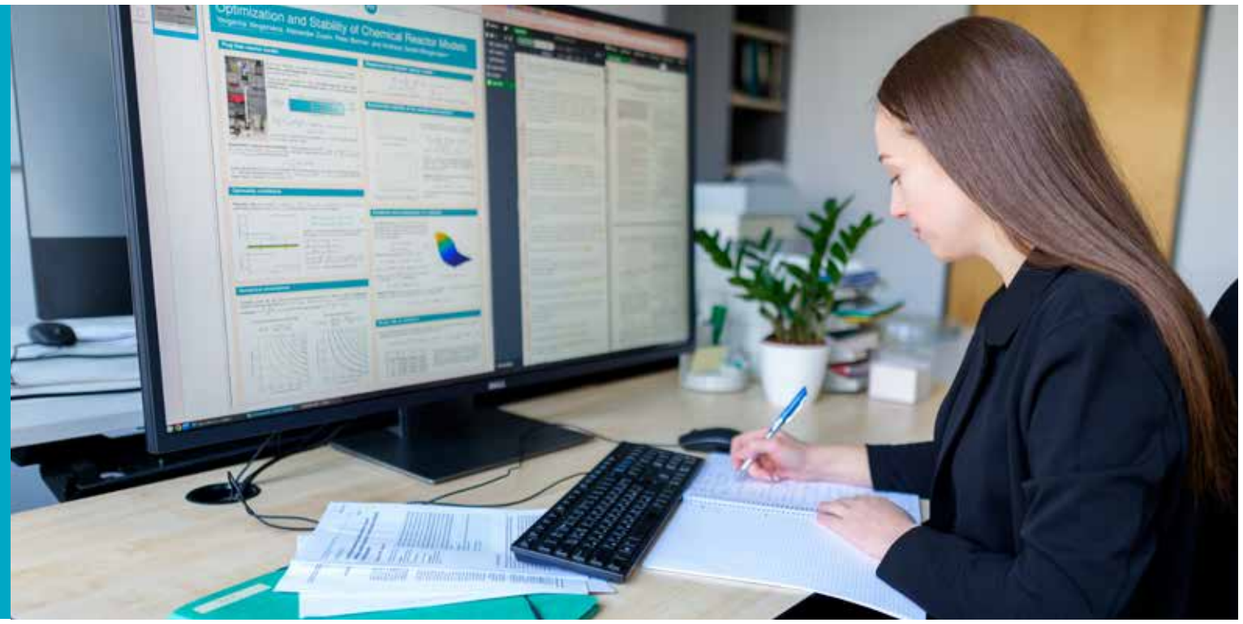

+ Yevgeniia Yevgenieva, mathematician in the CSC group, working at her desk on analyzing and optimizing chemical reactor models. Read more about her research results on the following pages.

PROF. DR. PETER BENNER | DIRECTOR

+ The CSC group's research key areas are modeling, simulation, optimization, control, and inference of time-dependent problems from the sciences and engineering. CSC researchers employ mathematical ideas and concepts to develop new computational methods for complex technical systems such as those investigated, for example, in the MPI's engineering departments. Specifically, we consider efficient simulation – enabling this via reduced-order models – as well as optimal and feedback control of dynamical systems, i.e. of mathematical models described by systems of differential equations. In recent years, we have strengthened our efforts on including machine and deep learning into our research portfolio, in particular for the inference of nonlinear system models from data. Our application areas range from chemical and biotechnological processes and electro-magnetic devices to energy networks and materials discovery. Workflows in the CSC group frequently incorporate advanced programming strategies for modern computer architectures, as well as energy-awareness in the algorithm design. We emphasize the **FAIR** principles of **F**indable, **A**ccessible, **I**nteroperable, and **R**eusable research data and software by engaging in the consortia MaRDI (for Mathematics) and NFDI4Cat (for Digital Catalysis) of the German National Research Data Infrastructure (NFDI) as well as in several efforts for sustainable research software engineering.

Our infrastructure is diverse, spanning multiple hardware platforms. At the core is the Linux cluster, *mechthild* [1], and we maintain several GPU-powered workstations. *mechthild* was updated in 2024 to boost its capabilities for training cutting-edge machine learning models using state-of-the-art GPU nodes.

CSC Teams

The CSC structure had comprised seven teams since 2021: **Model Order Reduction (MOR)** (headed by L. Feng) dealing with mathematical and machine learning methods to algorithmically reduce the complexity of mathematical models in order to accelerate their simulation, facilitate their optimization, enable control design, and to quantify uncertainties. The **Computer Aided Control System Design (CACSD)** team (led by J. Heiland until he moved to TU Ilmenau in April 2024; since then by A. Zuyev) considers analytical and computational methods for optimal and feedback control of dynamical systems. The **Simulation of Energy Networks (SES)** team (S. Grundel) focuses on the modeling and numerical simulation of energy transportation networks, including in particular hydrogen. Efficient **Numerical Linear and Multilinear Algebra (NLMA)** techniques percolate many aspects of CSC research. The NLMA team (P. Benner) deals with eigenvalue problems, preconditioning and tensor techniques, as well as the numerical solution of matrix equations. **Data, Infrastructure, Software & Computing (DISC)**, led by J. Saak, is concerned with the design of numerical algorithms and their efficient implementation on cutting-edge computer hardware. Moreover, the teams **Physics-Enhanced Machine Learning (PML)**, led by P. K. Goyal until October 2023, and **Structured Dynamical Systems (SDS)**, led by I. Pontes Duff until October 2024, dealt with several aspects of scientific machine learning and system identification. This area is currently re-organized, adapting to the fast development of AI methods for the sciences and engineering applications.

Highlights and Developments in 2023/24

The CSC group engaged in organizing numerous international scientific events, including the 10th Workshop on Matrix Equations and Tensor Techniques (METT-X) held in Aachen in 2023. A major effort went into organizing the 94th GAMM Annual Meeting in Magdeburg (see the detailed report on page 17). P. Benner also serves as the co-chair of the MPG committee on research data infrastructure. In this capacity, he organized the first MPG-wide workshop on this topic at Ringberg Castle (see page 14).

Notable awards were given to S. Monem (winner of the ACM Student Research Competition (SRC) at ACM SIGGRAPH 2023, Graduate Division) and S. Chellappa (best PhD dissertation, Faculty of Mathematics, OVGU). P. Benner was elected as spokesperson of the DFG Review Panel "Mathematics" for the period 2024-2028.

The following pages present a selection of our most notable research findings from 2023/24. In addition, the development of strategies for learning dynamical system models from data, in particular from noisy measurements, was recognized internationally through several publications in leading scientific journals and numerous invitations for CSC group members to speak at top-tier international conferences. We could also deploy novel surrogate modeling techniques for use in Digital Twins in smart process systems engineering, which will also serve as a major research direction in the coming years.

[1] Named after "Mechthild von Magdeburg" (c.1207- c.1282/94), a Beguine and the first mystic to write in German.

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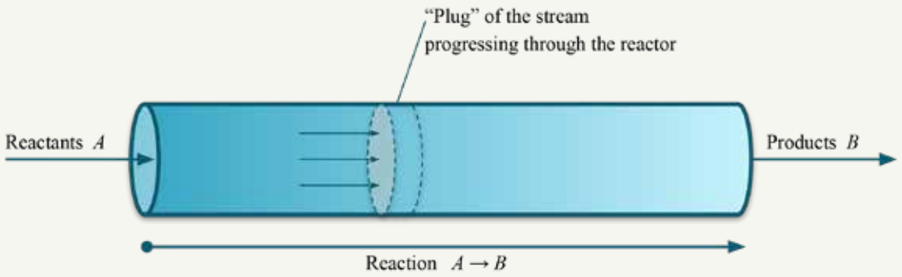

Figure 1:
The scheme illustrates the working of a plug flow reactor (PFR), where reactants A flow into the reactor, undergo a chemical reaction *A* —> *B*, and exit as products *B*. The color gradient represents the decreasing concentration of reactants and increasing concentration of products along the reactor's length.

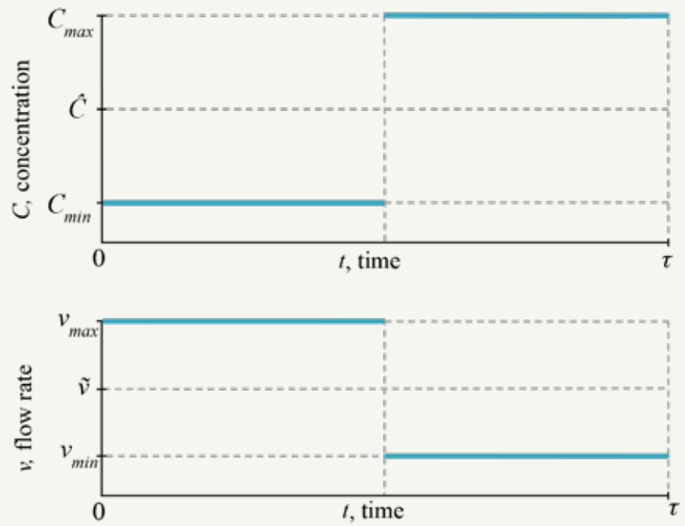

Figure 2: Illustration of the optimal bang-bang strategy for the plug flow reactor. The control inputs, inlet concentration *C(t)* and flow rate *v(t)* alternate between their extreme values over time. This switching pattern maximizes the product yield by operating the reactor at maximal concentration with a minimal flow rate and vice versa.

Optimal Control Strategy for a Plug Flow Reactor

Introduction

Optimal control of chemical reactions plays a pivotal role in enhancing efficiency and improving product quality across industrial processes. This article presents findings from our recent research[1], where we focused on the Plug Flow Reactor (PFR) model and solved the corresponding optimal control problem.

A Plug Flow Reactor (PFR) is a type of tubular chemical reactor where reactants move through the tube in a streamlined flow without mixing across the tube's cross-section, similar to the flow of liquid through a pipe. As the reactants progress from the inlet to the outlet, chemical reactions occur along the reactor's length, transforming them into desired products (see Fig. 1). Widely utilized across industries such as petrochemicals and pharmaceuticals, PFRs play a critical role in processes like polymerization, oxidation, catalytic cracking, ammonia synthesis, and oil cracking. Moreover, PFRs are increasingly employed in bioenergy production, such as biodiesel manufacturing, where their specific construction provides significant advantages. Highly valued for their cost-effectiveness, PFRs demand lower initial investments and operational costs compared to alternative designs, making them practical and environmentally friendly solutions for achieving modern sustainability goals.

The control of PFRs is a critical area of chemical engineering, aimed at optimizing operational parameters to achieve objectives such as maximizing yield and purity, enhancing selectivity, or improving energy efficiency. Our research aimed to identify the optimal strategy to maximize the product yield of a reaction occurring in a PFR. The project required expertise in both mathematical control theory and chemical engineering, fostering interdisciplinary collaboration between two institute groups: Computational Methods in Systems and Control Theory (CSC) and Physical and Chemical Foundations of Process Engineering (PCF).

The Optimal Control Problem

We studied the isoperimetric optimal control problem for the PFR model, which involves maximizing the product yield while controlling the flow rate and inlet concentration of the reactant under a fixed total reactant amount. A straightforward approach might use a stationary strategy, where the reactant is fed into the reactor with a constant concentration at a constant flow rate throughout the reaction. However, it has been proven that the periodic operation of chemical reactors can (sometimes) significantly enhance reaction performance. A commonly used periodic control strategy in chemical engineering is sinusoidal-like control, which delivers much better results compared to stationary operation. But is it optimal? To answer this, we aimed to find an optimal periodic control strategy.

The PFR model is described by nonlinear partial differential equations (PDEs), accounting not only for the time-dependent dynamics of the reactant concentration but also its spatial distribution along the reactor length. This makes the problem challenging and highly relevant within control theory and applied mathematics. Nonlinear PDE control is a broad and impactful field, with many sophisticated methods developed to address such problems.

For our analysis, we employed a method based on explicit solutions. Using the method of characteristics, we derived the exact solutions to the governing equations, enabling us to represent the cost functional analytically. Applying calculus of variations approaches, we determined the optimal control strategies.

Our analysis revealed that the optimal strategy is a switching (or so-called bang-bang) control strategy, where control variables alternate between their upper and lower limits. Furthermore, for maximum efficiency, the reactor should alternate between operating at maximal reactant concentration with minimal flow rate and minimal concentration with maximal flow rate. This switching strategy is illustrated in Fig. 2.

Simulation and Comparison

We simulated the switching control strategy and compared its performance to both stationary and sinusoidal periodic operations. The simulations showed that, with the chosen parameters, the bang-bang control strategy could achieve up to 25% higher performance compared to stationary operation. These results demonstrate the potential of advanced control strategies to significantly enhance reactor efficiency.

Outlook

Our research demonstrates the effectiveness of advanced control strategies, particularly the bang-bang control, for optimizing chemical processes in Plug Flow Reactors. By applying advanced control theory techniques for nonlinear PDEs, we determined an optimal control strategy that achieves significant performance improvements.

Future research will focus on extending these methods to more complex reactor models that incorporate temperature effects. We also aim to explore real-world implementation scenarios to bridge the gap between theoretical results and industrial applications, further advancing sustainability goals in chemical engineering.

Dr. Yevgeniia Yevgenieva

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Author **Dr. Yevgeniia Yevgenieva**

Yevgeniia Yevgenieva earned her Master's degree in Mathematics from Donetsk National University, Ukraine, in 2012. She completed her Ph.D. in Differential Equations in 2020 at the Institute of Mathematics and Mechanics of the National Academy of Sciences of Ukraine, where she subsequently worked as a research fellow. In 2022, Yevgeniia joined the CSC Research Group at the Max Planck Institute for Dynamics of Complex Technical Systems as a postdoctoral researcher. Her research focuses on the optimal control and stability of partial differential equations.

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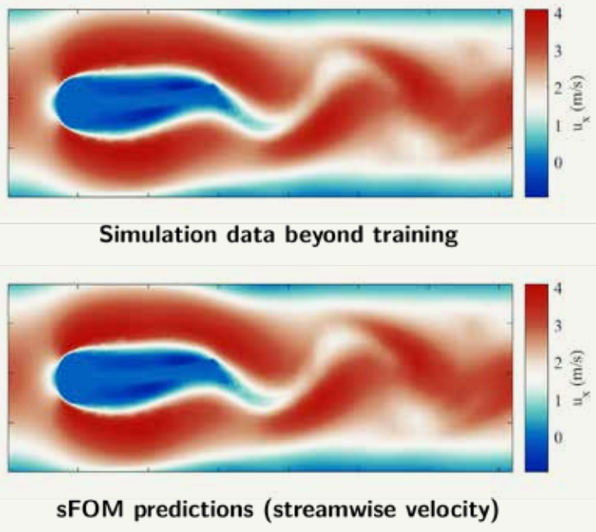

Figure 1:
Predictions on the coupled solid-fluid velocity field of the incompressible flow around a cylinder with a deformable "tail" (known as the Hron-Turek benchmark) via the inference of sparse operators at the full-order level.

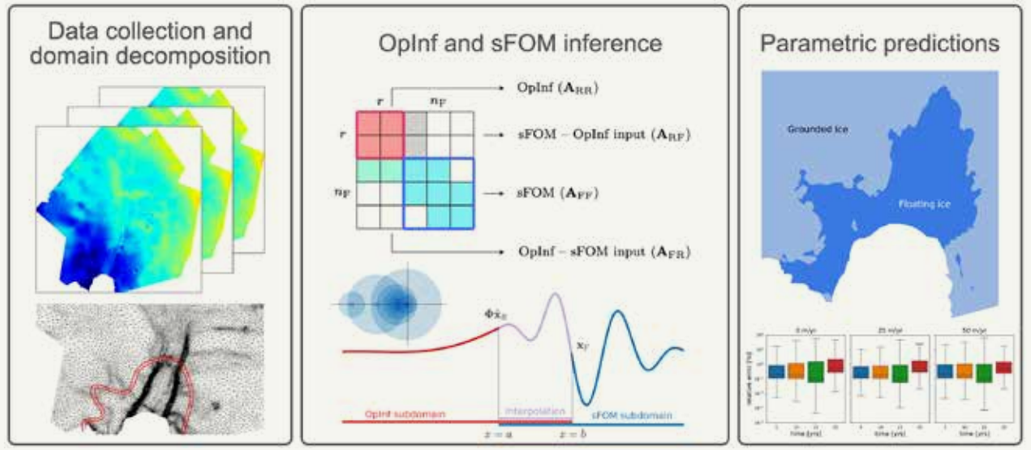

Figure 2:
Schematic of the domain-decomposition-based, physics-informed data-driven modeling framework in [3], with application to parametric predictions on the Pine Island Glacier ice thickness dynamics.

Leveraging Physics in Data-Driven Fluid Dynamics and FSI

Introduction

Data-driven modeling for dynamical systems refers to the derivation of mathematical models for dynamical systems using measurement data. Employing tools from linear algebra and statistics, such models can be cheap but trustworthy surrogates and can thus significantly reduce the computational cost of numerical simulations (or experimental campaigns) for demanding applications. Data-driven models are especially valuable in cases where the underlying, first-principle model that generated the data is not known or not accessible.

Systems in physics and engineering obey commonly accepted laws and principles. Therefore, the research field of physics-informed data-driven modeling aims to establish connections between first-principles and data-driven modeling by leveraging a priori knowledge of the physical properties of a system. Encoding this knowledge into data-driven methods and algorithms allows for more robust and accurate predictions on the dynamics of physics and engineering systems. The CSC Group is actively involved in shaping this novel, growing research field that strongly overlaps with the broader topic of Scientific Machine Learning.

Applications in fluid dynamics and fluid-structure interaction (FSI)

Target applications in my research come from the fields of incompressible fluid dynamics and fluid-structure interaction (FSI). Incompressible fluid dynamics considers the fluid motion under the assumption of constant fluid density, which results in an elegant mathematical formulation of the governing, Navier-Stokes equations. Incompressible fluid dynamics exhibit a wide range of dynamical phenomena which are of high practical interest to mechanical, aeronautical and process engineers. On the other hand, fluid-structure interaction considers the coupled motion of a fluid and a deformable solid. Such dynamical interactions arise under different conditions in many technological and physical systems, including wind turbines, blood vessels and aircraft.

The high interest in the optimization, control and engineering design of such systems drives the demand for compact, computationally efficient mathematical models that can accurately predict their dynamics. However, their numerical simulation is performed by resource-intensive computational fluid dynamics (CFD) finite element solvers, often hindering the efficient performance of many-query tasks. Physics-informed data-driven models can comprise fast, robust surrogates of computationally demanding CFD and FSI solvers that remain faithful to the system underlying physics, and can thus be integrated to real-time simulation, control and digital twin design.

We develop such models and test their capabilities on high-dimensional benchmark test cases and realistic applications with several thousand degrees of freedom. Such applications include the incompressible flow over a cylinder and around an elastic object (Figure 1) and the ice thickness dynamics of the Pine Island Glacier in Antarctica (Figure 2). Such test cases provide valuable insight into the capabilities and limitations of our methods.

Advances in physics-informed data-driven methods

In the last decade, the CSC group has been active in pushing the boundaries of physics-informed data-driven modeling in close collaboration with other world-leading research groups. Motivated by engineering problems, many of which are found in the aforementioned research fields, we are developing inference methods on both the full-order level, by exploiting the adjacency-based sparsity of discretized operators [1, 2, 3], and on the reduced-order level, in cases where the system dynamics evolve in a low-dimensional space [3, 4].

On both ends, we employ a physics-informed structure for the data-driven models and propose novel methodologies for the mathematical formulation of physical properties and their incorporation into the inference of models from data. Some of our more recent results address the problem of encoding aspects of dynamical stability to the inference task [3, 4] as well as the non-intrusive modeling for systems with spatially localized features, in collaboration with the Willcox Research Group at the Oden Institute of the University of Texas at Austin [3]. The developed methodologies aim to enhance the robustness of data-driven models used for engineering design and digital twins [5].

Leonidas Gkimisis

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Author **Leonidas Gkimisis**

Leonidas K. Gkimisis graduated in 2019 from the National Technical University of Athens with an M.Sc. in Mechanical Engineering. In 2021, he completed a research Masters in Fluid Dynamics at the Aeronautics & Aerospace Department of the von Karman Institute in Rhode-Saint-Genèse, Belgium. In the same year, he joined the CSC group at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg as a PhD student. He works on developing methods for physics-informed, non-intrusive modeling in applications of fluid dynamics and fluid-structure interactions.

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PCF | PHYSICAL AND CHEMICAL FOUNDATIONS OF PROCESS ENGINEERING

+ Chemical engineer Steffi Wünsche (left) and chemist Laura Lamkowski (right) are closely working together on the characterization of curcuminoid samples in the lab for Powder X-ray diffraction. Steffi prepares the samples so that Laura can place them into the diffractometer.

PROF. DR.-ING. ANDREAS SEIDEL-MORGENSTERN |
DIRECTOR

+ In 2023 and 2024, the PCF group contributed to the important field of providing enantiopure substances needed in the pharmaceutical industry. We developed dedicated crystallization-based and chromatographic processes. Significant progress has been achieved in demonstrating the potential of applying a conically shaped fluidized bed crystallizer in a continuous operation. To also exploit the commonly unwanted counter-enantiomers, efficient enzymatic racemization and recycling steps have been successfully incorporated (see pages 36-37).

Members of the group continued our research to develop strategies to isolate and purify valuable components from renewable resources. Efforts were made to improve the efficiency of extracting valuable natural products from plants. An effective way was developed to continuously extract the key ingredient of potent anti-malaria drugs from the plant *Artemisia annua* L using a screw-type extractor. To allow for rapid process design, a short-cut model was established and validated. We also studied crystallization and chromatography based isolation methods to provide certain ingredients of saffron (extracted from *Crocus sativus*) and curcumin (extracted from *Curcuma longa*, see pages 38-39).

Major efforts were undertaken to isolate and valorize lignin from black liquor originating from wood processing. In contrast to depolymerization of the large lignin molecules to synthesize small aromatic bulk chemicals, we contributed to the development of sequential precipitation methods capable of generating well-defined fractions of low and high molecular weight lignin. These fractions can be applied in various ways, for example as a substitute for fossil resources in the materials sector.

We also considered applying periodic operation principles to improve the performance of separation processes. In a project supported by the German Research Foundation (DFG), a new type of continuously operated chromatography separation process was studied using multi-column arrangements. In order to isolate a single target component out of a complex mixture, periodic shifts of the feeding positions were analyzed, modelled and implemented. The potential of several promising process configurations could be demonstrated experimentally.

The PCF group studied theoretically and experimentally the potential of a forced dynamic operation to improve the way reactions are carried out. The inlets of reactors are exposed to periodic modulations of feed concentrations and flow rates. This concept was investigated in cooperation with the groups of Achim Kienle (OVGU and MPI) and Daliborka Nikolic (University of Belgrade) and supported by the DFG (pages 48-49). As a relevant example, we evaluated the potential of forced changes of the ratio of carbon dioxide (available in waste streams and in the air), carbon monoxide and green hydrogen in gas streams which enter a reactor filled with a catalyst for the production of methanol. Applying suitable forcing frequencies and amplitudes, the applicability of this new regime could be demonstrated successfully. An observed gradual decrease of the catalyst activity is still one of the obstacles for industrial application and gives room for further research.

In another project, a novel carbon-negative process for the production of soda ash was studied (supported by the German Federal Ministry of Education and Research, BMBF). Essential features are the exploitation of carbon dioxide as carbonate source, which can be captured from air or exhaust gas streams, and a direct coupling with crystallization of sodium carbonate hydrate phases.

In the period covered by this report, the PCF group finalized nine PhD projects. After the restrictions caused by the coronavirus pandemic were lifted, our scientists were once again able to attend numerous national and international meetings in 2023 and 2024 to present their results. One highlight was the active participation in the 5th Indo-German Workshop “Advances in Materials, Reactions and Separation Processes” at the IIT Kharagpur in India. This successful workshop series was initiated in 2008 by the IIT Chennai and the MPI Magdeburg.

Due to the retirement of the head of the PCF group in August 2024, an intensive search was performed to identify a successor. We expect that the currently vacant position will be filled in the near future. The change in leadership will bring new, exciting research activities into the MPI. The successful activities in the field of crystallization will be continued under the supervision of Heike Lorenz.

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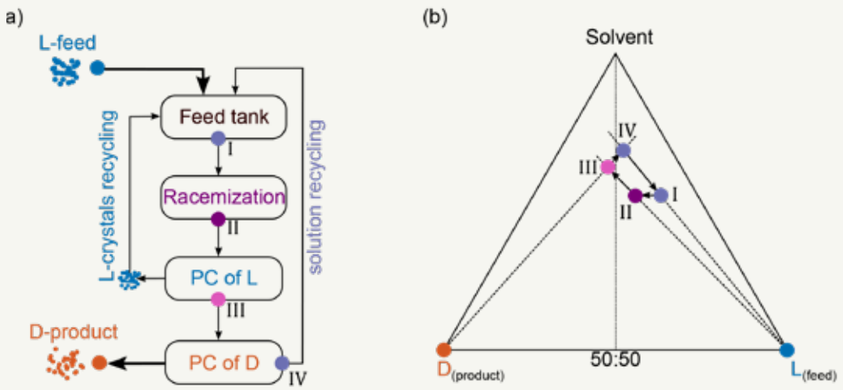

Figure 1:
Process scheme for continuous chiral inversion (a) and respective process trajectory within the ternary phase diagram (b).

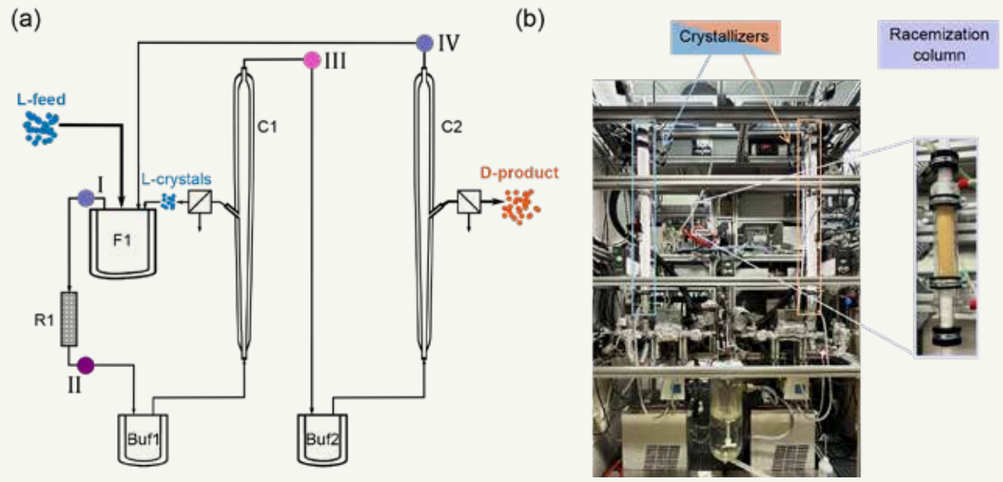

Figure 2:
Simplified flow chart of the coupled process (a) and experimental pilot plant setup with the crystallizers and the racemization column filled with immobilized racemase indicated (b).

Continuous Chiral Inversion in a Crystallization-Racemization Process

The production of enantiopure substances is increasingly essential in the pharmaceutical, fine chemical, and life science industries. In many chiral drugs, only one enantiomer provides the desired physiological effect, while the other is often inactive or potentially harmful. Regulatory authorities require chiral drugs to be administered in optically pure form. However, due to their chemical and physical similarities, producing single enantiomers remains technically challenging and cost-intensive.

In the absence of an economical asymmetric synthesis, a common strategy involves synthesizing a racemic 50:50 mixture followed by a resolution process. Since only one enantiomer is typically required, the yield is inherently limited to 50%. This limitation can be overcome by combining resolution with racemization.

Researchers at the Max Planck Institute Magdeburg are investigating chiral resolution processes, crystallization and chromatography based, as well as their coupling with racemization reactions. Preferential Crystallization (PC) enables the selective crystallization of one enantiomer from a racemic solution. It is a kinetically driven separation process that exploits the difference between the crystal growth rate of homochiral seed crystals and the primary nucleation of their chiral antipode [1]. Enzymatically catalyzed racemization interconverts enantiomers, establishing equilibrium at racemic composition. It exhibits high racemization rates under mild process conditions without the use of harmful substances. However, coupling these processes remains challenging due to the narrow operational window of PC, which requires conditions close to racemic composition.

A recently developed process coupling [2] enables the continuous production of a pure enantiomer from its inexpensive homochiral antipode feedstock. This concept is applicable, for example, to L-amino acids. The process scheme and trajectory are shown in Figure 1. In the racemization unit (I→II), an immobilized amino acid racemase (AAR) partially converts the L-enantiomer-enriched feed solution towards racemic composition. Afterwards, first, the undesired L-enantiomer is preferentially crystallized (II→III) and recycled by reintroducing the crystals into the feed tank. After depletion of the liquid phase in L-enantiomer, the mother liquor becomes enriched with D-enantiomer (point III). Next, the desired D-enantiomer is preferentially crystallized (III→IV). The L-enantiomer-enriched mother liquor (point IV) is returned to the feed tank and recycled. Product crystals are withdrawn from the outlet in the middle of the crystallizer. Due to the two-stage PC, this coupled process allows for a robust coupling of the resolution and racemization step even for low catalyst amounts while integrating waste recycling.

For experimental demonstration, D-/L-asparagine monohydrate (D-/L-Asn·H_2O) in water was selected as a model system. The pilot plant (Figure 2) employs a fixed-bed reactor filled with AAR (EC 5.1.1.10) from Pseudomonas putida KT2440 as an enzymatic catalyst (racemization column). Immobilization of AAR enhances robustness and enables continuous operation in a fixed-bed reactor. The two crystallization steps are performed in fluidized bed crystallizers (FBC). The upward flow of the supersaturated solution through the conical shaped FBCs enables size classification: larger crystals settle into a seeding bypass, where they are crushed and recycled to ensure a continuous supply of homochiral seeds. Smaller crystals exit with the top flow, redissolve in the mother liquor, and return to the feed tank, enhancing robustness against primary nucleation.

Using a further developed process model [3], we conducted simulation studies to determine optimal process conditions and design an experimental demonstration. A successful validation of the proposed configuration was performed in a pilot plant (Figure 2, b). We demonstrated the continuous chiral inversion process at pilot scale, achieving a productivity of 25 g/L/h of valuable crystalline D-Asn·H_2O product with >99% purity [2]. Future research will focus on applying this process to industrially relevant chiral systems for the production of high-value enantiopure substances.

Karina Oliynyk, Jonathan Gänsch

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Karina Oliynyk received her Master's degree in Chemical Engineering from Otto von Guericke University, Magdeburg, in 2022. She received a sponsorship award from the Association of German Engineers (VDI) for her outstanding Master's thesis. In the same year, she joined the PCF group at the MPI as a Ph.D. student. In her work, she focuses on the use of innovative selective crystallization processes for the continuous production of valuable products.

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Jonathan Gänsch received his Master's degree in Process Engineering from Otto von Guericke University, Magdeburg, in 2018. He was named the top graduate of his class. Since 2018, he has been a Ph.D. student at the Max Planck Institute, where he has investigated a promising but complex process concept for continuous chiral separation, namely the enantioselective fluidized bed crystallization. Currently, he is finalizing his dissertation.

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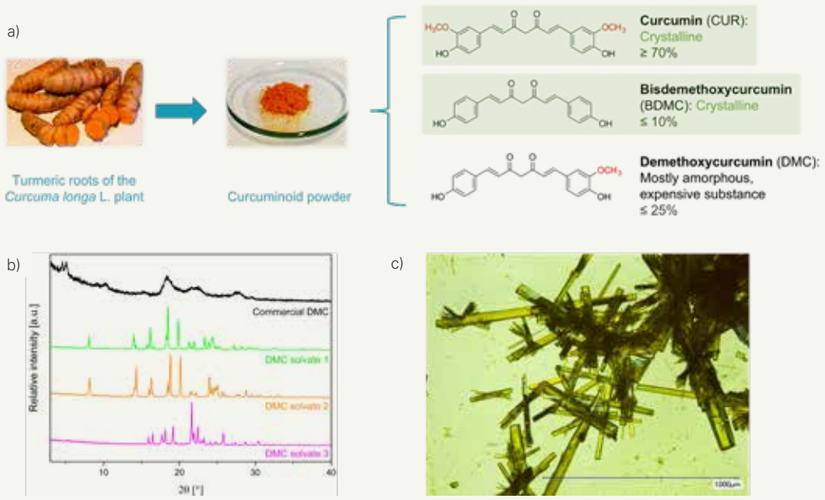
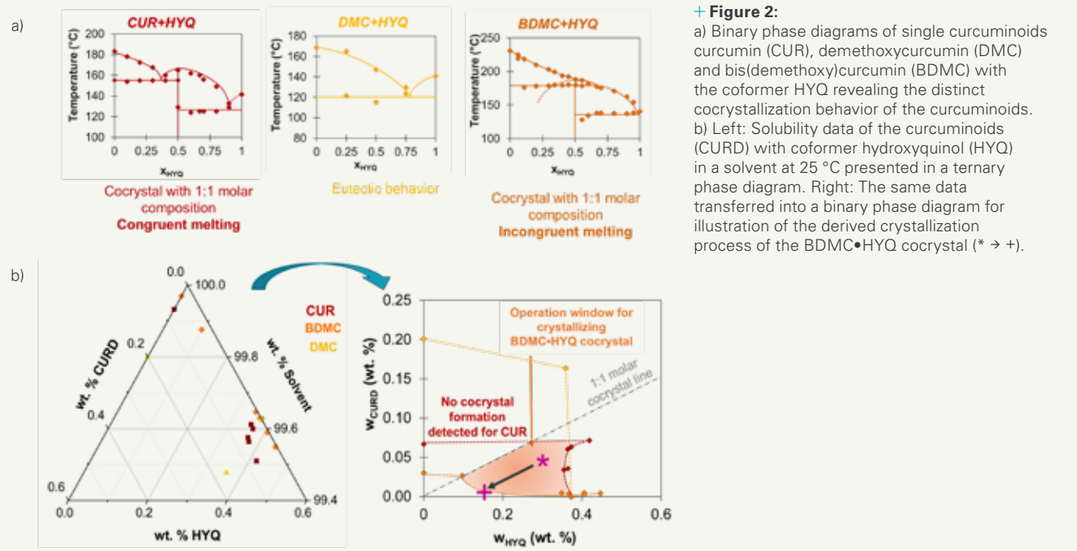


+ Figure 1:
a) Scheme showing the turmeric roots, which are processed to a powder. It contains three curcuminoids that have similar molecular structures: curcumin (CUR, ≥ 70 %), bis(demethoxy) curcumin (BDMC, ≤ 10 %), and demethoxycurcumin (DMC, ≤ 25 %). b) Diffractogram of commercial DMC and three synthesized DMC solvates. c) Optical microscopy image of the crystalline DMC solvate 1.



+ Figure 2:
a) Binary phase diagrams of single curcuminoids curcumin (CUR), demethoxycurcumin (DMC) and bis(demethoxy)curcumin (BDMC) with the coformer HYQ revealing the distinct cocrystallization behavior of the curcuminoids. b) Left: Solubility data of the curcuminoids (CURD) with coformer hydroxyquinol (HYQ) in a solvent at 25 °C presented in a ternary phase diagram. Right: The same data transferred into a binary phase diagram for illustration of the derived crystallization process of the BDMC•HYQ cocrystal (* → +).

Purification of Valuable Compounds from Plant-based Extracts

+ Natural products from plants serve as a rich source of valuable substances used in pharmaceutical and other life science industries, such as food additives, pigments and nutraceuticals. Prominent examples investigated in our research group are the antimalarial artemisinin,[1] the hemostatic rutin, and three curcuminoids extracted as a ternary mixture, namely: curcumin (CUR), demethoxycurcumin (DMC) and bis(demethoxy)curcumin (BDMC). The structurally similar curcuminoids only differ in the number of their methoxy groups and are the main bioactive constituents in turmeric roots (**Fig. 1a**).

Turmeric (*Curcuma longa* L.), native to South and Southeast Asia, has been used as a spice and in traditional medicine for centuries, for example in treating wounds or ailments such as colds and arthritic disorders. Several studies reveal different bioactivities for the individual curcuminoids, including varying anti-cancer and anti-Alzheimer effects. This is raising the need to deliver each of the curcuminoids in pure form and sufficient amounts. However, the isolation of the minor components DMC and BDMC remains challenging due to their structural resemblance and similar properties. Our research aims to purify the curcuminoid mixture via selective crystallization. Through detailed examination of physicochemical properties such as solubilities and solid-state forms, we develop and test potential separation strategies.

The physicochemical properties of the curcuminoids can be modified by formation of binary or multi-component compounds that facilitate their selective crystallization. The integration of a solvent in the crystal structure of a compound can result in a solvate, while integration of a coformer results in a cocrystal. Solvates and cocrystals often exhibit different properties than the individual single-component forms. For example, pharmaceutical cocrystals can enhance the bioavailability of a drug by increasing its dissolution rate. For the curcuminoids, we investigated solvates and cocrystals and how these can be utilized for separation. Therefore, we conducted a solid-state phase screening and characterization. This included crystallization experiments with a selection of potential solvents and coformers to synthesize the respective solvates or cocrystals. Crystallization techniques such as liquid-assisted grinding or crystallization from solution were used. We synthesized three DMC solvates and characterized them via Powder X-ray diffraction.[2] The diffractogram shows sharp signals for the crystalline solvates 1, 2 and 3 (**Fig. 1b**). Commercial DMC is for the most part non-crystalline as the signals come with a broad background and a low signal-to-noise ratio. Currently, we are evaluating single-crystal structure data of these solvates, which would be the first crystalline forms to be reported for DMC. The crystalline DMC solvates were observed to have a needle-like morphology (**Fig. 1c**). Further methods for characterization are nuclear magnetic resonance, thermal analysis and Raman spectroscopy. Future work will focus on the separation of DMC via DMC solvate formation.

Similarly, we were able to identify three cocrystals of BDMC.[3] Two of them contain coformers that also form cocrystals with CUR but not with DMC, while one of them exclusively crystallizes with BDMC.[4] This distinct cocrystallization behavior can be exploited for a separation process as shown for the coformer hydroxyquinol (HYQ) in **Fig. 2**. A solvent with preferably similar solubilities for the curcuminoids and coformer is required and can be found using computational methods like COSMO-RS. By experimentally determining the solubility behavior of the curcuminoids in the presence of the coformer HYQ, we mapped cocrystal regions in a ternary phase diagram. We found an increase in solubility for the eutectic systems of HYQ with CUR and DMC and a decrease for BDMC in the form of the cocrystal. Further, we derived a separation strategy that removes BDMC from the curcuminoid mixture in the form of a cocrystal (**Fig. 2b**).

These comprehensive studies on solvate and cocrystal formation of curcuminoids serve as a valuable example for future complex product isolations.

I Laura Lamkowski, Steffi Wünsche

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Author **Laura Lamkowski**

Laura Lamkowski obtained her Master's degree in Chemistry from Ruhr University Bochum in 2022 and became a PhD candidate at the Max Planck Institute in the same year. She is funded by the International Max Planck Research School (IMPRS ProEng) and has been a PhD representative of the IMPRS since 2024. Her research focuses on characterizing natural products to selectively crystallize them from mixtures for pharmaceutical and food applications.

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Author **Steffi Wünsche**

Steffi Wünsche studied Chemical Engineering at Otto von Guericke University in Magdeburg. In 2019, she joined the Max Planck Institute to pursue her PhD on developing purification processes for natural substances. Besides cocrystallization of curcuminoids, the efficient production of the antimalarial artemisinin from plant extracts through coupling of adsorption and crystallization is part of her research. Currently, she is finalizing her thesis.

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PSE | PROCESS SYSTEMS ENGINEERING

+ Edgar Ivan Sanchez Medina, chemical engineer, and Christoph Griehl, process engineer, both at PSE group, are discussing their recent approaches using different models for analyzing the thermodynamic behaviour of chemical mixtures. Graph neural networks (GNNs) are special neural networks used to solve challenging issues based on graphs that form a complex data structure.

PROF. DR.-ING. KAI SUNDMACHER | DIRECTOR

+ In recent decades, we have seen continuous progress in increasing the productivity and selectivity of (bio-) chemical processes and energy conversion systems. But to cope with the grand challenge **of defossilizing the chemical process industry to achieve the net zero CO_2 emission target by 2050** at the latest, new breakthroughs in Process Systems Engineering (PSE) are urgently needed to achieve drastic improvements of resource efficiency in existing processes, to invent dream process technologies for synthesizing chemicals at low energy demand, to strongly accelerate the substitution of fossil raw materials and energies by renewables, to make process operation much more adaptive and flexible, to organize a comprehensive circular economy for recycling as many material streams as possible, and - at the same time - to achieve even higher product quality and functionality objectives.

This vision forms the background to our PSE group's research mission. For the development of next-generation sustainable process systems, we closely combine **mathematical modeling** with theoretical methods for **process analysis, synthesis** and **optimization** as well as with **advanced experimental validation** techniques. In particular, our "Elementary Process Functions (EPF) methodology" supports design decisions on multiple levels of the process hierarchy (molecular level, phase level, process unit level, plant level). In recent years, we extended this methodology towards complex process networks ("FluxMax" approach) and applied the same to derive, e.g., green methanol production systems solely fed with renewables (see the research highlight by Tibor Svitnič).

As part of our research activities in the area of **Chemical Production Systems**, in September 2023 we started a new research project on sustainable multi-step catalytic process systems in fine chemistry for the production of precursors of active pharmaceutical ingredients. It is part of the interdisciplinary Research Unit FOR 5538 IMPD4Cat funded by the German Research Foundation (DFG). There, we closely collaborate with colleagues from the Universities of Magdeburg, Rostock, and Potsdam as well as the Leibniz Institute for Catalysis (LIKAT, Rostock). Our methodological contribution of this project is an integrated computer-aided molecular, material & process design (CAMPD) framework. For its development, we combine mechanistic with data-driven modeling concepts, e.g. for predicting thermophysical properties of solvents by use of Graph Neural Networks (see the research highlight by Edgar Sanchez Medina).

Regarding **Energy Conversion Systems**, we continued investigating innovative Power-to-X processes for efficient off- and onshore conversion of electricity to hydrogen and its follow-up products methane, methanol, and Fischer-Tropsch hydrocarbons. These activities are partly embedded in the BMBF lead project H2Mare in which the PSE group is involved together with more than 20 partners from academia and industry. Moreover, supported by another BMBF lead project (TransHyDE), in 2024 we started to explore a novel dynamic reactor-separator concept for the efficient decomposition of ammonia - a very promising chemical for storage and long-distance transportation of green hydrogen. First experimental results on pilot plant scale are be expected to become available in 2026.

Within our research area **Biological Production Systems**, we dealt with the model-based design of zero-waste biorefineries fed with green microalgal or lignocellulosic biomass. In 2023 we demonstrated the machine learning-supported solvent design for lignin-first biorefineries together with the group of Prof. Jeremy Luterbacher (EPFL, Lausanne) and showed how optimal solvents help to avoid energy-intensive biomass drying steps. In a second project from the same area, we continued targeting the bottom-up design of artificial life-like systems (ALLS) from functional biomolecular modules. Thanks to the former research network 'MaxSynBio' and the Max Planck School 'Matter to Life', we were able to establish a broad spectrum of (inter-)national collaborations to study the dynamics of various life-like processes in synthetic membrane systems.

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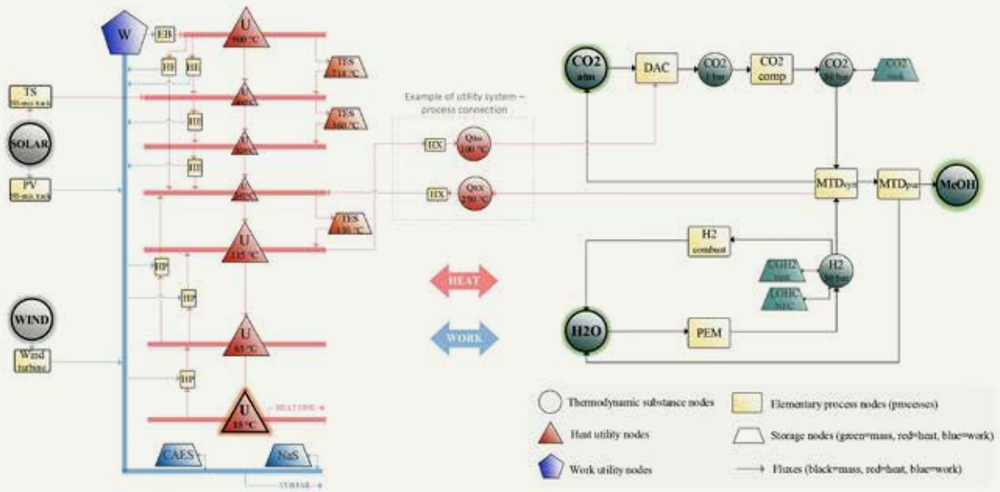
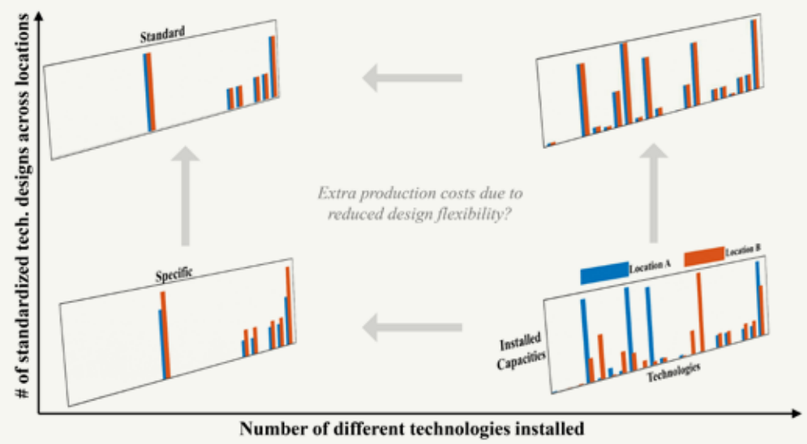


+ Figure 1:
Process network considered for the Power-to-Methanol designs [2].



+ Figure 2:
Visualization of the concept of design complexity reduction studied [2].

Optimizing Process Networks of Renewable Methanol Production

+ The transition to a defossilized chemical industry requires novel approaches to designing production systems that rely on renewable sources of mass and energy. However, this transition presents significant challenges due to the dynamic nature of these resources and the complexity of process networks, which integrate energy generation, storage, utilities, and chemical synthesis. Within the R2Chem project, we develop comprehensive design methodologies to address these challenges, and in the following we will present the work focused on the production of methanol – a crucial platform chemical that serves as a precursor for a wide range of carbon-based products and as fuel in various forms. Given its versatile applications, methanol represents a promising target for renewable production pathways.

A major challenge in Power-to-Methanol (PtM) processes is the high cost of renewable energy, necessitating efficient waste-heat utilization to improve overall energy efficiency. Technologies such as heat pumps, heat engines, thermal energy storage, and solar thermal energy conversion play an important role in this regard. Our recent studies extended the FluxMax approach [1] – a linear optimization framework that integrates heat recovery directly into process network optimization – to incorporate detailed utility subsystems, energy storage, and fluctuations in renewable energy availability (Fig. 1). This extension allowed for the simultaneous optimization of design, scheduling, and waste-heat utilization, leading to energy-efficient process configurations.

A case study for Port Arthur, Texas, demonstrated the effectiveness of this approach, using hourly renewable resource data to model solar and wind energy generation. The most cost-effective configuration featured a direct air capture process, parabolic troughs, thermal energy storage, and a steam turbine, achieving a levelized cost of methanol of approx. 1400 $/t in 2019, with an expected reduction to approx. 800 $/t by 2030 under projected future cost scenarios. Importantly, our analysis showed that incorporating waste-heat utilization and complementary energy generation can enhance economic feasibility, demonstrating the importance of a broadly integrated process network that spans all relevant subsystems [1].

As process networks expand, the increasing number of technological components introduces greater complexity in system design, deployment, and operation. A key trade-off emerges between minimizing the design simplicity and minimizing the calculated costs, which do not account for the negative-effects of design complexity in the early-stage of process design. To address this, we applied a multi-objective optimization framework to PtM processes, quantifying the impact of complexity reduction (Fig. 2) on the calculated production costs of methanol [2].

One study investigated the effect of reducing the number of major technologies as well as the potential for design standardization across geographically diverse locations with wind- or solar-dominant renewable energy conditions, specifically in the US and Chile. Results showed that the designs could be significantly simplified in terms of the number of installed technologies without a major effect on the production costs. Furthermore, standardizing the sizes of the major technologies across the locations led to increases in methanol production costs of 7–15%, depending on the quality of the individual locations in terms of renewable resources. If such cost increases could be compensated for by streamlining the plant construction and deployment, such a standardization concept may be a promising strategy for accelerating distributed PtM plant deployment, but more research is necessary [2].

Beyond technical and economic considerations, the deployment of renewable production systems also faces societal and political challenges. As part of the SmartProSys research initiative, we collaborated with political scientists from Otto von Guericke University to identify policy barriers and assess the land use implications of PtM deployment combined with biogas production under German conditions [3].

A multi-objective network optimization was conducted to explore land-efficient chemical production strategies. The analysis included agrivoltaics, wheat straw anaerobic digestion, heat pumps, and wind turbines – technologies that allow for intensified land use. Our findings showed that integrating methanol production with food and energy generation can achieve cost reductions of 19%, direct land use reductions of 9%, and greenhouse gas emission reductions of 12%. Further optimization demonstrated that land use could be reduced by up to 10% with only minor cost increases, highlighting the trade-offs between economic efficiency and land conservation [3]. Additionally, potential conflicts for agricultural land use and in deploying these sector-coupled production systems were discussed from the political science perspective.

Our overall findings demonstrate the added value that optimization methods have in helping to identify promising pathways and production concepts for chemical plants supplied with fluctuating renewable resources. Future work will focus on refining our process network methodologies, extending optimization frameworks to other Power-to-X processes, and on investigating the cost-scaling behavior of PtM plants to support the design decisions in this emerging industry and beyond.

I Tibor Svitnič

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Author **Tibor Svitnič**

Tibor Svitnič holds a Bachelor's degree in Chemical Engineering from the Slovak University of Technology in Bratislava and a Master's degree in Chemical Engineering from the University of Twente, Netherlands. He began his career with an internship at Air Liquide's Research Center in Frankfurt am Main, where he later worked as a Research Engineer. Currently, he is a doctoral researcher at the Max Planck Institute in Magdeburg, Germany. His research focuses on the design and optimization of renewable methanol production processes.

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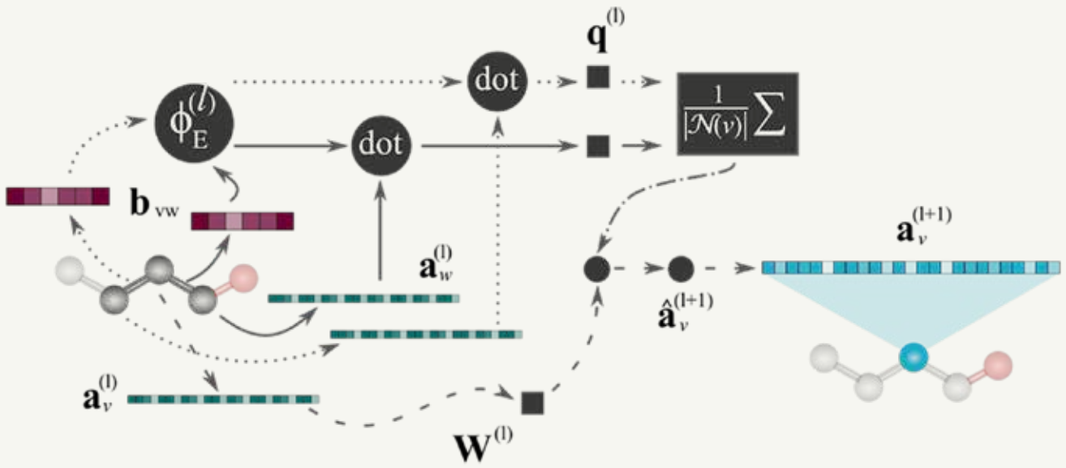
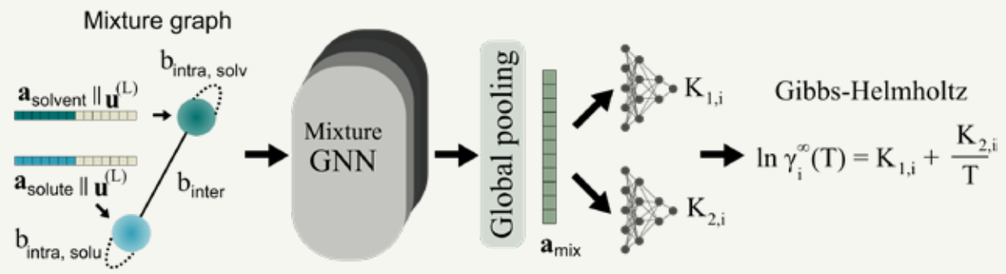


+ Figure 1:
Schematic representation of one message-passing step in a Graph Neural Network.



+ Figure 2:
Schematic representation of the Gibbs-Helmholtz Graph Neural Network after the construction of the mixture graph using the learned molecular embeddings from a molecular-level GNN.

Graph Neural Networks for Thermodynamic Modeling of Separations

For many years, scientists have been working on predicting the properties of mixtures based on the molecular structure of their components. Historically, a wide range of mechanistic models has been developed to predict the thermophysical properties of mixtures. These models have been instrumental in numerous successful applications across various fields of chemical and process engineering, such as the operation of large chemical plants that are vital to the global economy.

However, when it comes to novel and complex mixtures, such as those found in biorefineries or in the chemical recycling of plastic waste, or when developing sustainable processes for a future circular economy, existing models often fall short in terms of accuracy and predictive capability. This limitation is particularly evident in the modeling and calculation of phase equilibria, which is crucial for designing separation processes of molecular mixtures. To describe the non-ideal mixing behaviour of components in liquid mixtures, the activity coefficient concept is commonly used. This coefficient measures the deviation from ideality of components in liquid mixtures. Developing accurate and efficient predictive models to estimate these coefficients across a wide range of chemical species is essential for exploring alternative, and potentially more sustainable, separation processes.

The number of molecules that could be relevant for separation applications is enormous. Exploring such vast space using only experimentation and traditional trial-and-error approaches is simply not possible given our limited resources. Therefore, computational and predictive models are of great value to allow for better management of resources and to allow scientists and engineers to focus on only the most promising candidates. In a way, predictive methods can be seen as the road map for **molecular and material space exploration**.

In our group, we have investigated several predictive models that integrate the adaptability of graph neural networks (GNNs) with traditional mechanistic approaches to model the thermodynamic behaviour of mixtures, specifically activity coefficients. For this, molecules are abstracted as mathematical graphs where nodes represent atoms and edges represent chemical bonds. By using this specific molecular representation, distinct mathematical operations can be performed so that the information on each node of the graph is enriched by the information from its surroundings. This framework is popularly known as message-passing, and can be used to obtained tailor-made molecular representations for specific tasks.

By using backpropagation, the parameters of the GNNs are adapted to minimize an error function, improving the accuracy of the model predictions iteratively. Special care is taken during this optimization process to ensure that the GNNs are not only able to predict the observed data well but also, more importantly, to predict new mixtures accurately. In this way, effective and accurate predictive methods are obtained. However, as mentioned before, using GNNs is not enough. Thermodynamic constraints always need to be met and this is why hybrid mechanistic-machine learning models have been primarily researched in our group.

Two primary configurations of hybrid models have been explored. The **parallel configuration,** where the GNN acts as a corrector to the predictions made by a mechanistic model [1], and the **serial configuration,** where the GNN is embedded within a mechanistic expression to maintain the thermodynamical constraints of it and only produce thermodynamic-consistent predictions. Examples of the latter include the combination of GNNs with an expression derived from the Gibbs-Helmholtz relationship for the prediction of temperature-dependent activity coefficients [2]. Further hybridization of the previous model, named the Gibbs-Helmholtz Graph Neural Network, with a Gibbs-Duhem consistent model, the extended Margules model, is used for the prediction of both temperature- and composition-dependent activity coefficients.

Overall, the findings suggest that hybrid GNNs provide more efficient and accurate predictions of activity coefficients than standalone submodels. This was observed not only for systems with small organic molecules [1, 2], but also for polymer solutions [3]. We have also shown that these advantages can be leveraged in real-world scenarios, particularly in designing more sustainable separation processes through the intelligent selection of solvents for extractive distillation and biorefineries. The implementation of hybrid mechanistic-machine learning models holds significant potential for advancing sustainable separation technologies, and we hope to take this research even further to develop the next generation of predictive thermodynamic models that can assist our transition to a more sustainable chemical industry.

| Dr.-Ing. Edgar Ivan Sanchez Medina

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Author **Dr.-Ing. Edgar Ivan Sanchez Medina**

Edgar Ivan Sanchez Medina earned a Bachelor's degree in Chemical Engineering from the National Autonomous University of Mexico. During his studies, he participated in several research stays at institutions in the USA, United Kingdom, and Canada. He then completed his M.Sc. in Advanced Chemical Engineering with Process Systems Engineering at Imperial College London in 2019. Following this, he obtained his Ph.D. while working in the Process Systems Engineering department of Otto von Guericke University. Since 2025, he has been leading the Data Intelligence for Systems Engineering team within the Process Systems Engineering (PSE) group at the Max Planck Institute in Magdeburg.

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PSD | PROCESS SYNTHESIS AND PROCESS DYNAMICS

+ Johannes Leipold (PSD group) is meeting his colleague Lothar Kaps (PCF group) in the process control room of the MPI pilot scall hall. The experimental setup for methanol synthesis can be seen in the background. Johannes Leipold and Lothar Kaps are discussing on the implementation of theoretically optimized methanol synthesis conditions within the current plant setup.

PROF. DR.-ING. ACHIM KIENLE |
EXTERNAL SCIENTIFIC MEMBER

+ The Process Synthesis and Dynamics (PSD) group is headed by Achim Kienle, who is an external scientific member of the MPI. He also holds a professorial position at Otto von Guericke University. His MPI and university groups collaborate closely. The PSD group develops methods and tools for the synthesis, analysis, and control of complex process systems. It combines physical chemical insight with concepts from systems and control theory as well as applied mathematics. Process insight guides the way to suitable problem formulations and to feasible, efficient solution strategies. Whenever possible, theoretical concepts are validated experimentally. With this approach, the PSD group helps to bridge the gap between theory and application.

Process control has emerged as a major field of research for the PSD group in the last decade. Currently, the focus is on the control of particulate processes, advanced chromatographic processes, and methanol synthesis, which is an example of a particular important and challenging reaction system. Particulate processes are described by nonlinear partial differential equations and represent a highly challenging class of distributed parameter systems. Important topics addressed by the PSD group include mathematical modeling, nonlinear model reduction, and new approaches to robust, adaptive, and self-learning control of particulate processes. Novel crystallization, fluidized bed spray agglomeration processes have been investigated as interesting application examples. Chromatographic processes are switched systems with cyclic behavior. A particular focus of the PSD group in recent years has been on cycle-to-cycle online estimation and optimization of simulated moving bed (SMB) chromatographic processes, in cooperation with the Vande Wouwer group from University of Mons in Belgium. These SMB processes are applied for difficult separation problems in fine chemistry, including the pharmaceutical industry. Novel challenges for the control of methanol synthesis are posed by new applications for chemical energy storage under randomly fluctuating conditions. Furthermore, new modes of forced periodic operation are being developed together with the Seidel-Morgenstern group from the MPI and the Petkovska group from Belgrade University. Details on both aspects are given in the PSD group's Research Highlight.

In the field of **process design**, the PSD group is developing computational methods for a systematic design of complex process systems. Approaches range from shortcut methods based on analytical insight up to rigorous simultaneous mixed integer nonlinear optimization (MINLP) of process configurations, operating conditions, and auxiliary materials. During the period covered by this report, particular emphasis was placed on the robust design of novel multistage reactor concepts for power-to-methanol processes and on the design of novel SMB process for so-called center cut separations. These processes aim at isolating components of intermediate affinity from complex mixtures frequently occurring in fine chemistry. The latter was done in cooperation with the PCF group.

Biosystems engineering has been identified as a research area of common interest at the Max Planck Institute and Otto von Guericke University. The PSD group makes important contributions to biosystems engineering in the fields of modeling, dynamics, and control of biotechnological processes. During the period covered by this report, special emphasis was placed on multiscale modeling, soft sensor development, and optimal control of microbial biopolymer production processes led by Dr. Stefanie Duvigneau.

The PSD group has been involved in a number of highly visible larger joint research projects with external funding from the German Research Foundation (DFG), including the new research unit FOR 5538 IMPD4Cat on integrated molecular, material and process design of multistep catalytic production systems for fine chemistry with partners from Otto von Guericke University Magdeburg, Leibniz Institute of Catalysis (LIKAT), the University of Rostock, and the University of Potsdam. Furthermore, the group is contributing to several nationwide priority programs with funding from DFG, including SPP 2080 on catalysts and reactors under dynamic operating conditions for energy storage and transformation, SPP 2331 on machine learning in chemical engineering, and SPP 2364 on autonomous processes in particle technology. Finally, the group is also involved in the SmartProSys Research Initiative of Otto von Guericke University, the Max Planck Institute in Magdeburg, and LIKAT in Rostock. The objectives of SmartProSys concern smart process systems for green carbon-based chemical production in a sustainable society.

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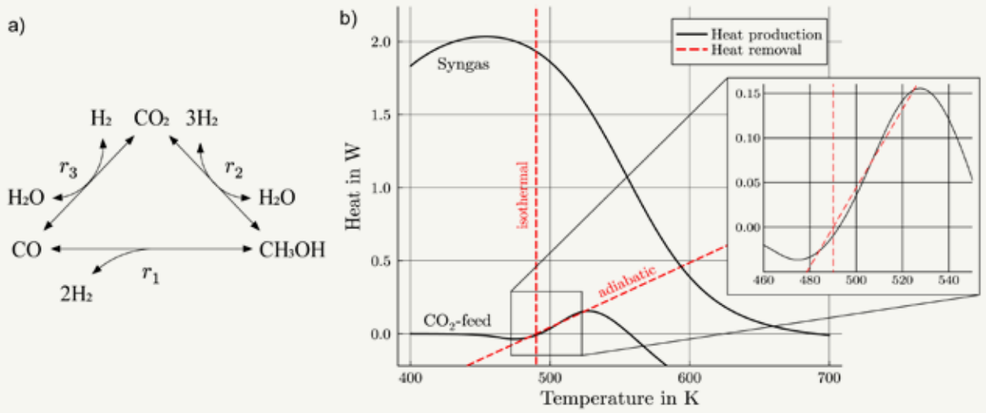
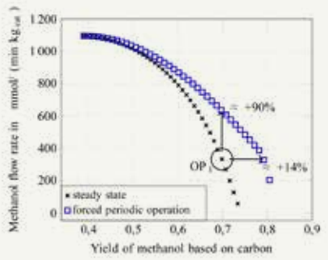
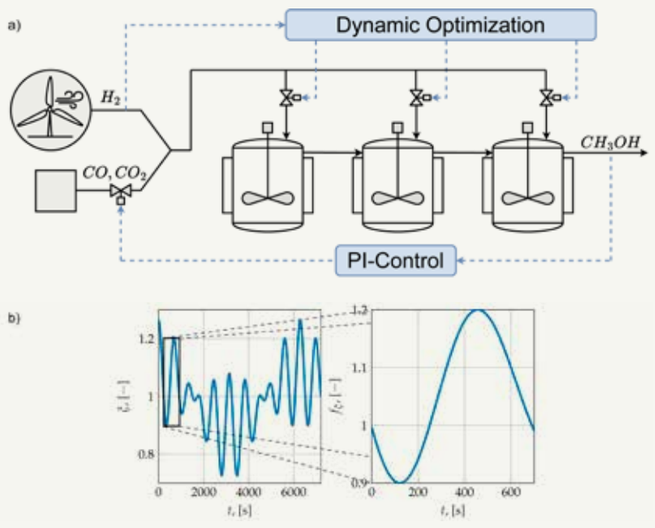


+ Figure 1:
Nonlinear dynamics: a) reaction network; b) heat production and heat removal curve of methanol synthesis from syngas and CO_2/H_2 feed. Intersections between heat removal and heat production indicate stationary points.



+ Figure 2:
Forced periodic operation: Pareto fronts of steady state compared to forced periodic operation with simultaneous but shifted square wave modulation of CO feed concentration and total feed flow rate in a nonisothermal reactor.



+ Figure 3:
Robust design and control:
a) flowsheet of multistage reactor with two degree of freedom controller to compensate fluctuations in hydrogen supply; b) hydrogen supply disturbance scenario.

Methanol Synthesis Under Dynamic Conditions

+ Methanol is an important platform chemical. Traditionally, it is produced on a large scale from syngas using $Cu/ZnO/Al_2O_3$ catalysts under pressures between 50–60 bar and temperatures between 200–260°C under steady state conditions. In contrast to this, the focus in our research has been on dynamics with a focus on nonlinear behavior, forced periodic operation, and robust design and operation of novel power-to-methanol processes.

Nonlinear Dynamics

Methanol synthesis is an exothermic reaction. Such reactions may give rise to self-accelerating dynamics including instability and multiple steady states. This was analyzed for a continuous stirred tank reactor (CSTR) by extending the classical heat removal and heat production curves (see Fig. 1) to the present heterogeneously catalyzed multistep reaction network. It was shown for the first time that for a CO rich feed under the typical conditions applied in practice multiple steady states and static instabilities will not occur [1]. The reason for this is that the overall heat production decreases with increasing temperature in the relevant range of operating conditions due to the water gas shift reaction. In contrast to this, the opposite behavior was found for a CO_2 rich feed, leading to instabilities and multiple steady states similar to the simpler CO_2 methanation.

Forced Periodic Operation

The objective of this project is to exploit the potential of forced periodic operation for improving methanol synthesis. The focus was on conventional CO rich feeds. This is a joint project with the PCF group and the Petkovska/Nikolic group from the University of Belgrade. It combines mathematical modeling (PSD and PCF groups), nonlinear frequency response analysis (Belgrade), rigorous numerical optimization (PSD group), and experimental validation (PCF group). It is based on the Langmuir-Hinshelwood kinetic model from our previous work [2], which accounts for dynamic changes of the catalyst and builds upon a comprehensive dataset of 140 steady-state and dynamic data previously obtained by the PCF group. Starting from a simple isothermal CSTR [3] investigations were extended step-by-step to computationally more challenging isothermal and nonisothermal fixed-bed reactors [4], which are commonly used in practice. To compare best possible steady state with best possible periodic operation, advanced multiobjective optimization was applied using the time-averaged methanol flow rate and methanol yield based on total carbon inlet as objective functions. In summary, it was found that
(i) not much improvement can be expected for periodic forcing of a single input, but significant improvements can be expected for simultaneous modulation of the CO feed concentration and the total feed flow rate with the some optimal phase shift [3],
(ii) additional constraints arising in practice can have a strong influence on the results and can be directly taken into account with our numerical approach (see, for example, [3,4]),
(iii) Square wave modulation is superior compared to harmonic forcing [4].

The most promising case is shown in Fig. 2. It shows significant potential to improve the reactor performance, especially for high yields. Experimental validation by the PCF group for an isothermal CSTR is on the way.

Robust Design and Operation of Power-to-Methanol Processes

The objective of this project is to exploit methods from machine learning for the robust design and optimization of novel power-to-methanol processes undergoing unavoidable fluctuations in the hydrogen supply. The focus is on hybrid models which combine a priori knowledge with machine learning using neural nets. This is a joint project with the PCF group, which has developed a flexible and powerful experimental setup for the challenging operating conditions mentioned above, and the OML group, which provides new algorithms for optimization and optimal experimental design of hybrid models. Contributions of the PSD group comprise:
(i) a new approach for the hybrid modeling of methanol synthesis, where partly unknown kinetics related to the effect of a change of active catalytic centers under dynamic conditions are replaced by a neural net [5],
(ii) optimization-based robust design of a new multistage reactor, sketched in Fig. 3, which allows flexible temperature management to avoid hot spot formation and achieve the desired conversion [6], and
(iii) a novel control strategy to compensate fluctuations of the hydrogen supply. The concept combines feedforward control, which is based on dynamic optimization with the hybrid model, with feedback control to compensate plant model mismatch of the hybrid model. The strategy is intuitive and can be extended in various ways as outlined in [7]. **I Johannes Leipold**

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Johannes Leipold studied Systems Engineering and Engineering Cybernetics at Otto von Guericke University, Magdeburg, and received his master's degree in 2022. In the same year, he joined the PSD group as a Ph. D. student. His research focuses on modeling, simulation, and control of methanol synthesis under dynamic operating conditions.

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OML | MATHEMATICAL OPTIMIZATION AND MACHINE LEARNING

+ Christoph Plate and Reinhold Wittmann are both mathematicians and members of the OML group. The main research areas of the group are presented on the following pages.

PROF. DR. RER.NAT. HABIL. SEBASTIAN SAGER |
MAX PLANCK FELLOW

+ The Optimization and Machine Learning (OML) group was established in November 2023 following the nomination of Sebastian Sager as a Max Planck Fellow. The Max Planck Fellow Program promotes collaboration between outstanding university teachers and scientists of the Max Planck Society. Sebastian Sager is full professor for mathematical optimization at OVGU.

The OML group

The group started in November 2023 with two Ph.D. students. **Christoph Plate** M.Sc. and **Reinhold Wittmann** M.Sc. both studied mathematics at OVGU and have shown great promise in mathematical research as well as interest in interdisciplinary engineering collaborations. They closely interact with colleagues at the MPI and also colleagues within Sager's MathOpt research group at OVGU.

The MathOpt group

The Mathematical Optimization research group was established at OVGU in April 2012. It currently comprises one postdoc and 11 Ph.D. students. They are funded via OVGU and MPI funds, via the DFG Research Training Group 2297 Mathematical Complexity Reduction, the DFG Special Focus Program 2331 Machine Learning in Chemical Engineering, the SmartProSys initiative of Saxony-Anhalt, the Center for Dynamic Systems of OVGU, the German Ministry of Health project "KlimaNot" (a cooperation with clinical emergency units in Magdeburg and Germany to forecast demand from weather data), the EFRE project "timingMatters" addressing digital twins in oncology, and the EFRE project "IntelAlgen" addressing algae production under realistic conditions. We closely collaborate with BASF SE in the area of nonlinear optimal experimental design.

Research focus

The MathOpt group's main focus is on the application-driven development of optimization methods, the close connection to machine learning, and an efficient implementation on computers. Main technologies and fields of expertise comprise nonlinear and integer optimization, as well as optimal control and optimal experimental design. A specialization is in numerical algorithms for mixed-integer optimization with differential equations. Many of our mathematical models arise from applications from chemical engineering, in particular from Power2X and SmartProSys processes. We are specifically interested in families of mathematical models and their interactions.

OML focuses explicitly on structures that are relevant in the cooperation with MPI groups. In many cases, a combination of first-principle models based on differential equations and data-driven surrogate models has shown to be an attractive modeling choice. This involves challenges for optimization technology on two levels.

Identifying hybrid models

The first level is to identify such models. Optimal experimental design (or active learning) can help to design experiments that provide enough information to identify model parameters and network weights accurately (see next page) or to discriminate (sub)models. This research is complemented by symbolic regression, aiming at interpretable algebraic formulations of input-output maps. Generalized inverse optimal control aims to infer optimality principles from data.

Using hybrid models

The second level is the question of how hybrid models can be (globally) optimized efficiently. In a cooperation with the PSE group (Ganzer), we analyzed the role of ReLU neural networks within mixed-integer nonlinear programs. We suggested a variety of different strategies such as bound tightening and an equivalent a posteriori-rescaling of network weights to analyze the correlation between the weights of a neural network and the runtime of modern MILP solvers. This fundamental research will be the basis for future cooperations to investigate superstructure optimization problems in process system engineering.

Applications in chemical engineering and cooperations

We successfully defended and prolonged a DFG SPP 2331 Machine Learning in Chemical Engineering project into the second funding period from 2025–2028. The project "Machine Learning for Power to Methanol Processes" was a collaboration between PSD (Kienle), PCF (Seidel-Morgenstern), and OML in the first funding period. The granted extension will be a collaboration between PSD, PSE (Zimmermann), and OML.

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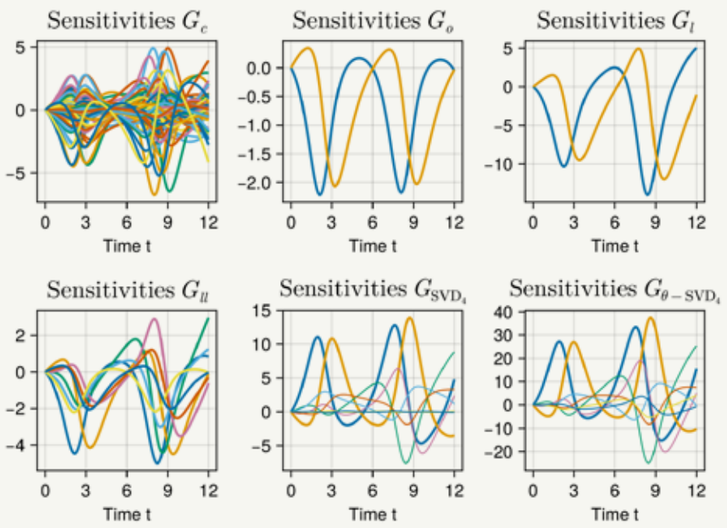

Figure 1:
Sensitivities with respect to weights and biases of the same neural network embedded in the Lotka-Volterra equations using different proposed dimension reduction methods. The dimension reduction hints at the possibilities of computational speedup while maintaining similarity of the time intervals of interest (those in which the sensitivities have high absolute values).

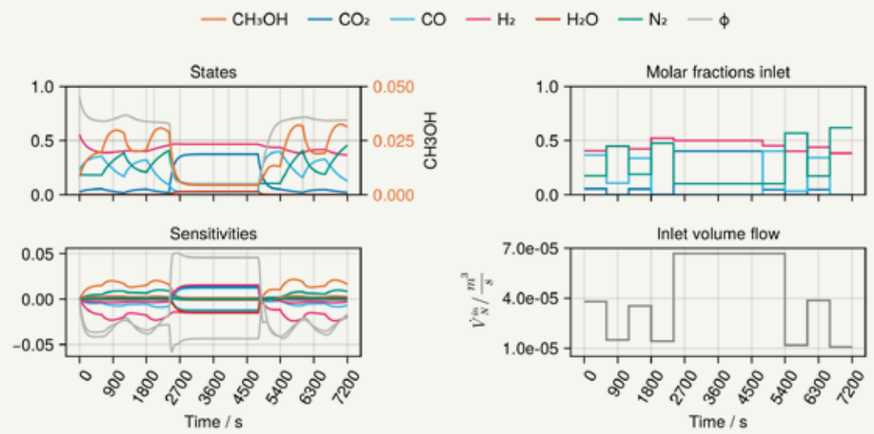

Figure 2:
Optimal experimental design for hybrid DAE modeling the synthesis of methanol. The degrees of freedom are the molar fractions of the inlet and the inlet volume flow as well as the temperature. The latter was considered as a control value, constant over time.

Hybrid Modeling and Its Challenges for Optimal Experimental Design

The Optimal Experimental Design

Model-based simulation and optimization is at the core of the solution process of many of today's engineering problems. However, all methods hinge on the validity of the mathematical model, and with this on the accuracy of the model's parameters. Learning model parameters for differential equations is traditionally related to the statistical approach of Optimal Experimental Design (OED), which is a systematic approach for obtaining useful data for parameter estimation, model identification, and model discrimination. The estimated model parameters are random variables; hence, they are endowed with a confidence region. The size of this confidence region depends on how the process was controlled and the decisions of which states are measured at what time. The OED problem, i.e. the problem of minimizing the size of this confidence region, can be cast as a specifically structured optimal control problem in which controls and sampling decisions are the degrees of freedom.

Hybrid Modeling

Hybrid modeling recently emerged as a powerful modeling approach aimed at combining the advantages of two different paradigms. First, the interpretability and data efficiency of rigorous modeling based on first principles and specific domain knowledge, usually expressed in parameterized differential equation models. Second, the flexibility of data-driven models such as neural networks, which are proven to be universal approximators. Under mild assumptions on their size and the used activation functions, they are able to learn unknown functional relationships from data to an arbitrary precision.

Thus, hybrid models typically consist of systems of differential equations with one (or multiple) embedded universal approximators, resulting in a parameterized model that is able to capture unknown effects from data. As data collection via performing experiments in real-world applications is costly, the need to carefully design these experiments is also relevant in this context. While strategies exist to come up with insightful data for parameter estimation/training for the two different paradigms considered independently (OED for rigorous ODE/DAE models as mentioned above, active learning for neural networks), developing algorithms for hybrid models is an open research question.

OED for Hybrid Models

In recent work [1], we considered Optimal Experimental Design for the special case of hybrid models. Embedding neural networks in differential equations has several implications for the OED problem. The first aspect is that, quantitatively, the number of weights and biases is typically very large in comparison to physical model parameters, increasing the computational effort needed for classical OED methods. In particular, setting up the necessary variational differential equations for the sensitivities of the solution of the differential equation with respect to the weights and biases quickly becomes prohibitive. Second, and more importantly, weights of a neural network are not uniquely identifiable. This is intuitively clear, as one can design equivalent transformations of weights and biases that leave the functional relationship of the neural network intact. However, this implies that the OED problem for hybrid models is usually ill-posed, as indicated by singular Fisher information matrices. We proposed to address this problem by considering different methods to reduce the complexity of the problem via means of dimension reduction of the sensitivities, illustrated in Figure 1. These dimension reduction methods range from the artificial scaling of all weights and biases to an identification of the most important weights via the singular value decomposition (SVD) of the Fisher information matrix. This way, singular Fisher information matrices can be avoided, rendering the OED problems solvable. With our open-source software DynamicOED.jl [2], these problems can be set up and solved efficiently, e.g. via the NLP solver Ipopt.

Application

In a current preprint [3], we applied the hybrid modeling approach and our proposed optimal experimental design methodology to the example of the synthesis of methanol from CO, CO_2 and H_2 over a $Cu/ZnO/Al_2O_3$ catalyst in a continuously stirred tank reactor (CSTR). The process is modeled as a DAE system, with an embedded neural network aimed at capturing the complex influence of reversible changes of the active catalytic sites on the reaction rates for the hydrogenation of CO and CO_2 and the reverse water-gas shift reaction. This influence is still not fully understood despite ongoing research and is thus far modeled via heuristics. With the built experimental setup from the group of Prof. Seidel-Morgenstern allowing the collection of time-resolved data under dynamic operating conditions, we were able to carry out the planned experiments and collect the data for the training of the hybrid model. With experiments specifically designed for the hybrid DAE model shown in Figure 2, we were able to obtain two results: 1) we could confirm the validity of two of the three used heuristics modeling the impact of the catalyst on the reaction rates, and 2) we observed an increase in model accuracy when including the data from the experiments planned via our proposed OED methodology for hybrid models in the training data.

Christoph Plate

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Author **Christoph Plate**

Christoph Plate received his Bachelor's degree in mathematical engineering and his Master's degree in mathematics from Otto von Guericke University, Magdeburg, in 2019 and 2021 respectively. In 2022, he started his Ph.D. at OVGU and joined the OML group in 2023. His research focuses on methods for optimal control and optimal experimental design, hybrid modeling, optimization methods for machine learning, and applications in chemical engineering

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ARB | ANALYSIS AND REDESIGN OF BIOLOGICAL NETWORKS

+ Katja Bettenbrock and Gerrich Behrendt are examining petri dishes filled with cultures of the bacterium *Zymomonas mobilis*.

DR.-ING. STEFFEN KLAMT | SENIOR SCIENTIST

+ Nowadays, it is widely accepted that understanding the complexity of life at the cellular level requires mathematical and computational tools. Taking this as a research leitmotif, the W2 research group **Analysis and Redesign of Biological Networks** (ARB) develops and applies methods from systems and computational biology and combines them with experimental investigations to analyze and rationally modify cellular (biomolecular) networks. One particular focus of our research is the modeling and computational design of metabolic networks in microorganisms with applications in metabolic and biosystems engineering. Other research areas include the theoretical analysis and optimization of microbial communities and of cell-free production systems, as well as the development of comprehensive toolboxes for the computer-aided analysis of biological networks (*CellNetAnalyzer* and *CNApy*).

Apart from theoretical developments, we use various genetic engineering and cultivation techniques to modify and study the physiology of different microorganisms under different conditions. Our experimental studies have a particular focus on *Escherichia coli*, one of the most important model organisms that serves as host in many biotechnological production processes. Another species studied in our lab is *Zymomonas mobilis*, a bacterium with tremendous production capabilities. The close integration of wet-lab and dry-lab investigations under one roof enables the prompt implementation and verification of model-based predictions.

Research in our group is thus highly interdisciplinary at the intersection of biology, informatics, mathematics, and engineering sciences. A long-term goal of our activities is to help pave the way for the routine use of advanced mathematical modeling approaches in the life sciences.

Highlights and trends in 2023/2024

In the last two years, the ARB group has made significant contributions to the field with publications in high-impact journals (*Nature communications, Nature Reviews Biotechnology, Metabolic Engineering*, and others). Highlights include theoretical studies on thermodynamic constraints shaping the specificity of redox reactions with respect to the redundant cofactors NADH/NADPH, concepts for bioprocess optimization based on metabolic cybergenetics, and new developments for computational strain design and associated software. With a stronger experimental focus, we have developed a framework for the optimization of cell-free enzyme cascades (with applications for synthesis of nucelotide sugars), tested and systematized oxygen-dependent promoters for dynamic metabolic engineering, and completed the development of a Golden-Gate cloning toolbox for *Zymomonas mobilis*. This genetic toolbox (called **Zymo-Parts**) is presented by Gerrich Behrendt and Katja Bettenbrock in our Highlight article on the following two pages. Using the production of lactate and alanine as an example, it is shown that this toolbox facilitates efficient metabolic engineering of this bacterium to exploit its enormous production potential.

The ERC Consolidator Grant project StrainBooster, which focused on the establishment of enforced ATP wasting as a strategy for rational metabolic engineering of microbial cell factories, was completed successfully. Funded by a newly awarded **ERC Proof of Concept (PoC)** grant, the transfer of this strategy into industrial processes was (and partially still is being) investigated with partners from two biotech companies in a follow-up project.

One particular aspect of our future research is **sustainable substrates** for bioproduction processes to replace sugar-based substrates (e.g. glucose) with alternative resources that are more cost-efficient and avoid the competition between the production of food vs. biofuels and biochemicals. With a new project financially supported by the state of Saxony-Anhalt, we will target the development of efficient bioprocesses for the production of platform chemicals from biogenic residues and waste streams (e.g. from the food industry, such as whey, molasses, and vinasse).

Our group is very grateful for the stimulating discussions with the **scientific advisory board** during their visit in fall 2024 and for the very positive feedback about our work.

The terrorist attack on the Christmas market in our city of Magdeburg in December 2024 has also deeply shocked all members of the ARB group. We mourn with the families of the victims and express our sympathy for the many seriously injured. At the same time, we firmly oppose the misuse of this horrific act as an excuse for xenophobia.

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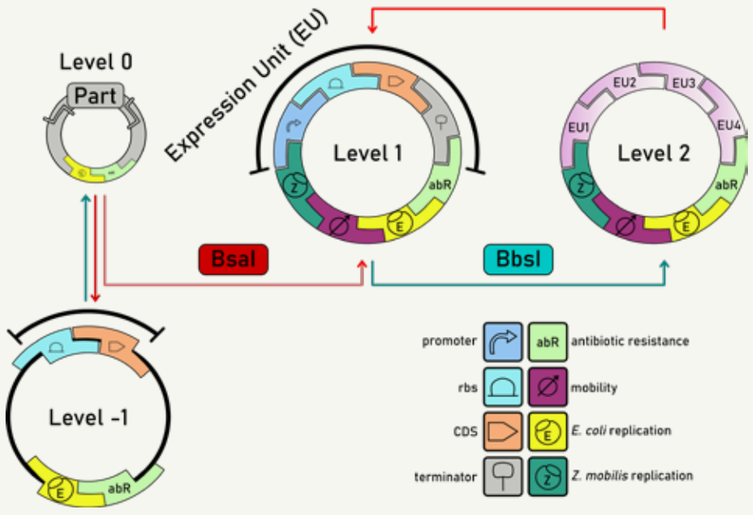
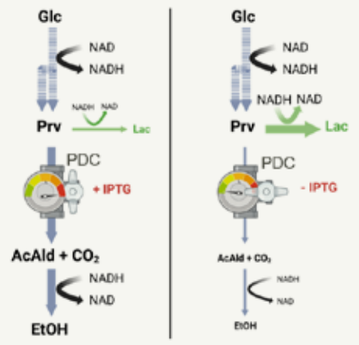


+ Figure 1:
The Zymo-Parts Golden Gate Cloning Toolbox. The Zymo-Parts toolbox is a modular cloning toolbox that allows easy cloning and combination of promoters, ribosome binding sites, genes of interest and terminators. The different elements have been tested for their functionality in *Z. mobilis* and can also be used for the construction of more complex constructs.



Strain	IPTG (µM)	µ (1/h)	r (mmol gCDW^{-1} h^{-1})			Y (mol/mol Glucose)	
			$r_{Glucose}$	$r_{Ethanol}$	$r_{Lactate}$	$Y_{Ethanol}$	$Y_{Lactate}$
WT	0	0.22	53	96.5	n.d.	1.9	n.d.
sGB027	0	0.05	25.7	45.1	n.d.	1.8	n.d.
	10	0.06	26.5	47.8	n.d.	1.8	n.d.
	20	0.07	39.4	69.9	n.d.	1.9	n.d.
	100	0.19	46.6	88.5	n.d.	1.9	n.d.
sGB029	0	0.09	47.4	18.4	66.7	0.35	1.5
	10	0.1	47.9	26.8	64,9	0.54	1.4
	100	0.13	47.1	56.5	32.3	1.3	0.67

+ Figure 2:
sGB027, a strain with controlled expression of the *pdc* gene. Shown is the design of sGB027, where the native *pdc* promoter has been replaced by a promoter that can be controlled by the addition of IPTG. Varying the IPTG concentration leads to different amounts of the PDC enzyme in the cell and therefore to different growth rates (see table). Low expression of *pdc* coupled with the expression of an alternative lactate producing enzyme (green pathway) in sGB029 allows the redirection of the metabolic flux away from ethanol towards lactate with very high lactate production rates ($r_{Lactate}$).

Enabling Metabolic Engineering of *Zymomonas mobilis*

+ The chemical industry is still largely based on fossil resources steadily releasing greenhouse gases. It is generally accepted that bio-based production processes, where microorganisms convert renewable resources into platform chemicals, could provide a major opportunity to reduce CO_2 emissions and enable more sustainable production routes. However, the range of products currently produced with biotechnological processes is still small. Bioprocesses that are more efficient are needed to cope with the large quantities of platform chemicals required and to keep the costs as low as possible. Metabolic engineering of microbes is key to improving microbial production processes.

The bacterium *Zymomonas mobilis* is well known for its outstanding ability to produce ethanol with a high specific productivity and a yield close to the theoretical maximum which even outperforms yeast, the traditional bioethanol production organism. In order to exploit the favorable properties of *Z. mobilis* for the production of chemicals other than ethanol, some requirements must be fulfilled. First, it is necessary to redirect central metabolic fluxes away from ethanol to alternative and more valuable products. However, this has proven to be problematic, mainly because knockout of pyruvate decarboxylase (PDC), the key enzyme in the ethanol production pathway, appears to be lethal. Second, the substrate spectrum of *Z. mobilis* needs to be expanded. In addition to its preferred substrate glucose, *Z. mobilis* is able to utilize sucrose and fructose present in sugar-rich waste streams such as molasses. An extension of *Z. mobilis'* substrate spectrum towards pentose sugars would allow the exploitation of other waste streams like lignocellulosic hydrolysates. In order to meet these requirements, efficient methods for the genetic engineering of *Z. mobilis* are needed and existing methods need to be improved and expanded.

To this end, we have developed the Zymo-Parts Golden Gate cloning toolbox[1, 2]. This toolbox contains a set of well-characterized genetic elements that can be used to drive gene expression in *Z. mobilis*. Most importantly, it contains a set of constitutive and inducible promoters that allow the variation of gene expression levels. It also contains a set of shuttle vectors (plasmids) optimized for *Z. mobilis*[2]. All elements of the toolbox can be easily combined by modular cloning facilitated by a new standardized assembly framework that enables the design of complex genetic constructs (Fig. 1). Overall, the toolbox enables the introduction of heterologous genes and fine-tuning of their expression levels, as well as introducing genome modifications.

Using the Zymo-Parts toolbox, we constructed a new platform strain (sGB027) of *Z. mobilis* in which the native promoter of *pdc* was replaced with an IPTG-inducible promoter, allowing the expression of *pdc* to be controlled from very low to high levels by the amount of IPTG added (Fig.2)[3]. These modifications were made at the genomic level, thereby avoiding the use of antibiotics and potential issues with plasmid stability. In this strain, the growth rate correlates with the amount of IPTG added and with the *pdc* expression level. High level expression of lactate dehydrogenase from *E. coli* in this strain combined with the omission of IPTG to ensure very low expression of *pdc* led to a very efficient redirection of the metabolic flux away from ethanol towards lactate. We achieved production of D-lactate with, to the best of our knowledge, the highest reported specific productivity of any microbial lactate producer (66.7 ± 0.6 mmol gCDW^{-1} h^{-1} in defined minimal medium, 92.5 ± 4.8 mmol gCDW^{-1} h^{-1} in complex medium with 2% glucose)[3]. As another proof-of-principle, the amino acid L-alanine was produced with a high rate by expressing the L-alanine dehydrogenase of *Geobacillus stearothermophilus* in sGB027. These results demonstrate the potential of our new platform strain sGB027 as a basis for the production of compounds other than ethanol [3]. Together with the developed Zymo-Parts toolbox, which also allows the introduction of more complex heterologous pathways, this strain may facilitate the establishment of *Z. mobilis* as a workhorse for a range of new bioproduction processes.

I Gerrich Behrendt, Dr. Katja Bettenbrock

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Author **Gerrich Behrendt**

Gerrich Behrendt studied plant biotechnology at Leibniz University Hannover, where he developed an interest in the fundamental aspects of genetics that enable the controlled manipulation of biological protein production. After his studies he started his Ph.D. work in the ARB group, where he is developing modular cloning techniques for the genetic engineering of microbial cell factories.

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Author **Dr. Katja Bettenbrock**

Katja Bettenbrock studied biology at the University of Osnabrück, where she also completed her doctorate in the field of bacterial genetics and metabolism. She joined the MPI in its founding year (1998) and has been a team leader in the ARB group since 2013. Her main interests are the investigation of fundamental metabolic and regulatory processes in bacteria and their application to the design and construction of optimized strains for bioproduction.

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MSD | MOLECULAR SIMULATIONS AND DESIGN

+ The Molecular Simulations and Design group in August 2024.

PROF. DR. MATTHIAS STEIN I GROUP LEADER

+ The **Molecular Simulations and Design** (MSD) group is led by **Prof. Dr. Matthias Stein**. It uses a comprehensive and advanced approach to study complex chemical and biological systems. Today, the computer is just as important a tool in chemical research as the test tube. Modern simulations have become so realistic that they can explain and sometimes predict the outcome of traditional experiments.

Multi-scale computer simulations allow for a detailed understanding of dynamics and reactions at various levels of resolution. The MSD group performs structure-based computer simulations using a multitude of appropriate methods from the fields of physics, chemistry, and biology. The methods range from structural bioinformatics through coarse-grained and full-atomistic molecular dynamics simulations to QM/MM and quantum chemical calculations. The results obtained from these quantum chemical and dynamic simulations help to control and regulate complex systems in biology and chemistry.

Between 2023 and 2024, the group established a number of new collaborative experimental and computational projects with other groups in Germany and worldwide

In 2024, **Froze Jameel** successfully defended his Ph.D. thesis entitled ‘Catalyst and Solvent Selection for Complex Homogeneous Metal-catalyzed Reactions’. It describes the development of new catalysts for a sustainable and green chemistry. Hydroformylation and reductive amination reactions were chosen as prime examples. In addition to EHS (Environment, Health, and Safety) criteria for the protection of the environment and its people, the effects of changes in solvent composition on thermodynamics, rates, selectivity, and yield of the modified processes need to be considered in detail when accompanying the transition of chemical processes towards sustainability and climate neutrality.

The stay of **Dr Yilmaz Özkilic** (Istanbul Technical University, Turkey) as a guest scientist from 11/2023 to 12/2024 was supported by a TÜBITAK fellowship. During his research in Magdeburg, he focused on the activation mechanism of the enzyme kynurenine 3-monooxygenase (KMO), which is an important target for the treatment of neurodegenerative diseases such as Huntington’s and Alzheimer’s.

Dr Ravi Kumar was the Ernst Dieter Gilles Fellow at the Institute from 07/2022 to 06/2024. He was also successful in joining the Postdoc Program of the Max Planck Society (MPG) and the Weizmann Institute (WIS) in Rehovot, Israel, to establish a long-term scientific collaboration with Prof. Leeor Kronik.

In 2024, the OVGU and the Silesian University of Technology (Gliwice, Poland) signed an individual **Cotutelle de thèse** for **Katarzyna Szleper**, which allows her to obtain a binational Ph.D. degree from both institutions. We already were and are going to host Katarzyna for work on her PhD topic. This enhances the visibility of our joint research and puts the collaborative work between MSD and Dr. hab. Artur Gora on a solid footing.

After the retirement of Prof. Seidel-Morgenstern in August 2024, the MSD group looks forward to the recruitment of another outstanding scientist in an emerging field as his successor. This presents an opportunity to shape the institute's focus for the coming years. With the appointment of the new director, new common research areas and scientific projects will be defined.

This summary captures the essence of some of the group's highlights during the last two years and some future plans, emphasizing their commitment to advancing research in chemistry and biology through innovative simulation techniques.

One Recent Example from our Work: Control and Regulation of Cell Growth and Degradation

X-ray structures represent only a static picture of a protein under crystallization conditions, leaving the structural dynamics under physiological conditions unexplored. Computer-based Molecular Dynamics (MD) simulations are able to sample those structural and conformational changes at finite temperature, providing insight into both global and local dynamics of protein motion.

MSc. Metehan Ilter addressed this topic for members of the deubiquitinating enzyme (DUB) family.

These enzymes regulate the deubiquitination process of post-translationally modified proteins, thereby controlling protein signaling in various cellular processes and are essential for maintaining the balance between protein synthesis and degradation. They are also the link between cancer and inflammation. Some bacteria and viruses mimic human DUB functions to evade the host’s immune response.

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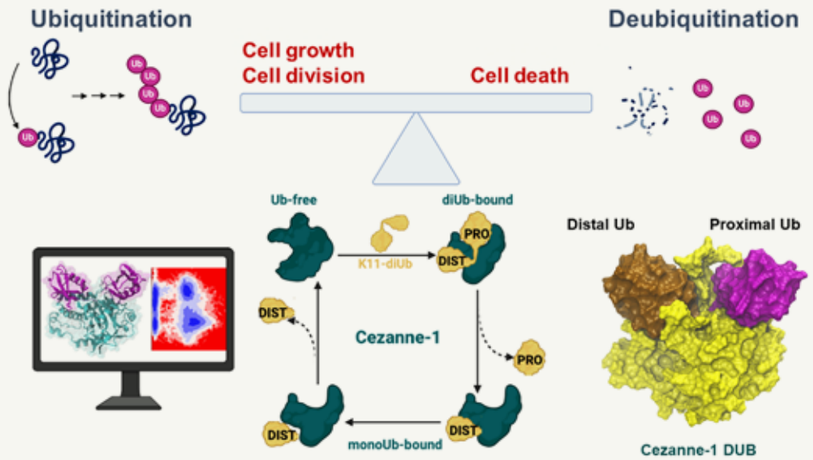

+ Figure 1:
The balance between cell growth, division and cell death is controlled by enzymes of the deubiquitinase family. Computer simulations are able to provide molecular insight into the conformational dynamics of molecular recognition and enzymatic action.

+ Figure 2:
Cezanne-1 and Cezanne-2 are distinct members of the deubiquitinase enzymes. They are not named after the French painter but their structure and function ('cellular zinc finger anti-NF-κB'). Both proteins are expressed in different tissues but behave very similarly.

The Structural Dynamics of Enzymes during Catalysis

+ The enzyme structures that we obtain from X-ray diffraction experiments only correspond to a static picture and the protein form under crystallization conditions. Biomolecular simulations have significantly enhanced our understanding of protein structures, their function, dynamics, and mechanisms. Molecular dynamics (MD) simulations offer insight into protein conformational dynamics that are inaccessible through X-ray crystallography, e.g. loop rearrangements, structural flexibility, and conformational transitions between inactive and active states by integrating Newton's equation of motion at an atomistic level.

The covalent attachment of ubiquitin molecules to target proteins, either as mono-ubiquitin or poly-ubiquitin chains, is a reversible post-translational modification in eukaryotes. This process is known as ubiquitinylation. Ubiquitinylated proteins carry such a label which designates them to be degraded by the 20S proteasome. Deubitquitinylases (DUBs) are proteases that counteract this protein ubiquitinylation, thereby maintaining cellular ubiquitin homeostasis and controlling several cellular pathways, such as DNA damage response and innate immune signaling. Some bacteria and numerous viruses have independently developed effector proteins to mimic the functions of human DUBs in order to increase their replication and infectivity.[1]

Dysregulation of DUBs is responsible for various diseases, and thus DUBs are currently becoming more recognized as attractive drug targets. There are particular members of DUBs called Cezanne-1 and -2, but they are not named after the French painter – their names stand for 'cellular zinc-finger anti-NF-κB'. Genomic alterations in Cezanne DUBs cause several diseases, including cancer and some neurological diseases.

The process of activation and catalytic turnover of Cezanne DUBs is a multistage cycle with several critical dynamic transitions that cannot be characterized based on protein structures alone. Our MD simulations covered several microseconds and showed that ubiquitin-free Cezanne-1 dynamically shuttled between catalytically competent and incompetent states. This suggested that its activation is independent of substrate binding. The catalytically competent substrate-free Cezanne-1 promoted distal ubiquitin substrate access to the catalytic center. The subsequent binding of the proximal ubiquitin shifted the equilibrium toward the catalytically competent state of the dyad, thereby promoting proteolysis of the ubiquitin iso-peptide bond. After cleavage of the scissile bond, sequential dissociation of first the proximal ubiquitin induced the inactivation of Cezanne-1. The subsequent release of the distal ubiquitin fully reconstituted the inactive substrate-free state of Cezanne-1.[2]

Cezanne-2 is a paralogue to Cezanne-1, i.e. an additional copy in the DNA originating from a gene duplication event. Analysis of computer simulations elaborated on similarities and differences between Cezanne-2 and Cezanne-1. From the MD trajectories, critical parameters for productive enzyme–substrate configurations suitable for proteolytic di-ubiquitin cleavage were identified based on carefully defined structural criteria and verified by hybrid QM/MM calculations. Using this combined approach of protein structural modeling, extensive sampling of several charge states and reaction intermediates by all-atom MD simulations, and QM/MM refinement, structural details of the enzyme activation and reaction were elucidated.

It was possible to assign a catalytic dyad of histidine and cysteine residues to be functionally involved in substrate bond cleavage, while the third glutamate residue close to the active center assisted in substrate recognition and positioning. A strictly conserved water molecule was identified that mediated the interaction between the active site histidine and glutamate residues. The water molecule polarized the histidine residue and thus promoted the formation of the catalytically active state. This was then also verified to be relevant for Cezanne-1.

Structural resolution of enzyme–substrate complexes is challenging since enzymatic turnover must be inhibited to co-crystallize the substrate in or close to the catalytic site. For cysteine proteases, activity-based probes or mutations in the active site are sometimes used to characterize a complex that is close but not identical to a physiological binding situation. In addition, mutations of the catalytic cysteine residue to a nonreactive alanine, for example, do not provide the full-resolution enzyme–substrate picture. However, these artifacts must be recovered, and a refinement by MD simulations is required. Likewise, protein–protein complex structural models from deep learning approaches have to be carefully inspected, and further MD refinement steps may also be necessary. The detection and interpretation of subtle differences in inter-residue distances (in order to issue statements about the state of enzyme activation) or substrate binding and orientation (to ensure a physiological binding situation) require curation by an expert scientist in this field.[3] **I Metehan Ilter**

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Author **Metehan Ilter**

Metehan began his Ph.D. at the MPI in 2021 after navigating a lengthy visa process. At that time, the ongoing SARS-CoV-2 pandemic, vaccination requirements, and travel restrictions were significant challenges. He earned his B.Sc. in 2019 from the Department of Biomedical Engineering at Istanbul University and went on to complete a Master of Science in Biomedical Engineering and Bioinformatics in 2021. He is an expert in computational biology and data analysis.

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EEC | ELECTROCHEMICAL ENERGY CONVERSION

+ Process systems engineers Monisha Sivasankaran and Antonio Sorrentino conduct dedicated experiments to validate model predictions for electrochemical CO_2 reduction reaction.

DR.-ING. TANJA VIDAKOVIĆ-KOCH I SENIOR SCIENTIST

+ A significant focus of the Electrochemical Energy Conversion (EEC) Group was on understanding electrochemical processes under alternating current (AC) conditions. Traditionally, AC conditions are used for analysis, such as in electrochemical impedance spectroscopy. Recently, a rapidly growing community has reported positive impacts of high-amplitude AC electrolysis on product selectivity in electrosynthesis. These different aspects of AC conditions are currently treated as unrelated within the scientific community. In the **EEC Group** we aim to establish a generalized framework, called nonlinear frequency response analysis (NFRA), to analyze and optimize electrochemical processes under AC conditions. Some major projects are described in brief below.

Fundamentals of Dynamic Electrochemistry

In this project, we concentrated on the applications of NFRA to enhance the understanding of reaction kinetics and improve selectivity under dynamic conditions. This research was undertaken in a large collaborative network funded by the German Research Foundation (FOR 2397), which included seven academic partners from both universities and non-university institutions. The network aimed to advance the understanding of reaction and transport processes in gas diffusion electrodes and concluded in 2023. The focus was on oxygen and carbon dioxide reduction reactions. Monisha and Antonio will discuss the details of the main achievements in our Research Highlight.

Energy Convertors under Dynamic Conditions

Polymer electrolyte water electrolysers (PEMWEs) are crucial for converting excess electrical energy from renewable sources into hydrogen. To understand their behavior at high current densities, we collaborated with project partners from OVGU with the support of IMPRS and SmartProSys. This work enhanced our understanding of PEMWE behavior and opened up the use of NFRA for PEMWE diagnosis.

In the German Research Foundation's priority programme "Bioelectrochemical and Engineering Foundations for Establishing Electrobiotechnology for Biosynthesis – Power to Value-added Products (eBiotech) (SPP 2240)", we collaborated with the University of Greifswald to address bottlenecks in electroenzymatic processes, such as product scale, productivity, and cofactor regeneration efficiency. We demonstrated that dynamic operation can enhance co-factor regeneration and confirmed product formation by integrating enzymatic reactions with electrochemical co-factor regeneration.

Data-Driven Analysis of Electrochemical Processes

We propose a novel data-driven analysis tool for electrochemical processes based on the Loewner framework (LF) approach. In collaboration with mathematicians and experts in the LF from MPI Magdeburg, we initiated this research with a joint Master's thesis student and continued with support from IMPRS. Our approach offers several advantages over existing tools: it is a direct, unbiased methodology with a high level of accuracy. We are currently investigating the effects of noise and applications on real-world data.

Events, Group Issues, New Projects

In 2023, Tanja co-organised a symposium on "Integrated electrocatalyst and electrode engineering for sustainable electrochemical processes" in the framework of the 74th Annual ISE Meeting in Lyon, France from 3 to 8 September 2023. In an excellent atmosphere and with a combination of keynote, invited and submitted contributions, we discussed the integration of smart catalyst and electrode design as a key to ensuring technology translation beyond the lab-scale. The topics included CO_2 reduction, ammonia electrogeneration, chlorine evolution, water splitting, water remediation, and electrosynthesis of organic products of added value.

In 2024, Luka moved to an industry position. We extend our gratitude to him for his significant contributions to NFRA applications in ORR and PEMWE, as well as his work on the dynamics of bioelectrochemical processes. Additionally, we appreciate his efforts in initiating collaborations for the use of LF in nonlinear analysis. Notably, Luka has demonstrated a commendable capacity for mentorship, guiding both Tamara and Mohammed. His contributions to inspiring discussions and organising group social activities are also highly appreciated. We send him our best wishes for his future success.

Starting from 2024, together with the collaboration partners from KIT and the University of Belgrade (Mercator fellow), we aim to advance NFRA for battery diagnosis. In another project supported by the DAAD and conducted with the partner from the University of Belgrade, we are looking into the use of pulses for catalyst and material synthesis.

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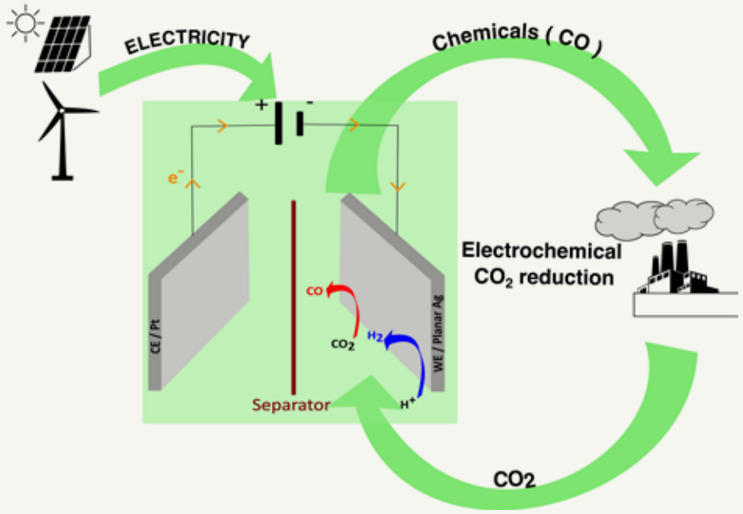
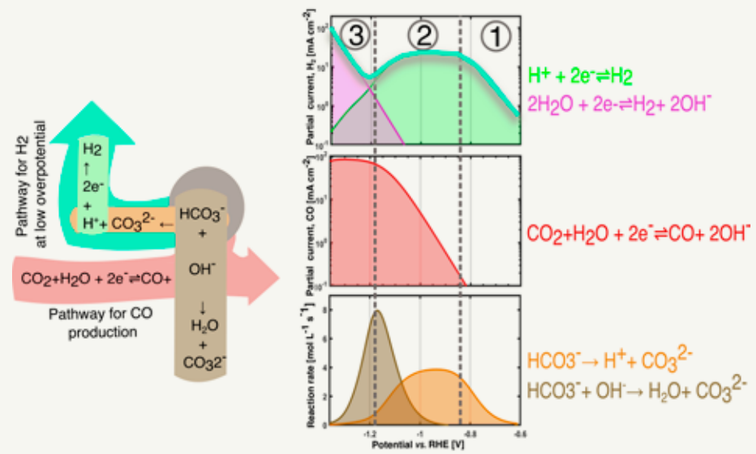


+ Figure 1:
eCO2RR Concept: Utilize renewable electricity, waste CO_2 feedstock streams, and water to sustainably produce carbon monoxide (CO). CE - Counter Electrode and WE - Working Electrode



+ Figure 2:
Complex reaction network of eCO2RR. (Left) two pathways depicting the production of CO and hydrogen in combination with buffer kinetics. (Right) top two figures show the partial currents of hydrogen (along with source of protons) and CO observed at different potentials; the bottom figure shows the buffer kinetics responsible for the change in the proton source.

Understanding and Driving the Electrochemical CO_2 Reduction Selectivity

+ Electrochemical CO_2 reduction (eCO2RR) stands as a cornerstone process for a sustainable future, offering a compelling pathway to mitigate climate change while simultaneously creating valuable resources. As illustrated in the schematic in Figure 1, by harnessing renewable electrical energy, eCO2RR can transform waste CO_2 from industrial emissions into a diverse range of useful chemicals and fuels. This includes not only the simple but industrially important carbon monoxide (CO), but also more complex carbon-containing compounds like methane, ethylene, and even higher-order hydrocarbons and alcohols. This versatility positions eCO2RR as a possible key player in the establishment of a circular carbon economy where CO_2 is not simply sequestered but actively recycled and transformed, closing the loop on carbon emissions and minimizing our reliance on fossil fuels.

However, driving the eCO2RR product selectivity and improving its efficiency remains challenging. This is partly due to a lack of understanding of the electrochemical mechanisms involved and the complex interplay of physicochemical processes influencing the reaction kinetics. Consequently, many observed experimental trends are not fully understood.

One intriguing phenomenon observed during eCO2RR, particularly on silver-based catalysts, is the "Z-shaped" behavior of the hydrogen evolution reaction (HER) current, which generally occurs as a side reaction when aqueous electrolytes are employed. An example is given in Figure 2 where the partial current densities of the main products obtained using silver as catalyst in bicarbonate buffer are depicted. This unusual trend (see the black curve) can be rationalized in three potential regions. The HER current initially increases (potential region 1), then decreases (potential region 2), and subsequently increases again with overpotential (potential region 3). This behavior directly impacts the Faradaic Efficiency of CO production (the main carbon product using silver as a catalyst), defining the potential window for its optimal selectivity.

Our research has delved into the underlying mechanism of this Z-shaped HER behavior, as it is a crucial step towards improving eCO2RR performance [1]. By developing a comprehensive model that integrates micro-kinetic and continuum approaches, we investigate the complex interplay between electrokinetics and homogeneous reactions within the bicarbonate electrolyte.

The decrease in HER current (see green curve in potential window 2), which gives rise to the Z-shape, is initiated after the onset of the eCO2RR (red curve). This is due to the generation of hydroxide ions (OH^-) during eCO2RR, which then react with bicarbonate (HCO_3^-) in the electrolyte as witnessed by the increase of reaction rate of the related reaction (see orange curve a). This consumption of HCO_3^- disrupts the equilibrium of the buffer reactions providing the protons (H^+) near the electrode surface (see brown curve and related reaction), leading to a decrease in their availability. Consequently, the rate of the HER, which relies on these protons, diminishes. However, at higher overpotentials (potential region 3), water reduction becomes the dominant mechanism for hydrogen production (see pink curve and related reaction), leading to a renewed increase in the HER current and completing the Z-shape.

Further, the use of dynamic operations to drive the selectivity of specific products was investigated [2]. It was found that the Faradaic efficiency to CO could be increased by modulating the electric input at specific frequencies and amplitudes. A theoretical investigation using the Nonlinear Frequency Response Analysis (NFRA) framework revealed that changes in selectivity are governed by the difference in the charge transfer coefficients between the CO2RR and the competing HER.

By elucidating the underlying mechanisms and identifying key influencing parameters, our work aims to pave the way for designing more efficient eCO2RR systems. Future research should focus on developing further refined mass transport models for more accurate prediction and optimization of eCO2RR performance across varying conditions.

| Dr.-Ing. Antonio Sorrentino, Monisha Sivasankaran

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Author **Dr.-Ing. Antonio Sorrentino**

Antonio Sorrentino successfully defended his PhD in 2021 within the Process System Engineering group at the Max Planck Institute in Magdeburg. He is currently working as team leader in the Electrochemical Energy Conversion group in the same institute. In his research, he combines modeling and experiments to develop diagnostic tools and to find optimal operating conditions for different electrochemical systems.

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Author **Monisha Sivasankaran**

Monisha Sivasankaran earned her Master's degree in Chemical and Energy Engineering from Otto von Guericke University in 2022. She joined the Max Planck Institute as a student assistant, contributing to the Molecular Simulation and Design and Electrochemical Energy Conversion groups, where she also completed her Master's thesis. Currently, she is pursuing her PhD in the Electrochemical Energy Conversion group, focusing on the dynamic operation in electrochemical CO_2 reduction.

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DMP | DATA-DRIVEN MODELING OF COMPLEX PHYSICAL SYSTEMS

+ Aerospace engineer Vahid Nateghi is working in the DMP group on data-driven techniques for modeling stochastic dynamical systems in the context of molecular dynamics.

DR. FELIKS NÜSKE I SENIOR SCIENTIST

+ The focus of the DMP group is the development and theoretical analysis of machine learning methods for complex (stochastic) dynamical systems, especially for applications in physics and chemistry. Dynamical systems play a central role in nearly all areas of science and technology. At the same time, they also pose a number of fundamental challenges. Modelers and practitioners must find ways of dealing with vast computational costs, high-dimensional data, and significant model uncertainties. Data-driven methods have gained traction in this context, as it has been shown that models learned from simulation or measurement data can be used to predict complex behavior, or to determine optimal control policies. The DMP group was established in August 2022 to strengthen MPI's research activities in this exciting area of research.

Research Scope

The main driving force for our research is understanding dynamics at the molecular scale. Molecular systems and their interactions essentially determine the function of biological organisms, the properties of materials, or the efficiency of chemical reactions. To simulate their dynamics on a computer, one would have to solve Schrödinger's equation in quantum mechanics, which can only be done for small systems. Researchers therefore need to rely on a cascade of approximations operating on different levels of resolution, such as classical molecular dynamics (MD) simulations. Besides the inherent model uncertainties, simulating even these classical approximations often exceeds the capabilities of current HPC systems.

A central building block for our research is the theory of Koopman operators. These have long been known as a class of linear models to forecast measurement values under an evolving dynamical system. They have found a renaissance with recent advances in machine learning, with the basic extended dynamic mode decomposition (EDMD) method becoming the workhorse algorithm. We use Koopman models to analyze and predict the dynamics of complex molecular systems, learn reduced representations, and optimize selected properties. The research topics we have addressed in the past two years include the following:

High-dimensional Approximation

Koopman models rely on an appropriate basis set, which is subject to the curse of dimensionality in high dimension. One approach we have pursued is to employ low-rank tensor representations. Although the Koopman learning problem usually does not come with a known low-rank structure, our work has shown that such representations can be learned from the data instead, and the resulting methods can be used to analyze molecular simulation data. An alternative approach is to define the basis set implicitly by a reproducing kernel and by the data. Here, we have investigated the efficient solution of resulting linear algebra problems, for instance using random Fourier features, consistently leading to parameter-efficient Koopman models even for challenging applications.

Finite-data Error Bounds

Another strand of our work concerns the derivation of probabilistic bounds for the finite-data estimation error of Koopman models. We have developed a theoretical framework to analyze this error with an emphasis on estimation from non-i.i.d data. We have derived estimation error bounds for different settings including kernel-based EDMD and for systems with control input.

Model Reduction and Sampling

We have worked on two ways to mitigate the problem of excessively long simulation times. First, coarse grained (CG) models are lower-dimensional surrogates aimed at representing the original system dynamics. We have presented an efficient kernel-based approach to infer the parameters of CG models using approximations to the Koopman generator; see the following spotlight by Nateghi et al. Another strategy to lighten the computational effort is to accelerate the system's exploration of state space by adding a bias to its original dynamical equations. We have started to explore ways of formulating this goal as a data-driven optimal control problem. We have successfully studied this problem using Funnel controllers, and using Koopman-based surrogate models for stochastic control.

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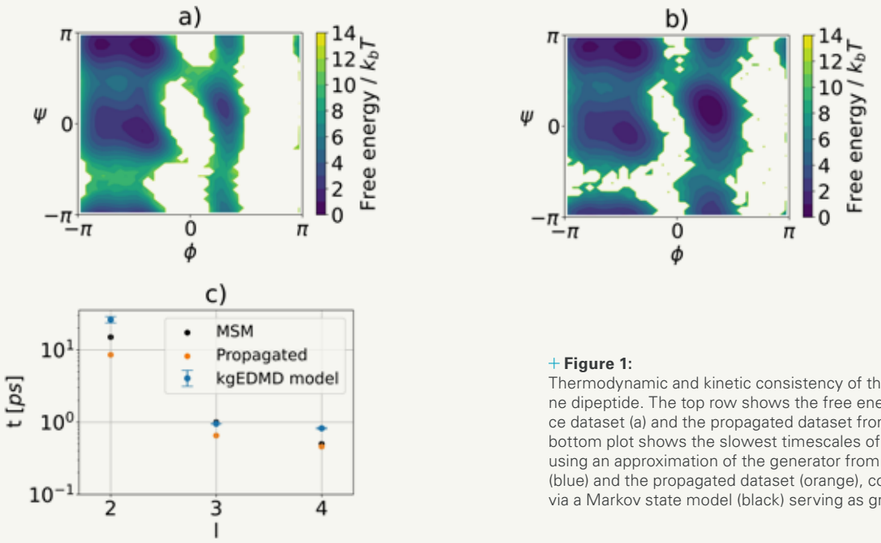

Figure 1:
Thermodynamic and kinetic consistency of the learned model for Alanine dipeptide. The top row shows the free energy surface of the reference dataset (a) and the propagated dataset from the learned SDE (b). The bottom plot shows the slowest timescales of the molecule calculated using an approximation of the generator from the reference dataset (blue) and the propagated dataset (orange), compared to those obtained via a Markov state model (black) serving as ground truth.

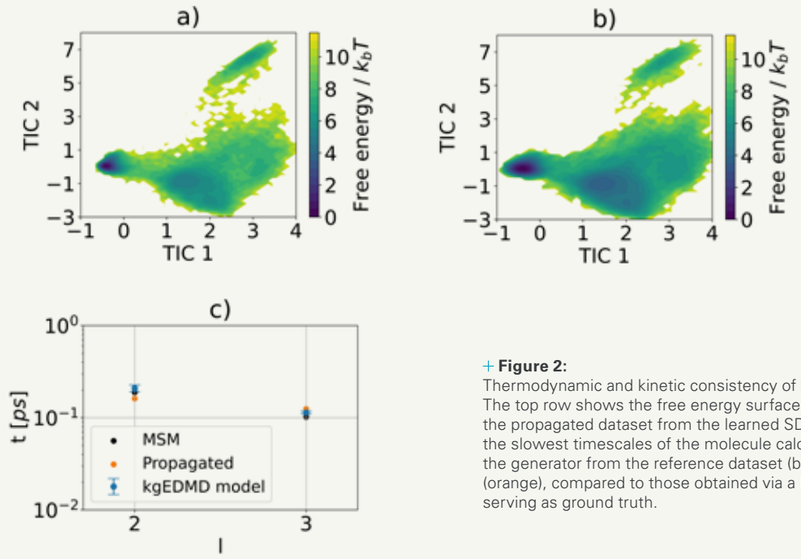

Figure 2:
Thermodynamic and kinetic consistency of the learned SDE for Chignolin. The top row shows the free energy surface of the reference dataset (a) and the propagated dataset from the learned SDE (b). The bottom plot shows the slowest timescales of the molecule calculated using an approximation of the generator from the reference dataset (blue) and the propagated dataset (orange), compared to those obtained via a Markov state model (black) serving as ground truth.

Kinetically Consistent Coarse Graining with Koopman Operators

Metastability

Stochastic simulations of large-scale dynamical systems are widely used to model the behavior of complex systems, with applications in computational physics, chemistry, materials science, and engineering. A common characteristic of such systems is high dimensionality coupled with metastability. **Metastability** implies that the system exhibits prolonged residence times within specific regions of its configuration space, rarely transitioning to other such regions. As a consequence, it becomes necessary to produce very long simulations in order to make statistically robust predictions. Specialized high-performance computing facilities are required to reach the sufficient simulation times, or it may just not be feasible at all.

Coarse Graining

Coarse graining (CG) tackles the aforementioned challenge by replacing the original dynamical system with a surrogate model in a (much) lower-dimensional space, in such a way that certain properties of the original dynamics are preserved by the surrogate model. CG models can enable scientists to achieve much longer simulation times because of the reduced computational cost, while maintaining the predictive capabilities of the full-order model.

Setting up a CG model typically requires two steps. First, selecting a linear or non-linear mapping (CG map) from full-state space to a lower-dimensional space, where the latter serves as the state space of the surrogate model. Second, definition of a parametric model class for the surrogate dynamics.

Kinetic Properties

Many existing methods are geared towards ensuring **thermodynamic consistency**, which means that the surrogate model is trained to sample the marginalized Boltzmann distribution in CG space, thus ensuring accurate estimation of average quantities. Ensuring faithful reproduction of **kinetic** properties, such as time-correlation functions or transition time scales, is a much less developed topic. In this project, we focus on recovery of the transition time scales associated with metastable states.

Transition rates and time scales are directly related to the leading spectrum of the system's Koopman operator ([1]) or its associated generator, which is the linear operator propagating expectation values of observable functions in time.

Kernel-based Koopman Generator Extended Dynamic Mode Decomposition

We parametrize the components of the CG model as a linear expansion using a fixed set of basis functions defined by a reproducing kernel. The leading eigenvalues of the Koopman generator can be inferred using an algorithm called kernel-based generator Extended Dynamic Mode Decomposition (**kgEDMD**), formalized in Reference [2]. The resulting transition rates serve as a reference to be reproduced by the CG model learned in the next step.

Identifying the Stochastic Differential Equations

In addition to transition rates, the project aims at identifying the dynamics of the system in CG space in the form of a stochastic differential equation (SDE). Our algorithm involves solving two optimization problems to derive the effective drift and diffusion terms, which are then used to formulate the SDE for predictive purposes.

Our approach only requires simulation data of the full system, the choice of the kernel function, and measurements of the local diffusion, which is analogue to the local mean force in the popular force matching method ([3]). Combined with the latter, this approach provides complete access to the effective dynamics associated to a reversible system.

Application to Molecular Systems and More

We tested the developed algorithm via two examples of molecular dynamics simulations, namely of the Alanine-dipeptide and the 10-amino-acid mini-protein Chignolin. The results showed that the learned effective dynamics is able to reproduce both thermodynamic and kinetic quantities of the full dynamics with high accuracy. The details can be found in Reference [4].

One of the future directions we are aiming at is to simultaneously optimize the CG mapping along with the parameters of the CG model, for instance by balancing the VAMP score ([5]) versus the complexity of the CG model. Scalability of the algorithm is another direction we are interested in to be able to tackle larger proteins with limited computational resources.

| Vahid Nateghi

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Vahid Nateghi received his Bachelor's degree in Aerospace Engineering from Sharif University of Technology in 2018. He then studied Space Engineering and graduated from Politecnico di Milano in 2021. In 2022, he joined the DMP research group as a Ph.D. student working on data-driven techniques for modeling stochastic dynamical systems in the context of molecular dynamics.

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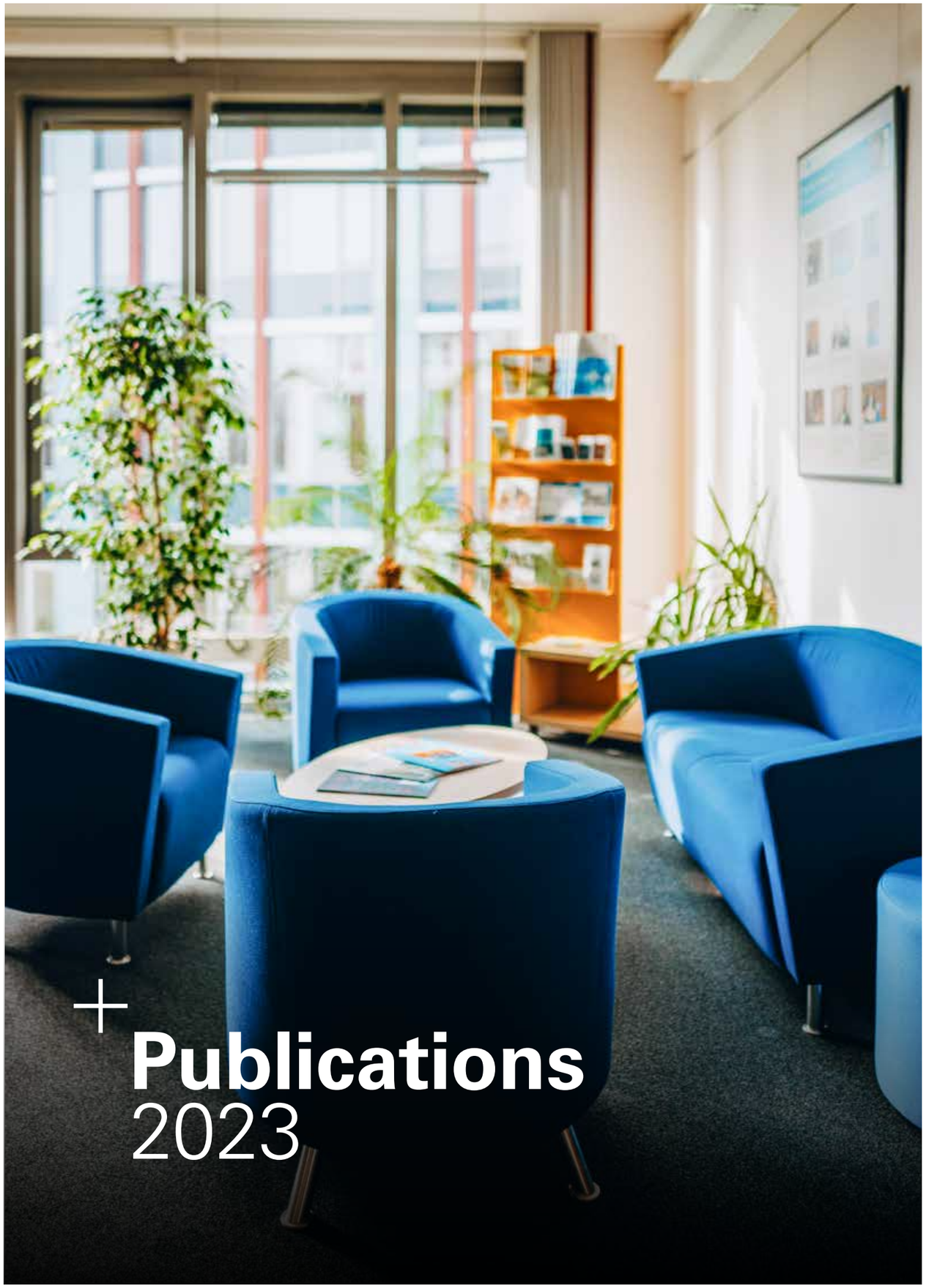

Publications 2023

The vast majority of publications can be downloaded from our website: MPI Authors are marked in bold letters.

SCAN ME

Journal Articles

Abayzeed, S., Anwar, T., Barnaveli, A., Bazant, M. Z., Bocquet, L., Donev, A., Dryfe, R. A., Faez, S., Janardanan, A., Jiménez-Ángeles, F., Kamsma, T. M., Kanoufi, F., Kornyshev, A. A., Lemay, S. G., Levin, Y., Marbach, S., Montes de Oca, J., Robin, P., Siwy, Z. S., Stein, D., van Roij, R., **Vidaković-Koch, T.** et al. (2023). Iontronic coupling: general discussion. *Faraday Discussions, 246*, 157-178. doi:10.1039/D3FD90031B.

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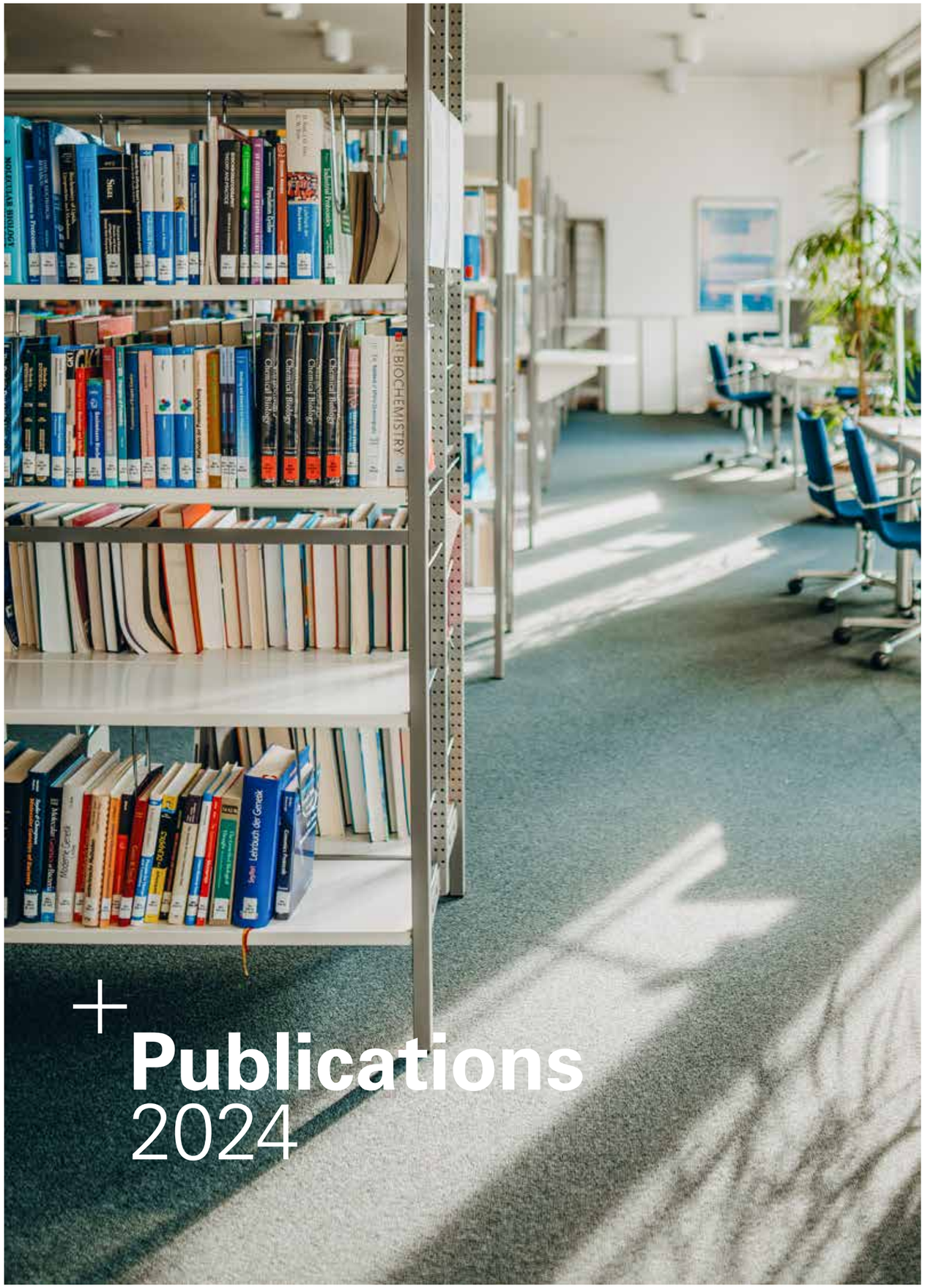

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