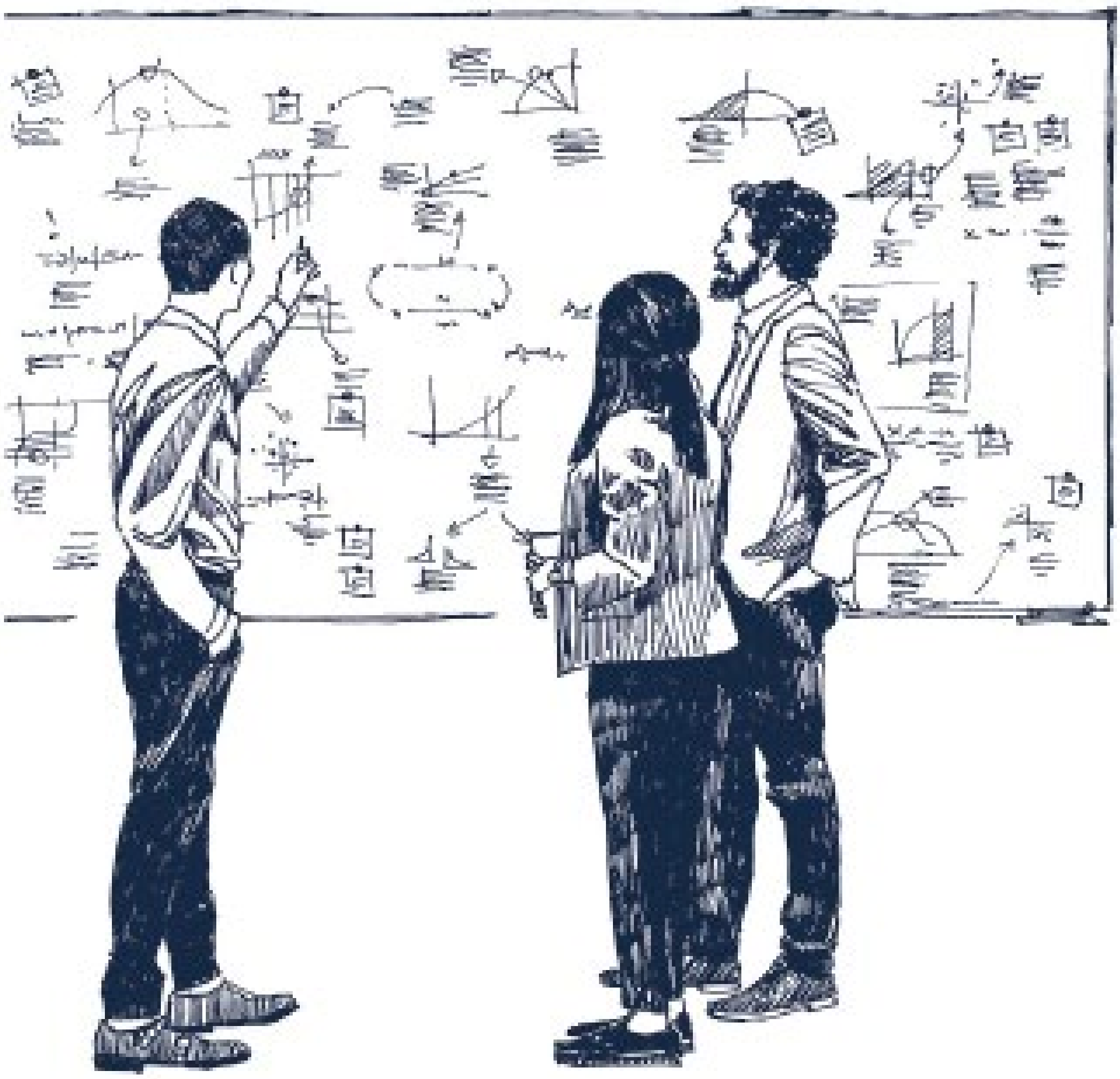
Institute for Advanced Study
Technical University of Munich



2024

Annual Report

Institute for Advanced Study

In 2025, our Institute is celebrating its 20th anniversary. Read more online about research, results, and successes from 20 years.

www.ias.tum.de/ias/institute-for-advanced-study/tum-ias-2005-2025

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TUM President's Foreword

A year ago, I called on us as scientists to uphold our values, lead by example, and take on our responsibility to future generations.

Twelve months later, this message holds greater relevance than ever. Germany is navigating a fundamental transformation of its industrial landscape amid rising geopolitical and social uncertainties. At the same time, trust in both politics and science is eroding. There is a widening gap between scientific facts and public discourse in large segments of society and politics. This growing divide poses a serious risk to the stability of our democracies.

In these challenging times, universities have a critical role to play. They educate the next generation – impacting 2.9 million students in Germany alone – while also ensuring the continuous creation of reliable knowledge, setting it apart from misinformation. Beyond this, they serve as key drivers of knowledge and technology transfer to society. Today, a new wave of entrepreneurial spin-offs is emerging from our universities, reinforcing the foundation of a strong and resilient economy.

Universities, with their broad research spectrum and innovative projects, have a responsibility to serve as a trusted point of reference for national and global challenges. Advancements in fields such as energy research, mobility, and quantum technologies do not stop at national borders. By fostering collaboration within Germany, across Europe, and around the world, universities help bridge divides and drive progress through cooperation.

Actions speak louder than just words!
Amid rapid technological, economic, and social change, universities are uniquely positioned to shape the future. Engaging young people early and deeply in research and its application to society is essential. That is why, at TUM, we are launching the TUMorrow Factory – a new facility designed for TUM Student Clubs. Equipped with workrooms, offices, and a large central workshop, it will provide students with the resources to turn their ideas into tangible prototypes and pioneering innovations.

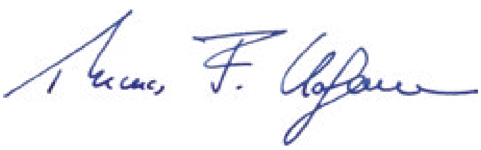
Aspiring entrepreneurs find a unique environment across 12 TUM Venture Labs, which span key research areas at our university. These labs provide opportunities to develop essential skills in future technologies, access venture capital, and connect with economic markets from diverse industries to support business development.

At the same time, we are firmly convinced that the future of teaching and research lies in interdisciplinarity. In a recent Times Higher Education (THE) ranking on research across disciplines, TUM secured the top spot in Germany and ranked 12th worldwide! Guided by the belief that future innovations emerge from a culture of interdisciplinary cooperation and the convergence of disciplinary strengths, TUM has prioritized these values. In recent years, it has established interdisciplinarity – alongside internationality – as a core principle of its development.

The TUM Institute for Advanced Study (TUM-IAS), the International Graduate School of Science and Engineering (IGSSE), and the TUM Innovation Networks have greatly enhanced interdisciplinary collaboration. Additionally, the shift to a matrix structure of Schools and Integrative Research Centers has further strengthened this approach. A prime example of this is the inaugural TUM-IAS Dieter Schwarz Courageous Research Grant in 2024, awarded to Jennifer Rupp (TUM) and Fikile Brushett (MIT). Their project on low-cost solid-state ceramic conductors and sustainable redox flow batteries combines chemistry, artificial intelligence, and sustainability.

Students have the opportunity to expand their talents and skills beyond their core disciplines through initiatives such as the TUM Student Clubs, TUM Project Weeks, and plug-in modules. These programs open doors to diverse career paths and encourage growth across multiple fields.

I am thrilled to see the success of these initiatives and TUM's transformative work culture now being clearly reflected in the university rankings. This achievement is a testament to the dedication of our entire TUM community. My deepest gratitude goes to our students, staff, professors, Fellows, and the many supportive friends and partners whose commitment and effort have brought our university to where it stands today. ■



Prof. Thomas F. Hofmann
President

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TUM-IAS Director's Message

2024 was again a successful year for the TUM Institute for Advanced Study: New programs were successfully implemented, partnerships further strengthened, and new Fellows warmly welcomed, while departing Fellows left with lasting relationships. The TUM-IAS also hosted several major conferences organized by its Fellows and their TUM host professors, attracting hundreds of international guests.

Our shared goal is to create new knowledge. In today's complex world, achieving this relies on scientific cooperation that transcends the borders of states, government systems, religions, and skin colors. I remain confident and optimistic because I believe in science's unifying spirit of cooperation. The year 2024 has reaffirmed this belief.

In 2024, we engaged with other German Institutes for Advanced Study, exchanging ideas and fostering dialogue. Despite differences in funding models and institutional connections, we are united by the commitment to supporting creative talent in transforming innovation into secure knowledge.

Our in-depth exchange with the IAS in Princeton through its Director David Nirenberg and the management team has been a source of encouragement – particularly in times of international tension and upheaval. It has reinforced our commitment to maintaining and perhaps even expanding spaces for shared reflection and scientific creativity to ensure the continuous flow of knowledge.

New knowledge will be essential in many areas, not only in the natural and engineering sciences but also in medicine and life sciences, as well as for shaping the future direction of our national communities and cooperation. Finally, and this will be a long-term endeavor, we will need the knowledge to embed sustainability into our economy, society, and daily lives.

Demonstrating its commitment to promoting sustainability and addressing related challenges across disciplines, the TUM-IAS has continued the Seminar Series of European Universities on Sustainability, launched in the autumn of 2023. Six scientists from the National Technical University of Ukraine, Poznań University of Life Sciences in Poland, Riga Technical University in Latvia, the University of Freiburg, and the Tallinn University of Technology in Estonia shared insights of their research as part of our weekly Scientists meet Scientists series.

For the first time in 2024, the TUM-IAS awarded the Dieter Schwarz Courageous Research Grant, uniquely combining sustainability and digitalization.

Thanks to our partnership with the Nobel Sustainability Trust (NST), TUM and the NST were able to jointly honor the winners of the Sustainability Award 2024. In December 2024, we mourned the loss of our friend and supporter, Michael Nobel. His passing is a great loss for the Nobel Sustainability Trust, of which he was a founder, as well as for TUM and global sustainability efforts.

In 2024, our successes would not have been possible without the generosity of our friends and supporters. I express my sincere gratitude to the Siemens AG, the TÜV SÜD Foundation, the Dieter Schwarz Foundation, the Nemetschek Innovation Foundation, and the Nobel Sustainability Trust. Your support has been crucial in turning our ideas into reality, getting new things off the ground, and potentially paving the way for future initiatives. ■

M. Molls

Prof. Michael Molls
Director

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Actions, Awards, Events

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Actions

Pioneering research and sustainability stand at the core of TUM-IAS. In 2024, we successfully implemented activities that we had initiated for the first time or drove programs forward, while also starting new initiatives.

Dieter Schwarz Courageous Research Grant

The Dieter Schwarz Courageous Research Grant is funded by the Dieter Schwarz Foundation to promote bold and visionary project ideas. This new Fellowship is open to outstanding international scientists from outside TUM who, together with a TUM research group, intend to use groundbreaking technology to propose a radical solution to a major challenge in **"Digitization and Sustainability."** The grant is comprised of a total amount of one million euros. The first recipient of the Dieter Schwarz Courageous Research Grant, awarded in 2024, is **Fikile Brushett**, Professor of Chemical Engineering at MIT. Together with their host, **Jennifer Rupp** (Professor for Solid-State Electrolytes at TUM), this Focus Group aims to conceptualize, synthesize, and integrate solid-state conductors with high conductivity and per-

SAP Research Center.

Siemens Technology Center.

fect selectivity into electrochemical energy systems. Through modeling and experiment, they aim to expand the library of fundamental knowledge on the behavior of solid-state conductors in contact with liquid electrolytes, establish design criteria for competitive embodiments, and pioneer proof-of-concept prototypes that illustrate the transformative potential of this approach (see also Chapter “Welcoming Our New Fellows”).

Industry on Campus

Together with top-tier research partners from industry and business, we at TUM are tackling future challenges and researching innovative solutions. Two long-standing partners, Siemens and SAP, have each opened new research centers on the TUM Garching Campus – investments exceeding 200 million euros and providing space for over 1,000 employees. More than 20 TUM professors have also relocated to offices in these state-of-the-art buildings. TUM-IAS has maintained a strong partnership with Siemens for many years. Since 2018, the company has funded 12 Fellowships at TUM-IAS, supporting cutting-edge research. Building on this partnership, Karin Nachbagauer and Wil Schilders, both Siemens Fellows at TUM-IAS, have already held several meetings at Siemens to advance their research collaborations.

Meetings with IASs in Germany and in Princeton/USA

There are 23 IASs in Germany, each with distinct focuses, objectives, funding structures, and institutional affiliation. However, they all share a common goal: to promote and support research excellence and talent. After the COVID-19 pandemic, interactions intensified again, with meetings held near Bremen in 2023 and Essen in 2024. ►


„INKUBATORFUNKTION FÜR DIE WISSENSCHAFT“

PROF. DR. KERSTIN SCHILL

DR. ULRICH MARSCH

These gatherings provided an opportunity to exchange experiences, discuss shared challenges, and evaluate the pros and cons of the various funding models.

In an extended interview with the "Deutsche Universitätszeitung" (German University Magazine, No 8/2024, circulation 20,000), **Kerstin Schill** (Professor for Cognitive Neuroinformatics and Director of Hanse Wissenschaftskolleg Delmenhost/IAS) and **Ulrich Marsch** (Managing Director of TUM-IAS) discussed the crucial role of IAS in German science, emphasizing its incubator function for emerging research topics.

IAS Princeton, New Jersey/USA

The first institute of its kind, the Institute for Advanced Study in Princeton, inspired the creation of the TUM-IAS. Strong relationships have existed for some time with other IASs in the UK and Canada. An initial meeting with **David Nirenberg** (Director and Leon Levy Professor at the Institute for Advanced Study) in Munich in February was later continued in Princeton in November. Together with his management team, questions and opportunities for collaborative research were discussed,

Linden-Tree at IAS Princeton, planted by Robert Oppenheimer.

Einstein statute at Princeton garden. Left to right: Michael Molls, Morwenna Joubin, Ulrich Marsch.

as well as potential consequences of Donald Trump's new presidency, ongoing scientific developments, and future collaboration prospects.

Seminar Series of European Universities on Sustainability

In its commitment to fostering sustainability and addressing related challenges across various disciplines, the TUM-IAS has continued the Seminar Series of European Universities on Sustainability, which was launched in the autumn of 2023. A total of six scientists from the National Technical University of Ukraine, Poznań University of Life Sciences in Poland, Riga Technical University in Latvia, the University of Freiburg, and the Tallinn University of Technology in Estonia presented an overview of their research during our weekly Wednesday Coffee Talk series. In 2024, we continued our seminar series with these talks:

- **Prof. Serhii Voitko (National Technical University of Ukraine)**
  Sustainable development methodology as a tool for researching the state of countries and making decisions, January 31, 2024

- **Dr. Victoria Takacs (Poznań University of Life Sciences, Poland)**
  Stakeholder engagement in nature conservation science – need or must?, May 29, 2024

- **Prof. Inga Zicmane (Riga Technical University, Latvia), Prof. Svetlana Beryozkina (College of Engineering and Technology, American University of the Middle East, Kuwait)**
  Go2Green – Towards Sustainable and Clean Energy Transition, June 26, 2024

- **Prof. Michael Zgurovsky (National Technical University of Ukraine, "Igor Sikorsky Kyiv Polytechnic Institute")**
  Main Threats to the Sustainable Development of Global Society in a Conflicting World, October 30, 2024

- **Dr. Neelesh Yadav (Tallinn University of Technology, Estonia)**
  Partial Power Converter and Its Emerging Applications, December 4, 2024 ▸

TUM-IAS Fellowship Call

Anticipating the arrival of our new Fellows in 2025, we reflect on the 16 Fellowships granted in 2024 distributed among various Fellowship categories: Hans Fischer (Senior) Fellowship, Dieter Schwarz Fellowship, Dieter Schwarz Courageous Research Grant, Rudolf Diesel Industry Fellowship, Anna Boyksen Fellowship, Albrecht Struppler Clinician Scientist Fellowship, and Philosopher in Residence Fellowship.

We are delighted to welcome these newly appointed Fellows from Australia, China, Denmark, Germany, Great Britain, Italy, Turkey, and the USA!

To learn more about our newest Fellows, please consult the chapter "Welcoming Our New Fellows."

Rudolf Mößbauer Tenure Track Assistant Professorships

For over a decade, TUM has been selecting promising young talents as Tenure Track Assistant Professors (W2) after a thorough selection process organized by the TUM-IAS. The TUM Faculty Tenure Track represents a performance-oriented career model for young scientists with international experience, providing the realistic prospect of advancing to a tenured W3 professorship from the beginning.

This TUM-IAS Fellowship is named in honor of TUM professor Rudolf Mößbauer (1929–2011), a Nobel Prize laureate in Physics (1961) for his groundbreaking research concerning the resonance absorption of gamma radiation and his associated discovery of the effect that bears his name. As the emphasis of the Professorship lies on the creative development of a new field of science and/or technology, and as we intend to offer those young researchers the best possible career start, they are equally affiliated with the TUM-IAS as Fellows.

In 2024, four new Rudolf Mößbauer Tenure Track Assistant Professors were appointed. For detailed information on our new Fellows, please see chapters "Events" and "Welcoming Our New Fellows."

Visiting Alumni Fellowship

Following the COVID-19 pandemic, we have relaunched the Alumni Visiting Fellowships to allow our Alumni Fellows to stay in touch with their former hosts, enter into long-term collaborations, or plan new projects. The Start-up Fund funds workshops and seminars to plan new projects and meet with participating researchers. 16 Fellows took advantage of these new offers in 2024.

TUM Ambassadors

Many international scientists have enriched our university with their expertise and experience over the past decades. Since 2013, once a year, the President awards the honorary title of "TUM Ambassador" to those who have particularly enriched TUM with their scientific expertise and international experience during their stay. They are links between TUM and the international academic research and industry community. The dedicated participation of TUM Ambassadors as ambassadors and advisors strengthens our global network and promotes the exchange of knowledge on an international level. TUM Ambassadors are Members of our TUM-IAS and can apply for annual funding to return to TUM for research and guest stays.

2024 Ambassadors are:

- **Gustavo Henrique Goldman,** Alumnus TUM-IAS Hans Fischer Senior Fellow and Universidade de São Paulo, Brazil
- **Ron M. A. Heeren,** TUM-IAS Hans Fischer Senior Fellow and Maastricht University, Netherlands
- **Noelle Selin,** Alumna TUM-IAS Hans Fischer Senior Fellow and Massachusetts Institute of Technology, USA
- Henrik Selin, Alumnus TUM-IAS Hans Fischer Senior Fellow and Boston University, USA
- **Iris Tommelein,** University of California, Berkeley, USA

Outreach

TUM-IAS has undertaken a variety of activities to promote its outreach further. We participated in the TUM Sustainability Day and the Open Doors Day with presentations. We continued and expanded the new series of video portraits of our fellows which can be watched on our website. Together with Siemens, we presented the work of our Siemens-supported Fellows in several podcasts. In our weekly "Wednesday Coffee Talks: Scientists meet Scientists," we presented current research topics of our Fellows from TUM to an interested scientific public. Three times a year, the "Garching Talks," organized by TUM-IAS, present scientific topics to a broader circle of interested citizens from the city of Garching.

Michael Nobel: An entrepreneur, philanthropist, and friend of the TUM-IAS

Michael Nobel (born February 3, 1940) was a great-grand-nephew of Alfred Nobel. He co-founded the Nobel Sustainability Trust (NST) in 2007 with other members of the Nobel family.

After studying psychology at the University of Lausanne, Michael Nobel worked as a researcher in social sciences at the Institute for Mass Communication at the University of Lausanne, as well as a consultant to UNESCO in Paris and the United Nations Division of Social Affairs in Geneva, focusing on methods for substance abuse prevention. As an entrepreneur, he played a key role in bringing a novel nuclear magnetic resonance imaging method to market maturity.

In later years, he dedicated himself to sustainability, especially in renewable energy and clean tech sectors, as an advisor and board member for international companies and NGOs.

In 2022, the Nobel Sustainability Trust officially entrusted TUM and its Institute for Advanced Study as an academic partner to lead the international selection process for the Sustainability Awards.

We mourn the passing of a dear friend and supporter. We will remember him as a warm-hearted, sharp-thinking, and creative individual whose vision of sustainability was rooted in the harmony of technological progress, nature conservation, and economic prosperity. ■

Michael Nobel and Michael Molls at the Sustainability Summit in Munich in 2023.

Awards

We are delighted and proud that our Fellows and Members have again received top-class awards in 2024.

ERC Synergy Grant for TUM-IAS Fellow Daniela Pfeiffer

Daniela Pfeiffer (TUM-IAS Albrecht Struppler Clinician Scientist Fellow and Professor for Radiology at TUM) and the project **SmartX** received an ERC Synergy Grant of up to 10 million euros.

The SmartX project is researching more detailed imaging procedures to diagnose lung diseases better and earlier. The focus is on chronic obstructive pulmonary disease (COPD). Conventional X-rays and CT scans are often inadequate for the early detection of COPD and are associated with high radiation doses. The project aims to develop a new type of detector for the dark-field X-ray procedure that requires 50 percent less radiation dose than the already low-radiation procedure. An X-ray detector is the counterpart to the radiation source and produces the X-ray image. While conventional X-rays are based on the attenuation of the X-ray light, the dark-field X-ray developed at TUM uses the so-called small-angle scattering of the X-ray light. This allows additional information to be obtained about the nature of the microstructure of the lung tissue.

Project partners are the Instituto de Biomedicina in Valencia/Spain and the EPFL in Lausanne.

ERC Consolidator Grant for Rudolf Mößbauer Tenure Track Assistant Professor Andreas Reiserer and former Mößbauer Professors Michael Knap and Matthias Nießner

Andreas Reiserer (Professor for Quantum Networks at TUM) won his Consolidator Grant for his project **OpENSpinS,** aiming to combine the wide bandwidth and long reach of photons (light particles) with the reliable and long-lasting storage of qubits in silicon. Silicon, well-known as the standard material in microelectronics, serves as the foundation. Instead of electronic spins, the team aims to use the durable nuclear spins of erbium atoms, which can be entangled using light. This approach seeks to enable qubits to be interconnected over greater distances – a critical step towards building larger quantum networks.

Michael Knap's (Professor for Collective Quantum Dynamics at TUM) project **DynaQuant** investigates how specific properties of quantum states can be leveraged to develop more robust and efficient systems. The focus is on topological quantum states with particularly exotic properties. The aim is to develop new methods to better understand the behavior of these states, especially under non-equilibrium conditions. The results could contribute to the development of new quantum technologies and significantly advance secure data processing.

Matthias Nießner (TUM-Professor for Visual Computing) is tackling the following challenge in his project **Gen3D: Learning to Create Virtual Worlds:** Until now, creating realistic 3D content has been very time-consuming and labor-intensive. Previous methods for automating the process do not come close to the quality of the work of artists who design virtual worlds by manual labor. Matthias Nießner develops generative models that generate 3D polygon meshes and their surface textures and material properties. These models can be used directly by modern graphics systems. He uses images and videos as training data. As these only partially show the 3D world, the models must also learn to deal with incomplete data.

Medical AI researcher Daniel Rückert receives the Leibniz Prize

IAS-Member Daniel Rückert (TUM-Professor of Artificial Intelligence (AI) in Medicine and Healthcare) has been honored for his research on AI-assisted medical imaging. The most important German research prize is endowed with 2.5 million euros by the German Research Foundation (DFG).

Daniel Rückert.

Daniel Rückert has developed pioneering methods with which AI algorithms can generate particularly informative images from computer tomography or magnetic resonance imaging, analyze them, and interpret them for improved medical diagnostics. Supported by the Alexander von Humboldt Foundation, TUM brought the top scientist from Imperial College London to Munich in 2020. Daniel Rückert studied computer science at the Technical University of Berlin and received his doctorate from Imperial College London in 1997. He was Professor of Visual Information Processing and Dean of the Department of Computing at Imperial College. He has published numerous highly cited scientific articles, led several large research projects, and is the founder of a start-up that uses his research results for faster and more precise clinical trials of drugs.

TUM Golden Ring of Honor for TUM-IAS Director Michael Molls

The highest award that TUM can bestow, the Golden Ring of Honor, was awarded to TUM-IAS Director Michael Molls. He receives the award in recognition of his many years of service to science. From 1992 to 2014, Michael Molls was Professor and Director of the Clinic for Radiotherapy and Radiation Oncology at the TUM University Hospital rechts der Isar. As co-spokesperson, Michael Molls has been responsible for the biomedical research area of the Munich Center for Advanced Photonics (MAP), a Cluster of Excellence of the German Research Foundation. In 2016, he was elected as chairperson of the TUM Senior Excellence Faculty, with a seat on the TUM Extended Board of Management and the Board of TUM. Since 2020, he has served as Director of the TUM Institute for Advanced Study. ►

TUM President Thomas F. Hofmann and Michael Molls.

TUM Golden Ring of Honor.

TUM President Thomas Hofmann said: “Although he officially ‘retired’ more than 10 years ago, his commitment remains undiminished. As Director of the TUM Institute for Advanced Study and Speaker of the TUM Senior Excellence Faculty, he continues to be one of the most dynamic and creative minds at our university. His work is living proof that scientific excellence and innovation are timeless.”

The Golden Ring of Honor of the TUM is a prestigious award that is presented to persons who have far surpassed their duty in making outstanding contributions to research, teaching, the promotion of young scientists, or educational and university policy. Personalities such as Eberhard von Kuenheim (former CEO of BMW AG) or Rudolf L. Mößbauer (Nobel Prize Physics 1961) also received the Golden Ring of Honor.

Highly Cited Researchers

When scientists write research papers, they cite the most important papers that have already been published. Therefore, the total number of times a paper is cited is a good indicator of the quality of the research. To identify the most highly cited researchers, the US company Clarivate annually analyzes its Web of Science database, which covers scientific publications in various disciplines.

The latest evaluation lists the scientists who were cited most frequently in their subject areas in the period from 2013 to 2023. Researchers frequently cited in multiple fields are listed in the Cross-Field category. The list contains the names of about 6,900 persons in no specific order, including the following TUM-IAS Fellows or Alumni Fellows:

- **Laura Herz** (Cross-Field), University of Oxford, Alumna TUM-IAS Hans Fischer Senior Fellow
- **Ingrid Kögel-Knabner** (Cross-Field), Alumna TUM-IAS Carl von Linde Senior Fellow
- **Bernhard Küster** (Cross-Field), Alumnus TUM-IAS Carl von Linde Senior Fellow
- **Melanie Schirmer** (Cross-Field), TUM-IAS Fellow as Rudolf Mößbauer Tenure Track Assistant Professor
- **Robert Schmitz** (Cross Field) University of Georgia, TUM-IAS Alumnus Hans Fischer Fellow
- **Thaddeus S. Stappenbeck** (Cross-Field), Washington University, Alumnus TUM-IAS Hans Fischer Senior Fellow
- **Ib Chorkendorff** (Chemistry), DTU Copenhagen, Alumnus TUM-IAS Hans Fischer Senior Fellow
- **Yang Shao-Horn** (Chemistry), MIT, TUM-IAS Hans Fischer Senior Fellow
- **Yang Shao-Horn** (Environment and Ecology), MIT, TUM-IAS Hans Fischer Senior Fellow
- **Naomi Halas** (Material Science), Rice University, Alumna TUM-IAS Hans Fischer Senior Fellow
- **Peter Nordlander** (Material Science), Rice University, Alumnus TUM-IAS Hans Fischer Senior Fellow

Euler medal for former TUM-IAS Director Ernst Rank

Ernst Rank, Professor emeritus for Computation in Engineering and former TUM-IAS Director, has been awarded the Euler medal by the European Community on Computational Methods in Applied Sciences (ECCOMAS). He was awarded the medal during the ECCOOMAS Congress in Lisbon/Portugal in June 2024. The Euler medal, one of the highest distinctions of the society, is awarded for outstanding and sustained contributions to the area of computational solid and structural mechanics.

Ernst Rank.

Carl Friedrich von Siemens Research Award for Noelle Eckley Selin

Noelle Eckley Selin (Alumna TUM-IAS Hans Fischer Senior Fellow and Professor at the Institute for Data, Systems, and Society at MIT) has been awarded the prestigious Carl Friedrich von Siemens Research Award by the Alexander von Humboldt Foundation. The prize is awarded to internationally leading researchers of all disciplines from abroad in recognition of their academic record. ▸

She is internationally known for her research contributions to atmospheric chemistry and sustainability science. Noelle Selin has developed and applied models tracing the conceptual pathways by which policies to mitigate air pollution and climate change affect the atmosphere, human health, and society. She developed the first global coupled land-ocean-atmosphere simulation of mercury pollution, using the GEOS-Chem chemical transport model, now used worldwide to answer this question. Working with political scientists, she has examined how science can inform policy processes, empirically testing how models affect decision-making and engaging with communities in shaping, conducting, and communicating research.

Polina Bayvel (University College London, UK) and Meisong Tong (Tongji University, Shanghai) honored with the Carl Friedrich von Siemens Research Award by the Alexander von Humboldt Foundation – and as such, Member of the TUM-IAS

Multi-wavelength optical networks form the foundation of the global digital information infrastructure. In 1994, **Polina Bayvel,** Professor of Optical Communication, founded the Optical Networks Group (ONG) at University College London, which developed into a leading research institution in high-speed communication over optical fiber networks. The Humboldt Research Award will intensify cooperation on using multi-mode fiber for long-range optical transmission technology and expanding communication via standard single-mode fiber to non-conventional bands to multiply transmission capacity. Gerhard Kramer hosts Polina Bayvel at the Technical University of Munich, Chair of Communications Engineering.

Meisong Tong is well known internationally for his outstanding research in computational electromagnetics and related topics. He has significantly contributed to developing the state-of-the-art Nyström and meshless methods for solving electromagnetic problems. He pioneered the derivation of closed-form formulas for calculating hypersingular integrals of electromagnetic integral equations, enhancing those numerical methods to a new level. During his stay in Germany, he intends to develop robust singularity treatment techniques for more challenging tetrahedral elements and apply them to inverse source methods. Professor Thomas F. Eibert hosts Professor Tong at the Technical University of Munich, Chair of High-Frequency Engineering.

As award winners of the Alexander von Humboldt Foundation, both are members of the TUM-IAS.

Lisa Adams (TUM-IAS Albrecht Struppler Clinician Scientist Fellow and Senior Physician at Radiology at TUM University Hospital) won two grants from “Bayern Innovativ,” totalling 700.000 euros.

Réne Botnar, TUM-IAS Hans Fischer Senior Fellow and Professor of Biomedical Engineering at King’s College London, gained the 2024 Research Award of the Faculty of Engineering, Pontificia Universidad Católica de Chile and a Gold Medal from the Society for Cardiovascular Magnetic Resonance, Washington DC. In addition, he receives a Fondecyt Regular 2025 grant from Chile, for his project “Towards a 20 min Cardiac MRI Exam at 0.55T: simple, efficient and affordable.”

TUM-IAS Alumnus Fellow **Ioannis Brilakis** (Professor of Civil and Information Engineering at the University of Cambridge) received the prestigious Tucker-Hasegawa Award of the International Association for Automation and Robotics in Construction and has been elected IAARC President by its Board of Directors in June 2024. **Dennis Christensen,** TUM-IAS Hans Fischer Fellow and

Professor of Energy Conversion and Storage at DTU Copenhagen, won the 2024 Promising Early Career Scientist award from the journal Materials Today Energy, rewarding “early career scientists” outstanding scientific work in energy materials.

Kim-Melanie Kraus (TUM-IAS Albrecht Struppler Clinician Scientist Fellow and Radiation Oncologist at the TUM University Hospital) received a research grant for 243,150 Euros from Varian, a major commercial player in radiotherapy. The project further advances treatment planning in Microbeam radiotherapy.

At the International Symposium on Quality Electronic Design 2024, TUM-IAS Rudolf Diesel Industry Fellow **Sani Nassif** gained the best paper award for his contribution “Toward Early Stage Dynamic Power Estimation: Exploring Alternative Machine Learning Methods and Simulation Schemes.”

Heather Kulik, TUM-IAS Hans Fischer Senior Fellow and Professor for Chemical Engineering at MIT, received US President Joe Biden's Presidential Early Career Award for Scientists and Engineers. Also, she was Sydney Ross Lecturer 2024, Rensselaer Polytechnic Institute, Department of Chemistry, Löwdin Lecturer for 2023 at Uppsala University, Sweden, Department of Chemistry, and TCI Hirschfelder Visitor/Lecturer, Department of Chemistry at University of Wisconsin.

Mathias Senge, TUM-IAS Hans Fischer Senior Fellow and Professor for Organic Chemistry, Trinity College Dublin, is evaluated as among the World’s Top 2 percent Scientists worldwide for 2024 by Elsevier Publishing and Stanford University. He also gave an invited keynote lecture at the Gordon Research Conference “GRC Tetrapyrroles” (2024).

TUM-IAS Hans Fischer Senior Fellow **Piotr Tryjanowski** (Poznań University of Life Sciences) received the “Gold Synapsy Award” on his book “ECOPSYCHIATRY” as the innovation book of the year. ■

Events

Seminars, workshops, conferences – these are core tasks of the TUM-IAS. Many of our Fellows had multi-day conferences on their research topics in 2024. In addition, TUM-IAS hosts over 200 workshops and conferences of TUM's academic community annually. Public outreach was an important focus last year, with a Sustainability Day, an Open Day, and lectures in our neighboring town of Garching. We continued our "Scientists meet Scientists" seminar series online on Wednesdays, with over 20 lectures annually.

General Assembly

At our annual meeting, we welcome our new Fellows, learn about ongoing projects in presentations, and create a platform for our Fellows to network. Doctoral students present their topics in poster sessions.

Will Schilders gave last year's Linde Lecture. He is one of the Hans Fischer Senior Fellows at TUM-IAS, funded by Siemens AG, and a Professor of Scientific Computing in Eindhoven. His topic was: **Mathematics: Key Enabling Technology for a Better World,** in which he addressed the key role of mathematics for almost all current and future applications.

Full Program

Simulation of Quantum Systems on High-Performance Computing Infrastructures, Örs Legeza, Wigner Research Centre for Physics, Hans Fischer Senior Fellow

The Role of Bacterial Oral-Gut Translocation in Inflammatory Diseases, Melanie Schirmer, TUM, Rudolf Mößbauer Tenure Track Assistant Professor

Women in the Industry 4.0 – Current and Future in Manufacturing, Jihyun Lee, University of Calgary, Anna Boyksen Fellow

From Injury to Integrity: From Biomechanics to Molecular Biology of Intestinal Wound Healing, Philipp-Alexander Neumann, TUM, Albrecht Struppler Clinician Scientist Fellow

China and the Changing International Order, Susan Park, University of Sydney, Hans Fischer Senior Fellow

Exploring Quantum Spin Liquids: From Majorana Fermions to Exotic Phases, Natalia Perkins, University of Minnesota, Hans Fischer Senior Fellow

Traffic State Prediction using Machine Learning and Automated Vehicle Data, Felix Rempe, BMW, Rudolf Diesel Industry Fellow

IAS Fellow Laura Herz at TUM-IAS General Assembly.

Nobel Sustainability Summit

The fourth Nobel Sustainability Trust Summit took place at the University of California, Berkeley, on November 20 and 21, 2024. The Nobel Sustainability Trust (NST), the University of California, and the Berkeley Center for Responsible, Decentralized Intelligence (Berkeley RDI) jointly organized the event.

The summit brought together a full assembly of thought leaders, innovators, and changemakers to address crucial technological, sustainability, and human development challenges. The Award Ceremony of the Sustainability Awards 2024, supported by the NST, took place on the first day after a morning session of roundtables composed of experts from the financial, entrepreneurial, political, and academic sectors. ►

Left to right Michael Molls (TUM-IAS), Mathis Wackernagel, Peter Nobel (NST), Klaus Butterbach-Bahl, Jiuhui Qu.

Rich Lyons (Chancellor of the UC Berkeley), Siddharth Chatterjee (UN Resident Coordinator in China), Eduard Barbier (Colorado State University), John Eleoterio (Global Head of Sustainability Banking, Goldman Sachs), Philippe Douste-Blazy (former French Minister of Health, and Foreign Affairs), Edward Russo (former Environmental Advisor of Donald Trump), James Mwangi (CEO and Group Managing Director of Equity Bank, Kenya), and many other persons were among the prominent international speakers and panelists.

The three winners of the Sustainability Awards 2024 are:

- **Dr. Mathis Wackernagel** (Global Footprint Network) is responsible for developing the ecological footprint concept and advisory work favoring sustainability for public organizations, businesses, and decision-makers.

- **Prof. Klaus Butterbach-Bahl** (Aarhus University/ Karlsruhe Institute of Technology) for his research on nitrogen cycles and greenhouse gas emissions at regional and global levels, particularly their agricultural and ecological impact.

- **Prof. Jiuhui Qu** (Chinese Academy of Sciences/ Tsinghua University) for his pioneering work in developing water treatment technology and risk management.

Furthermore, the NST presented its Outstanding Contribution to Sustainability medal, a recognition and symbolic prize for personalities engaged in sustainability projects. This year, the medals went to Dr. Claudia Sheinbaum (President of Mexico and former Mayor of Mexico City) and to Ban Ki-moon (former Secretary-General of the UN).

The second day was dedicated to the Nobel DAO. This technology accelerator brings together young talents worldwide in digitalization, artificial intelligence, longevity medicine, space technology, robotic automation, and green energy.

Mathis Wackernagel.

Klaus Butterbach-Bahl.

Jiuhui Qu.

TUM – Siemens Workshop

With the move of Siemens Corporate Research to the TUM research campus, the long-standing relationships are deepening even further. In the first workshop in January 2024, over 30 researchers from Siemens and TUM met to develop new fields of joint work and initiate projects.

Munich Battery Discussion

On March 4–5, the Munich Battery Discussions 2024 brought together 20 international experts in battery research to discuss the latest findings and the tone for the upcoming years with the audience, comprising international scientists from Academia, Research Institutes, and Industry. Close research and industry collaboration are critical to potent innovation and successful industrialization. In the framework of this collaboration, BMW and TUM jointly organized the MBD 2024, supported by TUMint.Energy Research.

The contributions addressed the challenges and opportunities of future lithium-ion batteries from different approaches, ranging from experimental to simulation studies, fundamental investigations, and the analysis of complex systems. In addition to the incremental developments in state-of-the-art lithium-ion batteries, a growing focus and increasing resources are also being invested in developing next-generation concepts such as the All-Solid-State batteries technology.

The 9th edition of the MBD was dedicated to the “Design and Production of Next-Generation Batteries: Challenges and Opportunities,” focusing on bridging the gap between fundamental science and scale-up to serial industrialization. For the first time in the satisfactory history of the conference, the topic of production technology also was in boosted focus.

Since its beginnings in 2013, the MBD aims to discuss the latest findings and the tone for the upcoming years with an audience comprising international scientists from Academia, Research Institutes, and Industry.

Embracing Nature’s Complexity Conference – How to communicate the value of water- and climate-regulating ecosystems?

Water transport and cloud formation are essential in climate regulation. In turn, they depend on vegetation covering the earth's surface. This plays a major role in weather patterns and extremes, especially floods and droughts. During the 5-days conference in April, physicists, hydrologists, ecologists, medical scientists, and atmospheric and climate scientists from over 20 countries strived to overcome the traditional separations among these disciplines. They exchanged new evidence on how human activities on land affect rain and climate and our overall well-being. ▸

Munich Battery Discussion 2024.

Embracing Nature's Complexity Conference participants at TUM-IAS in April 2024.

The conference was the culmination of **Anastassia Makarieva's** TUM-IAS Anna Boyksen Fellowship on "Drought mitigation through ecosystem restoration," which focused on the Bionic Pump concept she co-developed. In co-authorship with V.G. Gorshkov, Anastassia Makarieva formulated the idea of the biotic pump of atmospheric moisture, highlighting key ecological feedbacks on atmospheric moisture transport and, in cooperation with an international team of colleagues, demonstrated the existence of life's metabolic optimum (broadly universal rate of energy consumption across life's kingdoms). Combining theoretical work with field observations, Anastassia spent over sixty months researching forests in the Russian wilderness. Her current research interests focus on deepening the physical understanding of ecosystem feedback on the water cycle and moisture transport.

See also:
www.thebioticpump.com/tum-ias-conference-2024

Read session summaries and download transcripts at
https://bioticregulation.ru/life/conf2024.php

See videos from the conference at
www.youtube.com/@thebioticpump

Workshop "Advocates and Allies: Male Allies for Gender Equality"

TUM-IAS Hans Fischer Senior Fellow **Gregory D. Erhardt,** Professor of Civil Engineering in Kentucky, brought a new focus to TUM with this workshop in May 2024.

He claimed that we are all aware that women continue to be underrepresented in the sciences, the path toward addressing this issue differs across demographic groups. Traditionally, much of the advocacy is done by women. Since men dominate faculty demographics on campus, however, this group needs to be involved in any change in social norms. While many men do care about and understand gender diversity issues, they may not possess the understanding, vocabulary, or skills to turn their good intentions into actions.

This workshop took a new approach, focusing on how men can be better advocates and allies of women in the workplace. The course was taught by men, creating a depolarizing environment for a freer exchange of ideas. It covered topics including implicit bias, work culture, effective communication, and dealing with pushback. For each topic, best practices were discussed, allowing for the discussion of relevant examples and providing guidance for future activities.

Recent progress on tensor network methods

Hans Fischer Senior Fellow **Örs Legeza,** Professor at Wigner Research Centre for Physics, Budapest, and his host **Gero Friesecke,** Professor for Analysis at TUM, were organizing a four-day workshop at the IAS on “Recent progress on tensor network methods” together with colleagues Thomas Barthel of Duke University and Henrik Larsson from the University of California.

The workshop brought together condensed matter physicists, mathematicians, and theoretical chemists to continue the exploration of this active and growing field of research and to stimulate further developments of tensor network methods.

The workshop focused on innovative ideas for moving beyond the current limits of quantum many-body simulations despite the major challenges of high dimensionality and accuracy. Topics include the interplay between modes, rank truncation network topology, hybridization with other approaches, and parallelization.

Orbitrap Isotope Applications Workshop

TUM-IAS Anna Boyksen Fellow **Andrea Erhardt,** Professor of Earth and Environmental Science at the University of Kentucky, organized a workshop on the Orbitrap Isotope Solutions platform in April 2024. This one-and-a-half-day workshop covered innovations, new techniques, problems encountered, and potential solutions to this system. The second day of the meeting focused on live demonstrations.

Conference on Water Security in Africa – An integrated Water-Energy-Food-Ecosystems (WEFE) Nexus perspective

In May 2024, TUM-IAS hosted a conference on water security in Africa, supported by the Bavarian State Government. Increasingly severe climate change impacts, especially drought and flood conditions, coupled with inadequate management of water resources, negatively impact water security and livelihoods in parts of Africa. This is causing mass migrations of populations and violent conflict, fueling governance conditions' instability. Augmented water security is key for ecosystem regeneration and sustainable socio-economic development in Africa and beyond. Water reclamation with integrated resource recovery taking a Water-Energy-Food-Ecosystems (WEFE) Nexus approach to support the regeneration of ecosystems is also a significant opportunity to facilitate the achievement of the UN Sustainable Development Goals (SDGs). However, the operationalization of the Nexus approach is lagging.

The keynote speech was given by Tony Rinaudo, a multi-award-winning agricultural scientist from Australia who received the Right Livelihood Award in 2018.

The Deep Structure of Transatlantic Relations

In June, **Eugénia da Conceição-Heldt** (TUM-IAS Carl von Linde Fellow and TUM Professor of European and Global Governance) and international experts explored in this 2-day workshop, how much cooperation between Europe and the USA takes place, to what extent it is efficient, how profits and losses are distributed, and what the future of collaboration might look like. ▸

Tony Rinaudo at the Conference on Water Security.

Sustainability Day
The TUM-IAS was represented with scientific lectures at the first TUM-wide Sustainability Day on June 12. **David Egger,** TUM-Professor of Theory of Functional Energy Materials and part of IAS Focus Group Optoelectronic Properties of Perovskite Semiconductors, presented to Perovskite Semiconductors and solar pholtaic efficiency. **Manuel Spitschan**, TUM-IAS Fellow as Rudolf Mössbauer Tenure Track Assistant Professor of Chronobiology & Health, reported to "Light and Health."

International workshop on "Existential Elucidation. Jaspers and Spiritual Care"
TUM-IAS Philosopher in Residence **Rico Gutschmidt** conducted, together with his TUM Host Eckhard Frick (Professor of Spiritual Care and Psychosomatic Health), an interdisciplinary workshop on June 14–15 at the TUM University Hospital rechts der Isar. A group of international scholars (Philosophy, Psychology, Medicine, Literary Studies) interpreted Spiritual Care against the background of Jaspers' concept of the boundary situation.

The German philosopher Karl Jaspers (1883–1968) introduced the term "boundary situation," which refers to the limits of action and life, such as struggle, guilt, suffering, and death. Human life always remains within these boundaries, but this is experienced specially in particular situations. Patients who have to endure severe physical or emotional suffering or are confronted with their death due to a terminal illness can experience their situation as a boundary situation in the sense of Karl Jaspers. According to Jaspers, in confronting boundary situations, people can gain "existential elucidation," a new and transformative perspective on their lives.

At the workshop, Alice Holzhey-Kunz (Zurich), Giovanni Pietro Basile (Boston), Hilmar Schmiedl-Neuburg (Boston), Heidi Frølund Pedersen (Aarhus), Emmy van Deurzen (London), Godehard Brüntrup (Munich), An Ni (Beijing), and the two organizers discussed the question of how to support people in boundary situations from a philosophical, spiritual and psychological perspective. A central concern of the workshop was to establish ways of interrelating secular-existential and religious-spiritual forms of support. The workshop papers will be published in the series "Studies in Spiritual Care" by De Gruyter.

Multiphontonics Conference
The first **Multiphotonics** meeting took place on July, 4 and 5, 2024. **Elena del Valle,** TUM-IAS Hans Fischer Fellow and Professor of Theoretical Condensed Matter Physics in Madrid, initiated it. With over 40 participants various topics were discussed, e. g.: Multiphoton generation: Single and N-photon emission; Quantum light generation with properties such as entanglement or squeezing; Frequency filtering, statistics, coherence and correlation measurements; Quantum optics, cavity-QED, light-matter interaction and nanophotonics.

Workshop "Fabricating Archaeologies: Feminist Craft, Human Hands, and Intelligent Architectures"
Workshop by TUM-IAS Anna Boyksen Fellow **Nathalie Bredella** with Andrea Reichenberger (TUM School of Social Sciences and Technology, History of Technology), Rudolf Seising (Deutsches Museum), July 2024.

Evolving digital ecologies promise to situate technologies, software systems, and mixed actors within new epistemological approaches. Locating digital production processes within feminist labor histories, this workshop aimed at interrogating the narratives surrounding computation, the relationships between craft and digital production, and the subsequent interconnections between the human and the machine. In looking at histories of software systems as craft archaeologies, the organizers were interested in the hybrid modes of computation and construction, as well as in the methods of writing these situated histories.

Using a wide set of methodologies (oral history, media archaeology, technical re-enactment, archival research), the workshop brought together historical and theoretical investigations and to bridge the gap between the history of craft, computer science and artificial intelligence (AI). The questions immediately arose: What tensions have arisen around the automation of craft processes and mechanized calculation procedures? In what ways is the emphasis on productivity entangled with marginalization? How can we capture (situate) industrial and digital practices across disciplines? And what role do theories of contextual knowledge in a feminist framework play in the realm of diversity and epistemic (in)justice? Bringing together perspectives from architecture and technology studies, this workshop highlighted how technical, social, and societal elements interweave, investigating how material processes form communities.

Responsible Science Communication and AI

The rapid advance of AI over the last year has been greeted with both excitement over its possibilities and dismay about the rapidity with which it is being incorporated into various aspects of our lives. How can science communicators discuss such quickly evolving innovations when both potential benefits and potential negative impacts are unclear and future developments are impossible to predict?

This hands-on interactive workshop in July, organized by TUM-IAS Hans Fischer Senior Fellow **Maja Horst,** Professor of Science, Technology, Society and Dean of Arts at Aarhus University, explored what a Responsible Innovation framework might contribute to understanding some of the unique opportunities and challenges of responsible science communication in the field of AI.

Leibniz Quantum and Beyond

A workshop on Gottfried Wilhelm Leibniz in September 2024 dealt with his work on later quantum research and relativistic physics and his influence on medicine and philosophy. The workshop took place with the Leibniz Society, Hanover, and was organized by TUM Philosopher in Residence **Roberto Giuntini,** Professor of Philosophy at the University Caligari, Italy.

Open House

Over 15,000 visitors came to the Open Day on October 3 at the TUM Campus Garching, which had not been held for several years due to the COVID-19 pandemic. The TUM-IAS presented itself with selected lectures: Matthias Hebrok on how stem cells and organoids are revolutionizing medicine; Michael Zech with insights into our genome – how the genetic causes of rare diseases inform us about disease mechanisms; Rolf Moeckel on settlement development and transport: how we must transform our cities for sustainable development; and Werner Hemmert, hearing with a cochlear implant.

Stephania Centrone at Leibiniz Quantum Workshop.

Workshop “Link it and move it” at Deutsches Museum München

“Link it and Move it” is a collaboration between the TUMlab at the Deutsches Museum and TUM-IAS Anna Boyksen Fellow **Nathalie Bredella**, Professor of History and Theory of Architecture at Leibniz University Hanover. Together with Grayson Bailey, Merel de Coorde, and Jonah Marrs, she led a workshop exploring the history of Laura and Leonardo Mosso’s “Programmable Architecture” through robotic re-enactment. The workshop, directed at teenagers and young adults, brought together architectural history by presenting a comic illustrating the life and work of the Mossos, followed by an Arduino workshop.

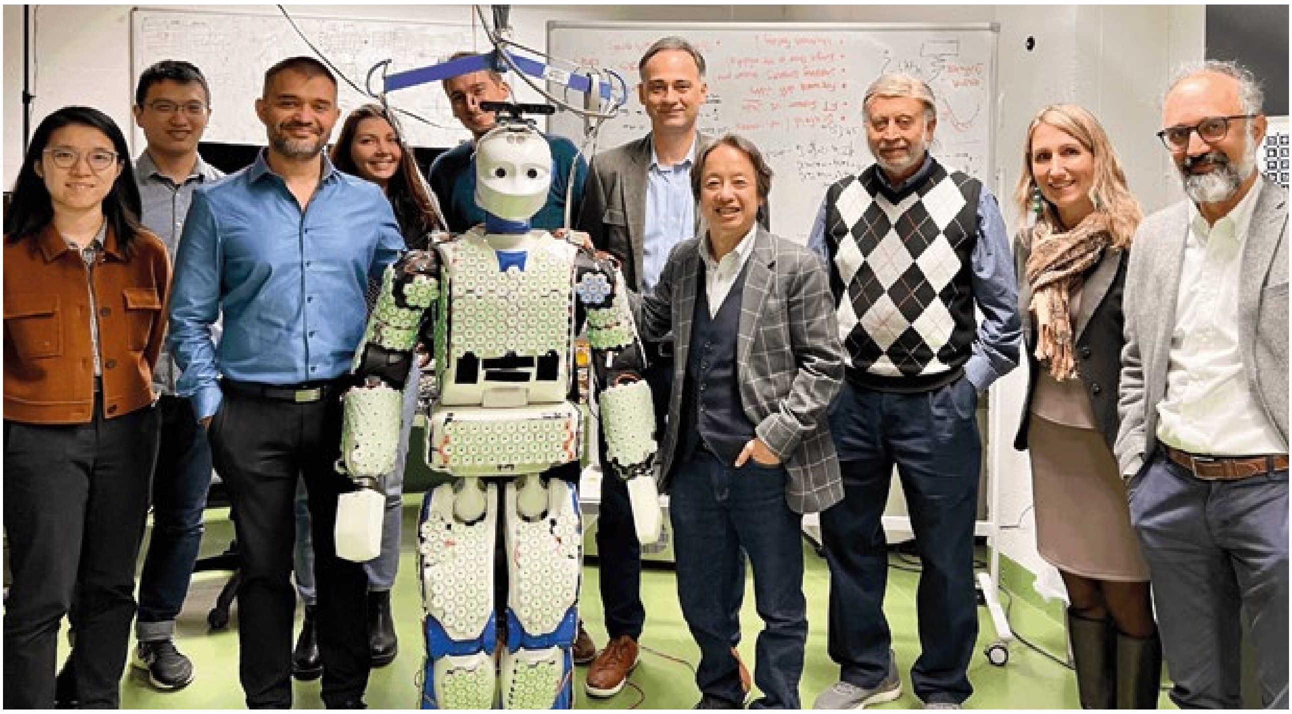
Advancing Scientific Machine Learning in Industry

In this joint academia-industry workshop, **Wil Schilders** and Dirk Hartmann explore recent advancements in implementing Scientific Machine Learning techniques.

Wil Schilders, whose Hans Fischer Senior Fellowship has been supported by Siemens AG, is a Mathematics and Computing Science Professor at Eindhoven University in the Netherlands. Dirk Hartmann is Head of Simcenter Technology Innovation, Siemens Technical Fellow, and a Siemens Top Innovator and Inventor of the Year. ▸

Scientific machine learning (SciML) has taken the academic world by storm as an interesting blend of traditional scientific modeling with machine learning (ML) methodologies like deep learning. While traditional machine learning methodologies have difficulties with scientific issues like interpretability and enforcing physical constraints, the blend of ML with numerical analysis and differential equations has evolved into a novel field of research that overcomes these problems while adding the data-driven automatic learning features of modern machine learning. Many successes have already been demonstrated, with tools like physics-informed neural networks, universal differential equations, deep backward stochastic differential equation solvers for high dimensional partial differential equations, and neural surrogates showcasing how deep learning can greatly improve scientific modeling practice. Consequently, SciML holds promise for versatile application across various scientific disciplines, ranging from investigating subatomic particles to comprehending macroscopic systems like economies and climates. However, despite notable strides in enhancing the speed and accuracy of these methodologies, their utility in practical and specifically industrial settings remains constrained.

If appropriately addressed, SciML, with its promise to accelerate innovations and scientific discoveries by orders of magnitudes, offers unique opportunities to address the insatiable desire for faster and more accurate predictions in many fields. This workshop was dedicated to exploring recent advancements in implementing SciML techniques. It brought together leading experts actively refining these methodologies to ensure their practical viability and scalability, particularly in industrial sectors where digital and physical components converge. The goal of the workshop was to produce a research roadmap for advancing scientific machine learning in industry, addressing application/industrialization challenges.



Gordon Cheng (center) and Nitish Thakor (3rd person from the right) at Workshop Sensory Integration.

Sensory Integration in Neuroprostheses and Rehabilitation

Nitish Thakor, TUM-IAS Hans Fischer Senior Fellow and Professor of Biomedical Engineering at Johns Hopkins University, had a joint workshop with Gordon Cheng, TUM-Professor of Cognitive Systems, in Munich on October 30, highlighting their years of collaboration.

Sensory integration, merging and coherently using sensory inputs, has become a frontier in robotics, rehabilitation, and sensory neuroprostheses. In prostheses and rehabilitation applications, different streams of sensory information are perceived and integrated by individuals with sensorimotor deficits to interact with the environment. In robotics, sensory information allows robots to achieve human-like behavior when interacting with objects.

This workshop aimed to discuss the latest advances and challenges in understanding sensory perception and integration in intact humans, evaluating sensory integration in individuals with sensorimotor deficits, and achieving sensory fusion for humanoid robots. From somatosensory feedback and cortical responses to robotics and algorithms that enable multimodal sensing in robots, participants learned about the latest advancements, methodologies, and scientific and technological challenges along these paths.

IAS meets Humboldt: Reception at TUM-IAS

TUM is one of the most successful universities in Germany when it comes to hosting internationally renowned Awardees and Fellows of the Alexander von Humboldt Foundation for research stays. Fellows and Awardees of the Alexander von Humboldt Foundation are automatically Members of TUM-IAS if their Host is a TUM Professor. In addition, the TUM-IAS is the central point of contact for applications for fellowships and awards from the Alexander von Humboldt Foundation. TUM-Senior Vice President Professor Gerhard Kramer invited all Humboldt Fellows and Humboldt Awardees at TUM and IAS Fellows, as well as their TUM Hosts, to a reception at the TUM-IAS Faculty Club on November 18, 2024, to strengthen the connection to the Humboldt Foundation and to support networking among Humboldt Awardees and Fellows.

Two Humboldt awardees of the Humboldt Foundation's Carl Friedrich von Siemens Research Award gave insight into their research:
Polina Bayvel from University College London and ICCS / Optical Networks Group, Department of Electronic & Electrical Engineering, is a highly accomplished professor specializing in optical communications and networks. She gave an interesting overview of her research with the title **"Maximising the capacity of optical networks – how far have we come and what else can we do?"**. She leads the Optical Networks Group at University College London (UCL), which she founded in 1994. Her groundbreaking research focuses on maximizing the capacity and speed of optical fiber communication systems, addressing fundamental challenges like nonlinearities in optical networks, and advancing multi-wavelength systems critical for modern digital communication infrastructure.

Andreas Winter from the Universita Autonoma de Barcelona, Quantum Information Group, who is also a TUM-IAS Hans Fischer Senior Fellow, is a renowned theoretical physicist and expert in the field of quantum information theory. His research focuses on the mathematical foundations of quantum information. In his talk, he offered a detailed illustration of the development of quantum information titled **"Quantum information: from foundations to 6G"**. He explores the intersection of quantum information theory and its potential applications in advanced communication technologies, such as 6G networks. He discusses how quantum principles can revolutionize secure data transmission, surpassing classical cryptographic systems by enabling physically verifiable privacy. This innovation is particularly significant given the potential of quantum computers to undermine current cryptographic methods. ►

Discussions, poster presentations, and a buffet concluded the evening. Mira Albus from the Humboldt Foundation was a valuable guest for the participants, who clarified questions and discussed ideas.

Workshop “Agentive Matter(s)”

Advanced digital technologies and research in architectural materials and construction processes transform work and life toward digitization and sustainability. These developments present opportunities to reduce environmental impacts and address long-standing labor inequalities, social injustices, and gender imbalances in the field. This workshop aimed to explore how social discourses and knowledge cultures shape and are shaped by new technologies. It examined design processes at the intersection of craft, systems thinking, and algorithmic cultures, explored how the knowledge embedded in technology can be made more accessible, and offered ways to engage with the ecologies of making.

Agentive Matter(s) is a two-phase initiative that aims to identify new approaches to teaching and learning about how technologies transport societal discourses from the past into the future. Phase 1 was an expert workshop exploring techniques for tracing discourses and knowledge across the past and present. Phase 2 will take the lessons learned from the workshop and translate them into an educational format that asks what societal actions the history of technological artifacts is producing today and how we can shape them to increase sustainable outcomes.

TUM-IAS Anna Boyksen Fellow Nathalie Bredella organized this workshop in November 2024 in collaboration with TUM-IAS Rudolf Mößbauer Tenure Track Professor **Pierluigi D’Acunto** (TUM School of Engineering and Design), **Kathrin Dörfler** (TUM School of Engineering and Design) and TUM-IAS Rudolf Mößbauer Tenure Track Professor **Anna Keune** (TUM School of Social Sciences and Technology).

Women@ED – A networking event for women of the TUM School of Engineering and Design

A new series of networking events at the School of Engineering and Design for Women started in November 2024. Its idea is to build a vibrant community, to spark inspiring conversations, and to dive into professional development featuring dynamic workshops, guest speakers, and engaging networking sessions.

The first event started with **Jihyun Lee,** a Mechanical and Manufacturing Engineering Professor at the University of Calgary and TUM-IAS Anna Boyksen Fellow. There was space for guided networking between women of the School of Engineering and design at all levels (students, scientists, professors).

Exploring New Horizons with Molecules on Surfaces

The scientific purpose of Focus Group of TUM-IAS Hans Fischer Senior Fellow **Lifeng Chi,** Professor of Functional Nano and Soft Materials at Soochow University, China, and Johannes Barth, TUM Professor of Molecular Nanoscience, was the development and exploration of a new materials base towards controlled electronic properties (electronic transport, optical absorption, excited state imaging) of highly ordered molecular monolayers, as well as polymeric organic wires and sheet structures, specifically using surfaces of wide bandgap semiconductors and non-conducting interface layers. The fabrication protocols of these innovative heterostructures rely on directed molecular self-assembly and on-surface synthesis, as well as comprehensive investigations and improved methods of suitable substrates.

The Closing Symposium in December 2024 was also an exploratory workshop where the project efforts and insights were discussed and put into perspective.

Moreover, it was aimed to establish a link to the extremely promising and closely related domain of "Engineering and design of interfacial nanographenes and carbon-based architectures as innovative nanomaterials." Synergies and ideas for further research initiatives evolved. To this end several recognized scientists in the field were invited, most of them providing comprehensive experiences in the field of on-surface synthesis and impressive records or seminal achievements regarding the engineering and design of interfacial nanographenes and carbon-based architectures. These include, for instance, innovative synthesis protocols and the realization of carbon nanomaterials with truly novel properties. Key examples are last-generation graphene-nanoribbons, biphenylene networks, graphyne- and graphite-type 2D materials, magnetism in surface-confined metal-organic sheets, and 2D materials. Many of these systems bear significant promise as do novo-designed quantum materials for quantum science and technology applications. ■

Polina Bayvel, Gerhard Kramer, Norbert Hanik, Andreas Winter at the Humboldt Reception.

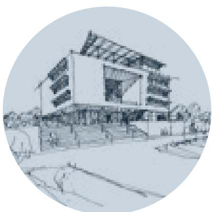
Welcoming Our New Fellows

Meet our new Fellows and get inspired by their research projects.

Fellowship Programs

Albrecht Struppler Clinician Scientist Fellowship
three years for excellent senior physicians working at the TUM School of Medicine and Health, the TUM University Hospital and the German Heart Centre Munich.

Carl von Linde Fellowship
two years for excellent TUM faculty members.



Philosopher in Residence Fellowship
one year for internationally leading and emerging representatives of the field of philosophy from outside TUM.

Rudolf Mößbauer Tenure Track Assistant Professorship
six years for outstanding, high-potential early-career scientists.

Rudolf Diesel Industry Fellowship
three years for highly qualified researchers from industry.

Anna Boyksen Fellowship
two years for oustanding female professors from outside TUM who intend to explore gender- and/or diversity-relevant topics within the TUM subject portfolio.

Hans Fischer Fellowship
three years for outstanding early-career international scientists from outside TUM.

Hans Fischer Senior Fellowship
three years for renowned international scientists from outside TUM.

Dieter Schwarz Fellowship
three years for renowned international scientists from outside TUM who intend to explore innovative, high-risk topics in the key research areas researched at the TUM Campus Heilbronn.

Dieter Schwarz Courageous Research Grant
three years for outstanding international scientists from outside TUM who intend to use groundbreaking technology to propose a radical solution to a major challenge in the area of “Digitalization and Sustainability.”

Dr. Lisa Adams

Clinic for Diagnostic and Interventional Radiology | TUM School of Medicine and Health

Fellowship: Albrecht Struppler Clinician Scientist Fellowship | **Focus Group:** Quantitative Imaging Biomarkers for Predictive Healthcare | **Research Area:** Advanced Computation and Modeling

The Focus Group explores the potential of personalized and predictive medicine through applications of multimodal medical imaging and artificial intelligence. Using large-scale public and institutional datasets, the team works to extract meaningful biomarkers beyond traditional anatomical assessments.
The Focus Group's research centers on developing AI-driven organ segmentation models, with an additional focus on body composition analysis. The aim is to establish new indicators of overall health and aging by creating organ-specific biological age prediction algorithms and quantifying various aspects of body composition. By integrating imaging biomarkers with clinical and genetic data, the researchers aim to improve risk assessment and validate organ age as a predictor for various diseases and treatment outcomes. Through third-party funding from EU Horizon, DFG, Bayern Innovativ, and the Wilhelm Sander Foundation, they aim to establish standardized, reproducible imaging biomarkers that can be translated to clinical practice.
This Focus Group's cooperation partners are Julia Schnabel (Computational Imaging and AI in Medicine, TUM), Daniel Rückert (AI in Healthcare and Medicine, TUM), and Keno Bressem (German Heart Center, TUM).

Prof. Kevin Brindle

University of Cambridge | Cancer Research UK – Cambridge Institute

Fellowship: Hans Fischer Senior Fellowship | **Hosts:** Prof. Franz Schilling, Prof. Wolfgang Weber (TUM School of Medicine and Health) | **Focus Group:** Imaging Cancer Metabolism Using Magnetic Resonance | **Research Area:** Bioengineering and Imaging

Molecular imaging is likely to play an increasingly important role in predicting and detecting tumor responses to treatment and thus in guiding treatment in individual patients. We have been using MRI-based metabolic imaging techniques to detect tumor treatment response, to monitor disease progression, and to identify tumor metabolic subtypes that display distinct therapeutic vulnerabilities. Initially, this was using hyperpolarized ^{13}C-labeled substrates. Nuclear spin hyperpolarization increases sensitivity in the ^{13}C magnetic resonance experiment by >10,000x, which allows imaging of injected hyperpolarized ^{13}C labeled cell substrates in vivo and, more importantly, the kinetics of their metabolic conversion into other cell metabolites. More recently, we have been using ^{2}H-labeled substrates; the relatively low sensitivity of detection is compensated by the very short T_1s displayed by this quadrupolar nucleus, which enables extensive signal averaging in the absence of signal saturation. In this Focus Group, we will focus on imaging tumor one-carbon metabolism using ^{2}H-labeled serine, with a view toward translating this into a clinical study back in Cambridge.

Prof. Fikile Brushett

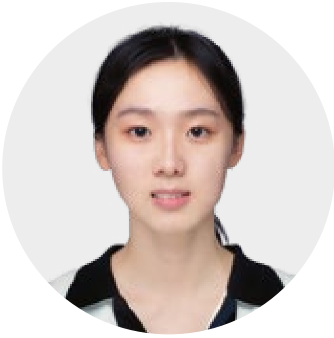
Massachusetts Institute of Technology

Fellowship: Dieter Schwarz Courageous Research Grant (funded by the Dieter Schwarz Foundation) | **Host:** Prof. Jennifer L. M. Rupp (TUM School of Natural Sciences) | **Focus Group:** Unlocking Transformative Electrochemical Systems Through Solid-State Ceramic Conductors | **Research Area:** Surface, Interface, Nano- and Quantum Science

This Focus Group seeks to conceptualize, synthesize, and integrate solid-state conductors with high conductivity and perfect selectivity into electrochemical energy systems. Through modeling and experiment, we aim to expand the library of fundamental knowledge on the behavior of solid-state conductors in contact with liquid electrolytes, to establish design criteria for competitive embodiments, and to pioneer proof-of-concept prototypes that illustrate the transformative potential of this approach. We are inspired by the following questions: How does the (electro)chemical environment impact the conductivity, stability, and selectivity of an ion-conducting solid-state ceramic material interfacing with a compositionally dynamic, multi-component liquid electrolyte? What structure-property relationships describe the rates and mechanisms of ion transport across the conductor, and how can the rate-determining processes be controlled by tuning of interfacial and bulk characteristics? Can dimensionally stable, continuous, and dense films and tapes of ceramics be manufactured and incorporated into flow cells that enable durable operation at high current, high efficiency, and with no crossover?

Dr. Jieshan Chen

Commonwealth Scientific and Industrial Research Organisation (CSIRO)



Fellowship: Dieter Schwarz Fellowship (funded by the Dieter Schwarz Foundation) | **Host:** Prof. Chunyang Chen (TUM School of Computation, Information and Technology) | **Focus Group:** Responsible AI for Trustworthy Technology and Automation | **Research Area:** Advanced Computation and Modeling

Our Focus Group is dedicated to developing trustworthy technologies that enable responsible software development and deployment. With the rise of AI and large language models (LLMs), researchers are leveraging these technologies to overcome software development challenges. However, ethical concerns regarding reliability and trustworthiness must be addressed, making human-in-the-loop accountability crucial. Our research focuses on software usability and accessibility testing, software engineering for LLM, and LLM-based agents. For example, we will tackle deceptive patterns in digital platforms by developing a comprehensive strategy to identify, track, counter, and eliminate these manipulative tactics. This approach will benefit various stakeholders and foster a more trustworthy, user-centric digital environment.

Dr. Dennis Valbjørn Christensen

Technical University of Denmark

Fellowship: Hans Fischer Fellowship | **Hosts:** Prof. Jennifer L. M. Rupp, Prof. Dominik Bucher (TUM School of Natural Sciences) | **Focus Group:** Seeing batteries from a new perspective | **Research Area:** Surface, Interface, Nano- and Quantum Science

Batteries play an increasing role in the green transition by enabling the electrification of transportation and balancing sustainable energy production with demands. However, batteries are notoriously heterogeneous in their operation, which arguably constitutes the largest bottleneck in understanding batteries and perfecting their operation. Our Focus Group aims at identifying and testing new methods for visualizing the functional processes within batteries. We particularly aim to be able to image the buried charge flow and heterogeneous redox reactivity of high-capacity solid-state batteries comprising layered oxide cathodes and lithium metal anodes.

Prof. Johanna Eichhorn

TUM School of Natural Sciences

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Nanoscale Microscopy and Spectroscopy of Energy Materials | **Research Area:** Surface, Interface, Nano- and Quantum Science

Photoelectrochemical energy conversion is a promising approach to convert sunlight directly into storable fuels. Economically viable and scalable photosystems are often based on semiconducting thin films. These photoelectrodes exhibit locally varying material properties, from the nanoscale to the microscale. To date, typical macroscale characterization techniques average the performance and fundamental properties over the whole photoelectrode and conceal important nanoscale insights. The Focus Group around Rudolf Mößbauer Tenure Track Professor Johanna Eichhorn leverages a complementary suite of advanced nanoscale microscopy and spectroscopy techniques to reveal the local processes of semiconductor photoelectrodes under realistic operation conditions. The resulting comprehensive portrait of the elementary steps associated with light-to-chemical energy conversion will provide the knowledge basis for rational development of efficient, stable, and scalable solar fuel devices.

Prof. Ghang Lee

Yonsei University

Fellowship: Hans Fischer Senior Fellowship (funded by the TUM Georg Nemetschek Institute) | **Host:** Prof. André Borrmann (TUM School of Engineering and Design) | **Focus Group:** AI-Based Design Compliance Checking (ADCC) | **Research Area:** Advanced Computation and Modeling

This Focus Group aims to advance automated design compliance checking (ADCC) theories and technologies while addressing management challenges to facilitate its practical adoption. ADCC involves automatically validating design information against specified criteria, which include not only codes and regulations but also contractual and client requirements. In the digitally transformed architecture, engineering, and construction industry, the quality of information produced and exchanged among project stakeholders is becoming more critical than the quantity. While the industry still struggles to ensure sufficient information for tasks related to the design, optimization, production, operation, and maintenance of built environments, it is essential to develop theories and technologies that can proactively enhance information quality.
The history of ADCC is intertwined with the development of artificial intelligence (AI) and computer-aided design (CAD). Although recent advances in large multimodal models (LMMs) and building information modeling (BIM) have enabled the interpretation of complex requirements and expert knowledge into machine-processable formats, these methods yet remain under active exploration.

Prof. Sossina Haile

Northwestern University

Fellowship: Hans Fischer Senior Fellowship | **Hosts:** Prof. Jennifer L. M. Rupp, Prof. Dominik Bucher (TUM School of Natural Sciences) | **Focus Group:** Unprecedented Visualization of Interfacial Phenomena and Carrier Dynamics in Energy Materials | **Research Area:** Surface, Interface, Nano- and Quantum Science

Ceria and its doped derivates play a pivotal role in a wide range of processes and devices, many of which are essential for a sustainable energy future. Despite its use in these applications, critical aspects of the surface and interfacial chemistry of ceria remain unresolved. Through this collaboration, we explore opportunities to harness quantum sensing via nitrogen vacancy (NV) diamonds to detect the presence and dynamics of interfacial species in ceria including protons, oxygen vacancies, and reduced cerium ions using model thin films. For the study of internal interfaces (grain boundaries), we evaluate nanocrystalline ceria films directly on NV-diamond substrates and use widefield imaging and NV-NMR spectroscopy to interrogate the defect state in the film. For the study of external surfaces, we grow single-crystal epitaxial films on lattice-matched single-crystal substrates and utilize scanning probe NV to detect the species on the film surface. This research contributes to proof-of-principle studies to explore critical method development on quantum sensing opportunities in solid-state ionic/protonic material model structures.

Prof. Max J. Hülsey

TUM School of Natural Sciences

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Catalytic Interfaces for Sustainable Chemical Energy Carriers | **Research Area:** Surface, Interface, Nano- and Quantum Science

Chemical energy carriers fed and fueled societies long before the industrial revolution. With the increasingly widespread and rapidly accelerating conversion of chemical energy carriers, a problem became apparent: the impact of fossil fuel combustion products on our atmosphere and environment. While the storage of energy in alternative forms shows promise for some applications, chemical energy storage compounds will continue to play a critical role in our society.

The interconversion of sustainable chemical energy storage compounds – such as methanol, hydrogen, and ammonia – depends on complex bond rearrangement processes at catalytic interfaces. The target of this Focus Group is to generate a deeper understanding of how sorption phenomena and chemical reactions on surfaces occur in a broad range of catalytic systems. Specifically, we aim to bridge the divides between thermochemical, electrochemical, and photochemical catalysis by developing comparative models that span these traditionally siloed disciplines. Through this integrative approach, we hope to provide new insights that can accelerate the implementation of sustainable chemical energy carriers.

Prof. Kejia Hu

University of Oxford

Fellowship: Dieter Schwarz Fellowship (funded by the Dieter Schwarz Foundation) | **Hosts:** Prof. Stefan Minner, Prof. Gudrun Kiesmüller, Prof. Stefan Wuttke (TUM School of Management) | **Focus Group:** Human-AI Collaboration for Decision-Making | **Research Area:** Advanced Computation and Modeling

Our Focus Group explores how humans and AI can collaborate more effectively in decision-making within operations management. As AI technologies continue to evolve, organizations face difficulties integrating them with human expertise, limiting the full potential of AI. Our research addresses this challenge by developing methods that combine human judgment with AI's processing power, allowing for better decision-making in complex scenarios. We aim to create a decision-support system that provides real-time recommendations, helping businesses enhance both efficiency and productivity. This system not only supports immediate decisions but also promotes continuous learning between AI and human collaborators, leading to more effective cooperation over time. By bridging the gap between advanced technology and practical application, our work will directly benefit industries ranging from manufacturing to consulting. Ultimately, our research will deliver both theoretical insights and practical solutions, enabling more productive human-AI partnerships across various sectors.

Prof. Zhen Li

Shandong University

Fellowship: Hans Fischer Fellowship (funded by the Siemens AG) | **Host:** Prof. Carlo L. Bottasso (TUM School of Engineering and Design) | **Focus Group:** Data-Based Maintenance of Offshore Wind Energy Conversion | **Research Area:** Advanced Computation and Modeling

The clean energy transition is the key motivation for concerted efforts by many nations to attain carbon neutrality within the next two or three decades. This goal requires replacing conventional fossil-fueled synchronous generators with renewable energy sources. Offshore wind energy has become one of the most promising renewable energy sources due to its many advantages. Power converters, as the core energy conversion equipment of wind energy systems, directly determine the operational and economic performance of offshore wind energy systems. However, the harsh operating environment and poor accessibility of offshore wind energy systems render them highly susceptible to equipment failures. Thus, it is crucial to ensure the reliable operation of power converters and protection devices in wind energy systems. This goal can be achieved by precise fault description, fast fault detection, and intelligent and predictive maintenance strategies. Therefore, in this Focus Group, we will propose effective maintenance solutions to ensure the operating reliability of offshore wind energy conversion systems.

Prof. Anke Meyer-Baese

Florida State University

Fellowship: Hans Fischer Senior Fellowship | **Hosts:** Prof. Jan Kirschke, Prof. Benedikt Wiestler, Prof. Claus Zimmer (TUM School of Medicine and Health) | **Focus Group:** Next Generation Deep Learning in Therapy Monitoring | **Research Area:** Advanced Computation and Modeling

AI-assisted multimodal brain imaging has the potential to improve diagnostic accuracy by automatically delineating tumor boundaries and diagnosing tumors, predicting treatment outcomes and revolutionizing personalized medicine. Despite significant progress, challenges persist in early diagnosis and recurrence prediction of brain cancer. The latter is extremely difficult because of tumor heterogeneity, resistance to therapy and incomplete excision of cancer cells. The interpretability of AI-based results, as well as the asynchronous nature of follow-up data, requires the development of novel multi-step deep learning systems to obtain continuous tumor tracking. The goal is to develop an AI-powered treatment monitor for recurrence prediction and clinical decision support, focusing on the interpretability of the results to achieve the highest possible level of acceptance among physicians and patients. This will be achieved by developing a novel AI system combining the generative stochastic modeling with “physics-informed” neural identification algorithms that enable end-to-end tumor tracking using spatial and temporal graph neural attention network transformers.

Prof. Cornelius Senf

TUM School of Life Sciences

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Earth Observation for Ecosystem Management | **Research Area:** Environmental and Earth Sciences, Building Technology

Prof. Cornelius Senf's research lies at the intersection of Earth observation and ecology, employing advanced remote sensing techniques to investigate the impacts of climate and land-use change on terrestrial ecosystems. His work focuses particularly on global forest resources, examining their vulnerability and responses to increasing climate extremes as well as the growing demand for wood as a natural resource. Driven by the goal of advancing sustainable ecosystem management, Prof. Senf bridges fundamental science and practical applications, collaborating closely with agencies to develop operational Earth observation-based monitoring systems. Methodologically, his expertise spans a wide range of tools, including large-scale processing of optical satellite data and in situ terrestrial laser scanning, enabling novel insights into ecosystem dynamics at scales ranging from landscapes to continents.

Prof. Raziye Tekín

ROKETSAN Inc.

Fellowship: Rudolf Diesel Industry Fellowship | **Host:** Prof. Florian Holzapfel (TUM School of Engineering and Design) | **Focus Group:** Smart GNC for Advanced Air Mobility | **Research Area:** Control Theory, Systems Engineering and Robotics

Guidance, navigation, and control (GNC) technology provides the essential algorithms and systems necessary for autonomous, stable, and safe flight of aerospace vehicles. Navigation determines the vehicle's attitude, position, and velocity, providing crucial input for guidance to generate commands. Control, in turn, executes these guidance inputs while ensuring stability. GNC is vital for the advancement of aerial systems, integrating automatic control, trajectory generation, and intelligent systems. Additionally, smart GNC focuses on achieving higher levels of autonomy for both single and multiple-vehicle missions through innovative algorithms. Therefore, Smart GNC must be capable of making real-time adjustments to facilitate safe operation in challenging weather and urban conditions.

The Focus Group is interested in advanced guidance, navigation, and control algorithms for the safe, efficient, and autonomous operation of future air vehicles. These systems are critical to ensuring that urban air taxis, drones, and other innovative aerial vehicles can safely operate in complex, highly dynamic environments while interacting with other airspace users and adhering to regulatory standards.

Prof. Yelda Turkan

Oregon State University

Fellowship: Hans Fischer Fellowship | **Host:** Prof. André Borrmann (TUM School of Engineering and Design) | **Focus Group:** Digital Twins for the Built Environment | **Research Area:** Advanced Computation and Modeling

This Focus Group is dedicated to advancing algorithms for developing digital twins (DTs) of existing bridges from point cloud data, known as the scan-to-DT process. DTs represent digital replicas of bridges and store detailed semantic and structural information, including components' geometry, materials, load bearing capacity, and other critical properties. The goal of this collaboration is to automate this process using machine learning algorithms that classify and extract key structural elements such as decks, piers, and abutments from point clouds. Once created, DTs will facilitate structural assessments, inform necessary maintenance or repair actions, and support asset management strategies. Additionally, DTs will enhance the long-term resilience of bridge infrastructure by enabling predictive maintenance and optimizing lifecycle costs. This work addresses a critical challenge for developed nations: managing aging transportation infrastructure. Timely inspections and proactive interventions are key to ensuring structural safety, minimizing disruptions, and extending the lifespan of bridges, offering significant societal and economic benefits.

Prof. Violetta Weger

TUM School of Computation, Information and Technology

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | **Focus Group:** Applied Algebra | **Research Area:** Communication and Information

Coding theory and cryptography build the two main pillars on which we base our modern digital world. The communication channels and systems we rely on daily are not only vulnerable to errors but also to attacks. Coding theory addresses these challenges by enabling error correction in data transmission, ensuring reliability in data storage and retrieval. Cryptography, on the other hand, ensures the security and privacy of these interactions. Both disciplines are based on algebraic concepts and are rich in mathematical structures.
As technology evolves, so do the challenges. Among the most critical is the threat posed by capable quantum computers, which render all of our current public-key cryptosystems insecure. Addressing this urgent need, our Focus Group specializes in post-quantum cryptography – designing cryptosystems that can withstand quantum attacks. One of the most promising candidates for such a cryptographic system is based on algebraic codes. Our Focus Group works on constructing and analyzing the security of these systems and exploring novel mathematical frameworks to advance their development.

Dr. Zhenchang Xing

Commonwealth Scientific and Industrial Research Organisation (CSIRO)

Fellowship: Hans Fischer Senior Fellowship (funded by the Siemens AG) | **Host:** Prof. Chunyang Chen (TUM School of Computation, Information and Technology) | **Focus Group:** Software Engineering for AI | **Research Area:** Advanced Computation and Modeling

The Focus Group explores the intersection of software engineering, human-computer interaction, and artificial intelligence to build next-generation AI-driven systems that are efficient, explainable, and trustworthy. A key aspect of our research is addressing the emerging need for natural language programming paradigms, where AI enables users to interact with systems through intuitive, human-friendly languages. This shift demands new software engineering methods and tools that stand on the shoulders of AI to streamline development, enhance productivity, and ensure responsible AI practices. Our research is highly relevant as AI plays a growing role in critical fields such as health, safety, and environment. Trust in AI systems is essential to ensure compliance, reduce risks, and improve safety. Through this Focus Group, we aim to advance responsible AI development, focusing not only on AI's high performance but also on creating adaptable and transparent software engineering frameworks that empower users and developers alike, unlocking the full potential of AI-driven systems.

Prof. Zhenbin Zhang

Shandong University

Fellowship: Hans Fischer Fellowship | **Host:** Prof. Carlo L. Bottasso (TUM School of Engineering and Design) | **Focus Group:** Efficient and Reliable Energy Conversion Technique for 20MW-level Offshore Wind Energy | **Research Area:** Control Theory, Systems Engineering and Robotics

Harvested by advanced technical systems honed over decades of research and development, (offshore) wind energy has become one of the mainstream energy resources. Currently, 16MW offshore wind turbines have been installed, and 18-20MW wind turbines are under investigation and on the way to be integrated to the power grid. Major concerns lie in reducing costs so as to improve the economic benefits and mitigating its diverse impacts on the grid. In this Focus Group, we will collaborate in a multidisciplinary manner (aero-mechanical-power electronics-control) on two aspects of techniques:

1) how to maximize the wind energy capture ratio and reduce the turbine load for 20MW level wind turbine systems;

2) how to enhance the stability of large wind power-grid systems under wide-range stiffness variability and weak grid conditions.

Tackling the scientific and engineering problems of the first target will yield techniques to improve overall power conversion efficiency and extended system lifespan, with the potential to lower the cost, while work the second should lead to solutions to mitigate large diverse impacts on the modern stiffness-varying grid.

Prof. Tao Zhang

Dalian Institute of Chemical Physics, Chinese Academy of Sciences

Fellowship: Hans Fischer Senior Fellowship | **Host:** Prof. Fritz E. Kühn (TUM School of Natural Sciences) | **Focus Group:** Single-Atom Catalysis | **Research Area:** Surface, Interface, Nano- and Quantum Science

The emergence of single-atom catalysts (SACs), first proposed in 2011 by Tao Zhang and coworkers, marks the downsizing of nanocatalysis to an atomic level. Such catalysts, featuring isolated metal species ligated on defined solid supports, maximizing the metal's atomic efficiency and providing both uniform and well-defined active sites, can exist now in many coordination environments. Accordingly, it should be possible, starting both from "classical" homogeneous (molecular) catalysts by synthesizing appropriate precursor molecules and from "classical" surface chemistry, to engineer active atomic sites on a very well-defined and appropriate support surface.
The team will focus on rationally designing the synthesis of uniform SACs with excellent catalytic activities. The structure-performance relationship and dynamic evolution of the active sites at an atomic scale is to be investigated, focusing on the novel SAC concept. Principles established for highly selective but also usually sensitive and short-lived homogeneous catalyst systems will be transferred to much more stable SACs to combine the advantages of homogeneous and heterogeneous catalysis in an unprecedented way.

Prof. Walther Ch. Zimmerli

Humboldt Universität zu Berlin

Fellowship: Philosopher in Residence (funded by the TÜV SÜD Foundation and as part of the Excellence Strategy of the federal and state governments) | **Hosts:** Prof. Claudia Eckert (TUM School of Computation, Information, and Technology), Prof. Urs Gasser (TUM School of Social Sciences and Technology), Prof. Michael Zäh (TUM School of Engineering and Design) | **Research Area:** Political, Social, and Technological Change

The project aims at developing an adequate understanding of the process of digitalization as the main characteristic of today's technological culture, bottom up from different perspectives of both engineering and social sciences, as well as by trying to integrate them top down in a comprehensive philosophical approach at the same time. The underlying paradigm shift consists in the assumption that the process of digitalization is also affecting some of the main philosophical ideas of the implicit epistemology, ethics, and anthropology, guiding our thinking from "behind our backs." Thanks to the different expertise of the TUM Hosts, it will be possible to test this general hypothesis in a case study approach by scrutinizing cases such as digital twin technology in manufacturing, privacy techniques in cybersecurity, or smart contracts and intellectual property issues in the legal system. In order to achieve sustainable results, it will be helpful to first develop an operatively feasible clarification of the concept "digitalization" before looking at some of the most important effects the process of digitalization has with respect to traditional philosophical reasoning.

In Focus

Green Oceans of the Blue Planet

Not only are forests more complex than is commonly realized, they also do more. Their active role in transporting moisture thousands of kilometers inland from oceans, argues Anastassia Makarieva of the Petersburg Nuclear Physics Institute, should not be overlooked in studies of global climate change. This is one focus of her TUM-IAS collaboration with TUM Professor Anja Rammig, as discussed in an interview.

Petersburg-based physicist Anastassia Makarieva is a pioneer in examining large-scale effects of the interactions between living things and the environment. She focuses on phenomena such as long-distance moisture transport, chiefly within the framework of theoretical concepts known as biotic regulation and the biotic pump. An Anna Boyksen Fellowship from the TUM-IAS has facilitated her collaboration with Anja Rammig, Professor of Land Surface-Atmosphere Interactions at TUM. Science journalist Patrick Regan discussed this research with them in an interview.

Q: As I understand it, Anastassia, you have been studying mechanisms through which major tropical and boreal forest belts can play a role in both global climate trends and events such as hurricanes and droughts. You describe a biotic pump, for example, by which forests draw water vapor far inland from the oceans and thus help to preserve the conditions for life. Could you explain this with an example?

Makarieva: An important development we made during my time with the TUM-IAS, published in *Global Change Biology*, is that we have now identified two regimes: one where the biotic pump works, so plant transpiration increases atmospheric moisture transport and moisture import; and another one we call the dry regime, when plants transpire but there is no condensation, and hence the biotic pump dynamics is not initiated. In this case we can see that with increasing transpiration we have decreasing atmospheric moisture import to the considered area from the surrounding regions, including the ocean. So we have two regimes with distinct reactions to increased plant transpiration. This means there is a tipping point in the functioning of the ecosystem, and if, for example, by logging, we disturb it in such a way that it gets drier and drier, at a certain point this can lead to a self-destructive loop wherein the ecosystem won't be able to contribute to sustaining its own water cycle.

An example of an ecosystem in Central Asia degraded by overgrazing and fallen into the dry regime. Transpiration from the remaining scarce vegetation does not lead to changes in atmospheric dynamics necessary to enhance moisture import.

Example of a natural ecosystem in the wet regime (boreal forest in the Yenisei river basin, Siberia). The low-level clouds with their high albedo are an important mechanism of temperature regulation by forests.

Conversely, we could help the ecosystem. When we begin to restore a dry place, for example initially with irrigation, there is hope that it will pass through this tipping point again and become self-sustainable. This is an important thing that we had not explicated before. We used data for the Amazon, for the wet regime, and for China, where there are examples of both dry and wet regimes.

Q: How does this mechanism affect or involve atmospheric currents, the so-called flying rivers?

Makarieva: I can explain on the example of the Amazon. Here this effect was described independently, not connected to the biotic pump, by other researchers. When the forest, after the end of the dry season, begins to transpire, the atmosphere moistens and there is condensation, and the air begins to move from the Atlantic Ocean to the forest. So forest transpiration triggers condensation over the forest, and it leads to the appearance of the air motion from ocean to land. This occurs two months earlier than the geophysical rain band, which is the Intertropical Convergence Zone. The question is, what is the physics of that? What we're saying is that it is because of the pressure drop from condensation, from precipitation, basically there is less atmospheric mass, and when it occurs on a very big scale, like over 1,000 kilometers, this facilitates air motion.

Q: If there is strong evidence that the biotic pump affects both weather and climate, why isn't it taken into consideration in global climate models or policy discussions?

Rammig: The main critique that I always hear is that this effect is not large enough that it would really make such big air masses move. This is the main critique you got, right?

Makarieva: It is difficult to say what the main critique is. As a recent independent study puts it, the biotic pump "has been heavily contested, yet seemingly without a definitive resolution." Specifically for the Amazon, we did show that our prediction fits the data. This was published in 2014. The data are not very precise, but to the precision that we have, they fit with our expectations. It is not a weak effect. It is very sizeable. We are always doing parallel research on tropical storms. Forests are incredibly complex. You can't easily pinpoint what's going on there. But tropical storms are physical systems, and fairly simple compared to living systems. We can point out what happened there, and if it worked there, it should work in the forest as well.

Rapid intensification of tropical storms is a very big problem for meteorological science. It is recognized that this is very poorly predicted. So there is a weak tropical storm, and suddenly there is a Category 5 hurricane. Sometimes it goes very rapidly, and the hurricane models ►

Anastassia M. Makarieva, Anja Rammig, Patrick Regan.

fail to predict it. We were the first to point out that this rate of rapid intensification, how fast the pressure falls, is closely related to the precipitation in the storm center. Precipitation removes mass, so there is less and less air pressure, and this coincides with the maximum rate of intensification. This was not known. Nobody even looked at this, from that side. If it is so, how can people claim the effect is unimportant?

Q: One way you've described biotic regulation is "the key role of natural ecosystems in stabilizing a life-favorable environment." That sounds like something that should be considered in confronting the global climate crisis and the issues it raises – including impacts, adaptation, and vulnerabilities as well as mitigation. Are you concerned that faulty assumptions or incomplete models could lead to counterproductive policies?

Makarieva: Yes, and I can give you a very current example. We all know that 2023 and 2024 were abnormally warm, such that mainstream climate science can't explain it. As leading climatologists confessed, we are on uncharted ground. We don't know what happened, why there was this uptick of temperature. Some claim that they need more resources to get real-time data to understand what's going on. But when there is this recognition from the climate modeling community that none of the models have predicted that this is even possible, now is a good moment to look at the alternatives. Among potential causes of anomalous warming, some scientists hinted at teleconnections, oceanic and atmospheric currents. So something in the oceanic and atmospheric currents could represent a tipping point, which could be behind this abrupt extra warmth.

Now we know that during the same time, the Amazon has been suffering one of the worst droughts, if not the worst, in history. So it is precisely long-distance moisture transport that was disrupted. On nearly a global scale, in a critically important climatic region – the tropics. So it could be that this was the cause, piled on top of the regular greenhouse gas accumulation.
If you look at global climate models, and how they describe the Amazon moisture transport, it is all parameterized. What is parameterization? When a modeler applies his or her own ideas, for example about how the atmosphere should produce rain, this is introduced manually into the model after fitting to observations. In the case of the Amazon, if you remove convective parameterization, the dynamics of many global climate models are such that they don't transport moisture to the continent at all. This is a well-known fact. So basically all the transport into the Amazon in the models is manually fit-

ted to the observations, which means that the capacity to predict things is severely limited. Parameterizations fitted to data under normal conditions may go totally wrong when the Amazon forest becomes sick enough.

So we have unexplained warming, terrible drought in the Amazon, and severely limited predictive value of the models with respect to long-distance moisture transport. It is a good time, a very good moment, to look seriously at alternative explanations – precisely, that the forest itself regulates moisture transport, and that when it's disturbed beyond a threshold by human overexploitation, we can see all these consequences.

Q: To what extent is the biosphere part of the climate models?

Rammig: Current Earth system models that simulate climate change have integrated land surface models. They simulate the feedbacks from the land surface, the carbon cycle, and also the water cycle. Often, the feedbacks are very coarsely represented. Earth system models are large and complex, often constrained by the runtime and available computational power, and it has always been necessary to make a lot of simplifications. The modelers needed to be pragmatic. Often, Earth system modelers have their background in atmospheric sciences, so there is ususally more emphasis on the development of atmospheric processes.

Q: Until Suki Manabe and others linked the atmosphere to the oceans.

Rammig: Exactly. And then came the link to the land surface, and then came the link to the carbon cycle. Every process you introduce causes some feedbacks in the Earth system, which requires the modelers to readjust other parameters and try to make the model stable again.
I'm working only with land surface modeling. We have now developed a new version of our model where we simulate in more detail how the plants take up the water from the soil and pump it through their system, through the stem, and then release it to the atmosphere. Trees have different strategies, and we have implemented this now in the model. You have to adjust all the other processes, like how evapotranspiration and carbon uptake are simulated, and it often makes the model unstable. In the end, the goal is to reproduce the observed pattern. And of course, as Anastassia says, you can always tune parameters so that you can reproduce the observed patterns, but it can also be for the wrong reasons.

We can now show, with our land surface model, that we can simulate drought effects in the Amazon and show that this has a strong impact on tree growth and tree mortality. So we now can reproduce observations that other models without hydraulic processes cannot.

Implementing this into the Earth system model would be even more complicated. And there are many processes that are not well understood. And if you wanted to implement this biotic pump theory, you might have to change the basic principles of the models.

Makarieva: Yes, this is challenging. But think about this concept of Spaceship Earth. When it comes to a real spaceship, engineers always say to plan for the worst-case scenario. And in industries like information technology, it's common for companies to pay for research that exposes vulnerabilities. My view is that the climate community should endorse and welcome disruptions instead of always defending the current understanding.

Rammig: I want to add something. You mentioned adaptation and mitigation of climate change. This relates to the paper Anastassia mentioned earlier, which we wrote together. Currently, it is assumed that afforestation is a very efficient method to mitigate climate change, and now everyone is planting forests everywhere. I think it is very important to keep in mind that a forest is not just some machine that sucks up a lot of carbon. There are many other feedbacks, ▸

especially with regard to the water cycle, that are not at all considered in these afforestation efforts. There is much more to consider when you do afforestation or reforestation projects. There are many more processes that you are not aware of – which are not intuitive and straightforward – that should be considered.

Q: Could you elaborate?

Makarieva: This was the motivation behind our second paper, published in *Frontiers of Forests and Global Change*. This received quite a bit of resonance. We objected to the idea that boreal forests are bad for climate because they make the surface dark and have a small albedo. That idea could lead to dangerous practices. We proposed a moratorium on exploiting old-growth forests, on a global scale. It was picked up by American scientists, and 100 of them signed it and made an appeal to then-President Biden. When you put boreal forests into the climate models, it gets warmer because they absorb more sunlight. So you might think that doing away with the forests gets the Earth cooler. So basically even though they store carbon, it is better without them – according to global climate models. What we wanted to call attention to is that transpiration, besides moistening the atmosphere and influencing the dynamics of circulation, also has an important function of cooling the surface. According to the models, it doesn't lead to global cooling, but it could – and we suggested how it could.

You see, there isn't transpiration or evaporation without precipitation. There is a very small amount of moisture in the atmosphere. Everything that goes in goes out. They are always matched, to a very high precision.

So what's going on when we have a transpiring forest? Solar energy is absorbed at the surface, and it is not converted to heat. It is absorbed and spent on evaporation, tearing the molecules from the water phase. Then this moist air goes up, and then this latent heat is released, first to thermal energy of molecules, and then from this higher level it ultimately radiates to space. This solar energy is converted to heat, high in the atmosphere, and goes to space, leaving all the greenhouse absorbers beneath. So basically this radiation escapes the greenhouse gases, and thus the planet is cooler.

Now suppose you turn off the transpiration. Now all the solar energy is turned to heat at the surface, sensible or just radiation – sensible heat also dissipates close to the surface – and so all this radiation now goes through the greenhouse gases and is trapped and partially returns to the surface. So the greenhouse effect increases, and the planet warms as a whole. We calculated that this can be quite significant.

We identified a physically plausible mechanism that shows that the models can be incorrect. And this could lead to a reconsideration of the role of all forests, including boreal. We actually showed that this can be pronounced, and that you can see it in observations and can discriminate between warming solely due to greenhouse gases and warming due to reduced transpiration. The problem will be in trends in temperature at different altitudes. Speaking simply, if you remove heat from an upper level and put it to the ground, at the ground the temperature will grow faster than at the height from which you removed the heat. So we have these different rates of temperature trend at different heights. This is shown in observations, and this is another thing the models can't explain. We have shown that if you have a reduction in transpiration, it should have this effect.

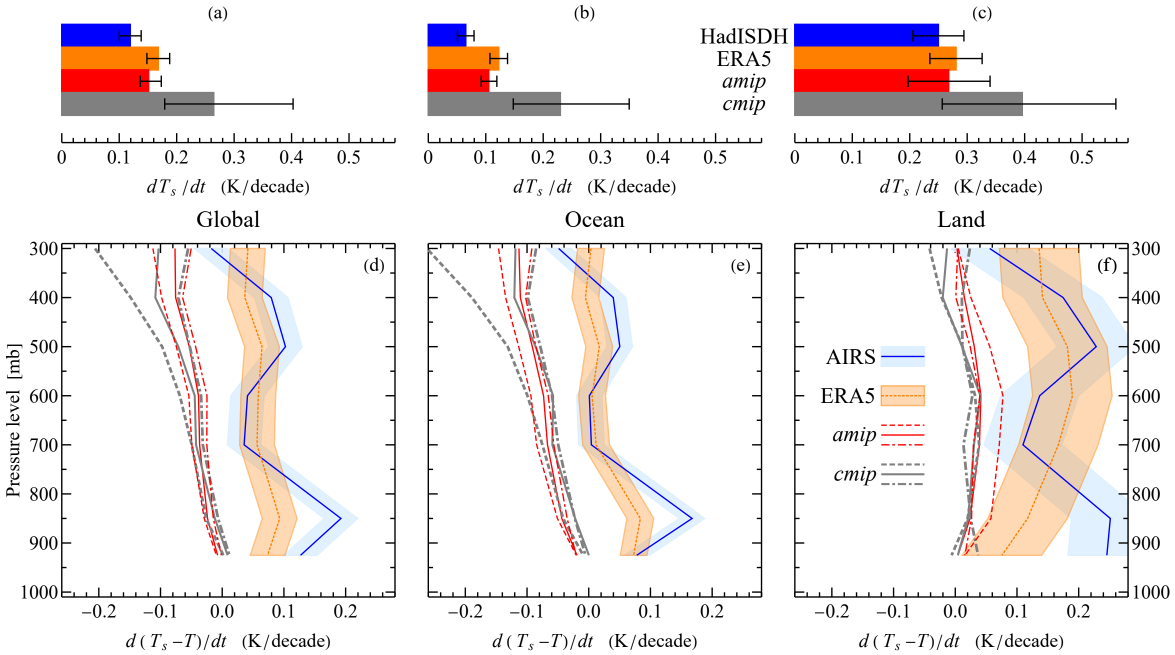


Illustration of the discrepancy in temperature trends at different atmospheric levels between observations (AIRS, ERA5) and global climate models (*amip, cmip*) during 1988–2014. Panels (a), (b), and (c) show trends in surface temperature globally, over the ocean, and over land, respectively. Panels (d), (e), (f) depict the difference between surface temperature trends and atmospheric temperature trends.

It is a profound revision of our understanding of global warming. I've always wanted to do something real to save forests. This *Frontiers* paper, "Reappraisal of the role of natural forests," is the most real thing that could work to save these forests – if it gains wider traction.

Q: Both of you, in addition to your work on physical analysis and ecosystem modeling, spend a lot of time in forests. Could I ask you to talk about how that experience affects you and influences your scientific work?

Rammig: We held a conference here, on Embracing Nature's Complexity. When you work in the forest, you get a feel for it. It sets a very high standard for complexity. Some people, with good intentions, propose technical solutions for ecological problems. But it is unproven that we can replace even a single element of the system, say, by inventing an artificial bee. When we look at the system as a whole, its complexity is totally beyond our capacity. If we look at this mechanism of climate regulation, we won't be able, ever, to make a technological substitute.

Makarieva: I do think that implicitly many people can't accept that forests have a greater and far more complex role than just being there as carbon sinks. We have embraced artificial intelligence and supercomputers, yet when faced with the supercomputer of life itself, we reduce it to simple chemical reactions – CO_2, carbohydrate production – little more. This is a dangerous perspective.

Rammig: I agree. It is very important to acknowledge this as a revolutionary idea. The forests are not just there because they have been planted by humans. The old-grown forests are there because of a long evolutionary pathway that brought them there. I would divide all people into those who know what complexity is and those who have never really faced it. The complexity of life is absolutely unprecedented, and we need to keep it intact as much as we can. ►

Q: This is easier said than done, with a variety of pressures on not only heavily exploited forests, but also on areas that remain in something more like the natural state created by evolution. How can you put all this into perspective?

Rammig: The Amazon forest always gets a lot of attention. I realize this because I am working on these forests for quite some time now, and there is a lot of interest, often in the news, and I get requests from journalists, from TV, and so on. The boreal forests don't have this standing somehow. This makes it more difficult to highlight that this is also an old-grown, huge forest biome, one of the largest existing forest biomes besides the Amazon rainforest, but it doesn't have these lobbies, so to say. This makes it even more difficult to communicate that this is also a very important forest system that needs to be saved.

And it doesn't make any sense to cut it down and then restore it, because then you lose all the functions that this old-grown forest has. It will never come back to this state. This is also something I learned from Anastassia. I always was aware of it, and I always wanted to work in the boreal forests – from the beginning of my research, I was much more focused on the cold forests than the tropical ones. Anastassia explained to me that Russia is still relying on the natural resources of the forest, to cut it down and sell it. This also happens in the Amazon, but I think this is very important to consider, that there is not the same kind of public and institutional support for the boreal forests that there is for the Amazon.

Q: Like the status of endangered animals that aren't seen as charismatic?

Rammig: Exactly.

"The complexity of life is absolutely unprecedented, and we need to keep it intact as much as we can."

ANJA RAMMIG

Q: Haven't you written that cutting down forests in Europe could affect agriculture as far away as China?

Makarieva: Not just Europe, but this entire Eurasian forest belt. It's 7,000 kilometers across. There are studies, by other researchers, showing that indeed China receives a lot of moisture through this moisture recycling and also the biotic pump, which in the boreal forest takes a different form than in the tropics. There moisture is transported in the form of atmospheric vortices, and so the intensity of precipitation is what matters.

Our message to China is that by cutting old-growth forests in Siberia they disrupt the moisture flow to China. Then they plant trees in China to stop aridity. However, plantations are no substitute for the vast natural forests that have evolved the capacity to stabilize the terrestrial water cycle. What is actually needed to stabilize the Eurasian water cycle is investment into highly productive plantations somewhere close to cities, to satisfy economic demand, and simultaneously setting aside massive territories with natural old-growth forests totally exempted from exploitation, to stabilize the climate and the water cycle. It is totally doable.

What is optimistic about the strategy of relying on the biosphere to solve global change problems is that our economy no longer critically depends on the destruction of the biosphere, as it used to depend say a couple of centuries ago.

Rammig: But it actually is becoming more and more the basis of economy, saying that forests are important for mitigating climate change. This is something we have in Europe now. There are several different kinds of pressures on forests: They should store carbon; they should also be there for construction; wood can now be used as a substrate for many other materials. Because it is acknowledged now that forests are good for the climate.

Makarieva: But in which sense? In North America now they have forests that approach old-growth conditions, that have recovered from disturbances 100 to 150 years ago, but these forests are now logged for pellets and transported to Europe for a greener economy.

Rammig: This is exactly what I mean. We can stop deforestation, but our economy has started to change a bit to get away from fossil fuel burning, and the role of wood is acknowledged more – and then these strange kinds of things happen. This could again threaten old-growth forests, because there you have all this wood. You can easily cut it down and sell fuel pellets somewhere where you can earn a lot of money, and it's "green."

Makarieva: And it's subsidized. So it's becoming green to destroy forests. Words fail me, how destructive this is. Cutting down forests for pellets is the first thing that should be stopped.

Q: So is this where there's a role for industrial forestry, to grow trees specifically for such purposes?

Rammig: No, that's not straightforward either. Where should you do that? In Europe, we now have this credo of having multifunctional forests, where you do all these things at the same time: carbon storage, high biodiversity, timber for construction or pellets or whatever. There are many discussions going on about how to manage forests. In the United States they have a land-sharing land-sparing approach – you discuss it at least, so you can have some areas where there can be large-scale plantations. But here in Europe we have national and regional differences in laws, we have different ownership. There are a lot of private people who own small pieces of forest, so they could be advised how to manage their forests, but you cannot implement any large-scale preserves or plantations.

Q: You've mentioned that the framework offered by the TUM-IAS has been a strong support for your productive collaboration. How so?

Makarieva: The main thing that contributes to productive work – meaning when you get results – is an atmosphere of academic freedom. Here you are very free. In our collaboration, nobody told us what to do or how to do it. We are totally free, and there are all kinds of support. When we wanted to organize this conference, we had overwhelming support. Generally people at the TUM-IAS are supportive of any initiative. This is what I valued most. The motto is "risking creativity," and they try to make the atmosphere as stimulating as possible.

Rammig: Anastasia was very well supported by the TUM-IAS, and I didn't have to manage things like visas or accommodations. You know your guest will be treated well. And I think it's important that women work together and build up a strong, independent network of female scientists to support each other. The Anna Boyksen Fellowship is specifically oriented toward promoting female networking.

I have a lot of female students, from the Amazon actually, so I can see how it works. I brought them here from Brazil, and they are bringing more female scientists here. It is a safe space here for them to be themselves and give their opinions and feel free from whatever influences might prevent them from doing their science the way they want to do it. This is very important, and it makes me happy to see these networks growing. ■

In Focus

Modeling Molecules

A hundred-year-old equation is at the heart of an effort to better understand the dynamics of molecules that do interesting and potentially valuable things. Physics, mathematics, and computer science are united in the collaborative research of Örs Legeza and Gero Friesecke.

Hans Fischer Senior Fellow Örs Legeza heads a research group at the Wigner Research Center for Physics in Budapest that focuses on "strongly correlated systems" – compounds and materials with unexpected and often useful properties. Legeza's Host is TUM Professor Gero Friesecke, who uses mathematical tools to analyze, among other things, the electronic structure and dynamics of molecules. Their collaboration is pushing the envelope for simulations of quantum physical phenomena and extending the limits of what is computationally feasible. They recently spoke with science journalist Patrick Regan.

Q: It's easy to understand why it might be difficult to model molecules and materials. Why is it worth the effort? And is it within reach?

Legeza: In the history of all mankind, better understanding of materials always leads to a big change in society. Think about the stone age, bronze age, iron age, steam engines, electricity, semiconductors, nuclear technology – and now we see more and more emergent evolution in quantum technology. If we understand quantum technology, then we can manipulate other things on the atomic and nano scale. That means we may be able to understand and control some processes that lead to new products that can later change everybody's life.

"They have a life of their own. They're not just dead objects. They act, they move, they perform tasks. They keep the world running."

GERO FRIESECKE

To understand how this is related to numerical simulations, think about how aircraft are designed and manufactured today. In the engineering world, nobody is building hundreds of actual models. Instead they do simulations on computers. When you design the new Airbus, for example, perhaps millions or hundreds of millions of simulations are performed on the different parts before the computer suggests solutions that seem to be the best. It's only then that people start to build the actual models and put them into wind tunnels and perform other tests to measure whether the parameters match with the computer simulations.

In a chemical reaction path, there are many intermediate steps as you go from system A to system B. If you could selectively model and manipulate key steps, there would be many potential applications. We want to do the simulations in the same way as in the classical world, just like with these CAD programs in engineering. It would be good to have something like a quantum CAD to do all these things.

In quantum physics, we are not at this stage yet. We understand many things, but there are still many things that we can't describe, or we don't have complete knowledge about. But the kind of knowledge that we already have, this we can program. That is exactly what people are doing in computer simulations for quantum systems.

Örs Legeza, Patrick Regan, Gero Friesecke.

Q: And one of your main tools, and a focus of your research, is an equation that was devised and published around a hundred years ago?

Friesecke: Yes, the Schrödinger equation. The reason Erwin Schrödinger invented it is the same reason we're still studying it today. He wanted to be able to make predictions about the behavior of atoms and molecules and materials. They have a life of their own. They're not just dead objects. They act, they move, they perform tasks. They keep the world running. They keep biology running. And the quickest access is often through theory, because sometimes you can't access what they're doing with experiments.

A good example is FeMoco, short for iron-molybdenum cofactor, which plays the crucial part in nitrogenase. That's the enzyme used by microbes, which often live in symbiosis with plants, to take nitrogen out of the air and "fix" it, transforming it into plant food. Plants can't use N_2 from the air. It needs to be broken apart to form NH_3, ammonia.

Q: I can't tell you how many times scientists have told me that plants are the best chemists in the world.

Friesecke: I agree with that. You can use the Haber-Bosch process to make ammonia – under high heat and pressure – in the lab or on an industrial scale, but that requires a huge amount of energy. Or you can put your plant in the sun on the balcony, and the enzyme just makes it happen. How? With better understanding, it should be possible to emulate this and drastically reduce the cost of fixing nitrogen. As we reported in a paper published in a computational chemistry journal, Örs managed to do a good simulation of the enzyme's quantum electronic structure that could shed some light on this.

Legeza: This is "only" a simulation of the electron cloud of the enzyme by itself. Simulating a whole dynamic process like nitrogen fixation, which involves the interaction of the enzyme both with the N_2 molecules in the air and other parts of the environment, is one of the great future challenges. ►

Friesecke: That enzyme is a pretty big beast. Until very recently there was a disconnect between this world of theory, with the Schrödinger equation, and the world of living things and interesting biomolecules that perform tasks. At the quantum resolution, it wasn't possible to do a Schrödinger equation simulation. Each time you add a particle, the computing time doubles, and doubles again, so this has been like a brick wall.

People in the field of quantum chemistry had already done the first simulation of an atom in the 1920s. But an atom is not so interesting for chemistry. It's just a basic building block. By the 1960s, people got to maybe benzene, and by the 1980s they were still stuck at benzene. You really need high accuracy to resolve the behavior to the scale where interesting transitions happen, where bonds break, and if you want to simulate that reliably you need the Schrödinger equation.

Q: Over all the decades before the advent of powerful computers and clever algorithms, how did researchers approach this?

Friesecke: I would say there were two schools. There were the exact modelers, and there were the simplifiers. And the first group was saying, we need to stick with the equation. We only make some very careful approximations that are not too crude, and then we can simulate small systems. And then there was the second group who said, oh, no, the equation is too complicated. Let's remodel it, get a simplified model, and then run simulations of complex systems – so we're going to lose accuracy, but we can predict something about, say, a metal surface or a metal-organic compound.

These two schools both got the Nobel Prize in 1998. From the precise school, it was John Pople, who started the first computer program which is the ancestor of today's programs like Örs's but for much smaller systems. He could simulate things like benzene with some accuracy. And the other was Walter Kohn, the founder of a field called density functional theory. This relied on a cruder approximation of the Schrödinger equation but could be extended to a thousand particles or so. It wasn't 100 percent reliable, but it gave a lot of good insight into what's happening. So the Nobel committee was wise and gave the prize to both.

Q: That was for work done over what period of time?

Friesecke: The award was for 30 years of cumulative work by the community, starting in the 1960s, and two of the founders got the Nobel Prize – the first ever given for computational quantum mechanics.

It's only due to cumulative advances in the past 20 years that this brick wall is beginning to be cracked, between the Schrödinger equation and getting to the size of interesting biomolecules. I think we made a big advance in simulations of such systems at chemical accuracy.

Q: So two of your own stated goals are accuracy and efficiency. If you're measuring efficiency in terms of computing resources, that seems fairly straightforward. But how do you gauge the accuracy of a simulation?

Friesecke: That's very easy. Experimental data. The thing that distinguishes the different quantum states of a molecule is the energy level. The level the system adopts when you don't have any external forces is the lowest energy state. And energy can be measured from spectroscopy, so we have wonderfully accurate measurements by five, six, seven, eight digits. At the end, you really benchmark against experiment.

> ***"It's only due to cumulative advances in the past 20 years that this brick wall is beginning to be cracked, between the Schrödinger equation and getting to the size of interesting biomolecules. I think we made a big advance in simulations of such systems at chemical accuracy."***
>
> GERO FRIESECKE

In quantum science, the accuracy of data on the real-world energy level is fantastic. The trouble is, you know the energy level of the molecule, but you don't know the quantum state. So you measure just the energy. That's the check you use. The methods are constantly competing against the measurements, and if you get the third digit wrong, you're out. It makes a big difference which state a system is in, ferromagnetic or non-magnetic, polarized or not polarized, rotated this way or that way. Especially in designing chemical reactions, the accuracy has to be good enough to decide which reaction path the system is actually taking. And that dictates to how many digits you want for the energy levels. It's not like chasing the hundredth digit of Pi, but you want them accurate enough to distinguish different transition paths and different quantum states.

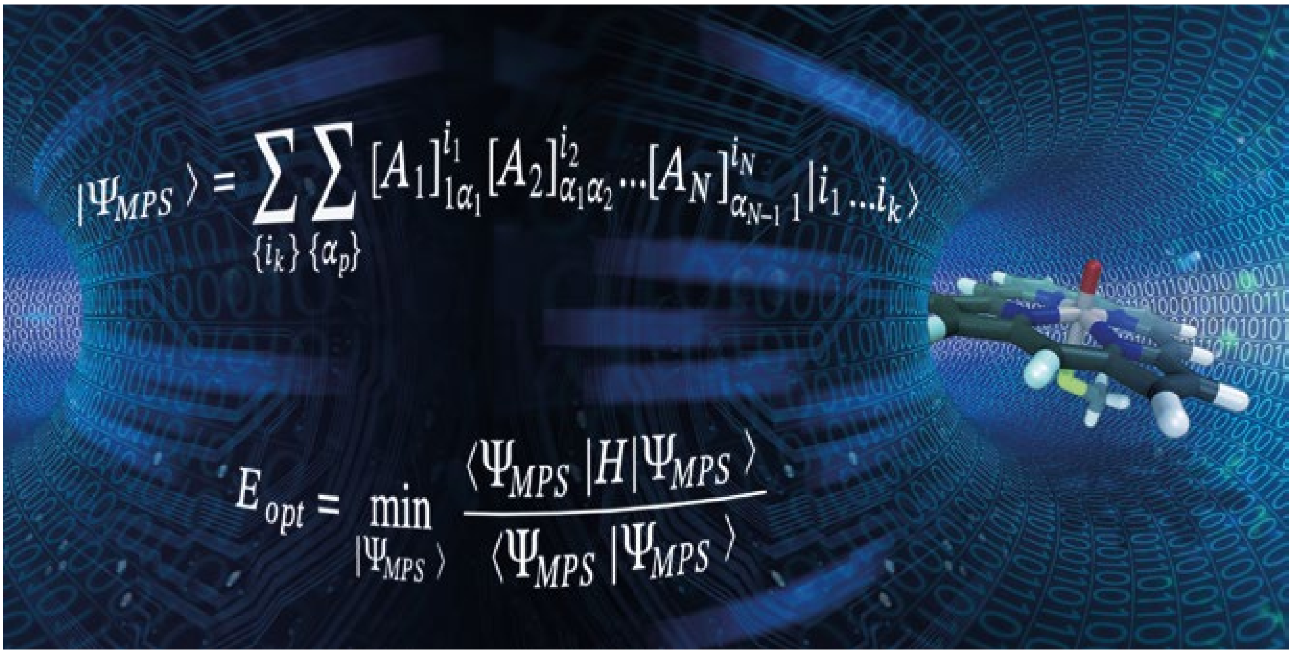
Q: So the methods that you're using can make this kind of detail accessible?

Friesecke: Exactly. I would say that is where Örs is one of the pioneers in bridging the two schools. He brings much bigger systems within the reach of this kind of chemical accuracy.

Legeza: Maybe there are originally these two worlds, physics and chemistry. I'm coming from physics. In physics we are looking at very complicated systems, and we want to make a model that can describe a physical process. For example, if you tune the temperature or the magnetic field or the pressure, you see some kind of change in the material properties. You can for example show that the magnetic properties change. In physics, we are very happy if we can show the material properties change, even if the transition temperature that we calculate is far off. It still can give you good qualitative descriptions. If you want to fine-tune it, then you have to refine your models, and you have to take a far more accurate and precise approach – and this is what comes from the quantum chemistry side.

The two worlds are coming together now. In physics you can study very large models with less precision and still get a good description of many things. In the quantum chemistry world, you really describe these energetic properties and other things on a very accurate scale. And of course if you can do larger and larger simulations, you can improve the models and model larger systems. The two will approach each other at some point.

This is why my code for computer simulation has both features. It is flexible, because we ▸



Mathematical formulae for the quantum state and the energy of a molecule modeled by tensor networks.

are using it for model systems in physics, but I'm also applying it to quantum chemistry. You can fine-tune these two approaches and use the extreme power of the machines that we have nowadays. You get improvements in speed of a factor of tens, hundreds, thousands, so that you have the chance to study larger systems or more accurate models. This is how things advance, step by step.

Q: What are the most serious issues limiting further progress?

Legeza: One major issue is scaling. Richard Feynman said that when simulating quantum systems on classical computers, the problems scale exponentially with the system size and complexity. Of course a quantum computer could solve this, breaking down this complexity issue. But what Gero and I and many others in math and physics are doing is to design mathematical algorithms that by some approximation can help us bring down this exponential scaling to the so-called polynomial form. For people who are coming from other fields, exponential refers to a function that increases extremely rapidly, and polynomial to a function that is manageable using computers available today.

Once you have the algorithm, then the question is how to implement it on the latest modern technology from IT and computer science. And if you do this, then you can further speed up this polynomial form, and that is exactly what we're doing.

Friesecke: It makes a huge difference which way you run an algorithm. You can do it in a basic way. You can do it in a smart way. Every algorithm we have now could be made to run in an even better way. And the best implementation depends on the hardware, and that's one of the reasons I admire Örs so much. He's a modern interdisciplinary scientist, a physicist who can talk about the mathematics of the algorithms with me and then talk with people from NVIDIA and AMD about how to implement these methods on their new hardware – machines that are not based on CPUs, but rather on GPUs, graphics processing units.

Q: This could be interesting to a number of different industries, right?

Legeza: It has many aspects. Accurately simulating the behavior of larger systems could eventually be valuable for a range of applications, from biological research to industrial catalysts and pharmaceuticals. Perhaps the most immediate benefit, however, is that our algorithms can help advanced computer manufacturers test and improve their technology. For example, I did some calculations that helped NVIDIA to validate some of their very recent developments on both the hardware side and the software side. They even mentioned us in an announcement. So not only is the algorithm a tool to run simulations in chemistry or physics, but it's also contributing in computer science to benchmark efficiency of hardware.

Friesecke: It's a two-way interaction, where these hardware companies, NVIDIA, AMD, and others, also need users who provide feedback which can help them optimize their design.

Legeza: With Gero, these mathematical algorithms are very well controlled in terms of math, so you can really have very direct means of accessing the accuracy, and there are many things that you can fine-tune by changing the parameters. It's not just a matter of running a calculation and getting something out. Physics, chemistry, and math – everything comes together. We can focus on the mathematical properties and the detailed analysis. And if you have this, you can validate all the calculations and also provide immediate benchmarks for the industry.

Q: Your work on algorithms, to make models more efficiently computable, strikes me as being analogous to the crucial role of information theory in making the most of technological advances such as semiconductor lasers and optical fibers. Is that a valid way of looking at it?

Friesecke: Absolutely. It's 100 percent accurate. You have the two sides. You need to compactly encode the information. There are millions of parameters, and many of them are important, but you don't know in advance which ones. You pick the right encoding of the information to capture the important pieces and then process that. And then at the same time you need the hardware. The hardware technology and the efficient encoding of the information, they have to be advanced together. I would say it's 50-50. Sometimes you gain by better encoding and processing of the information, and sometimes you gain by changing the hardware.

Q: Could you explain how the so-called tensor network methods make this possible?

Friesecke: In a sense these tensor network methods try to split up a very high-dimensional problem, which means you have many unknown parameters. It tries to split it up into many smaller problems with fewer parameters. And then these smaller problems communicate with each other across the edges of some graph. So then there are many issues that could be optimized. One is the design of the size of the blocks in which you split up the big problem. Then which pieces need to communicate with which other pieces. And then ▸

at which accuracy do you need to resolve the individual pieces and then bring these together at the end to get the results.

There's one way in which Örs is different from other researchers who use these methods. We met in 2018, at a meeting in Berlin. Örs was the only speaker who talked about these methods in a very global way. People have done really important work, but usually they focus on one ingredient and optimize that. Örs was saying look, we have to optimize all these things together. So his code constantly adapts the size of the sub-problems, how they are connected, the basis functions, and so on.

Q: What kinds of measurements can help you gauge your own progress?

Legeza: There are, for example, computational benchmarks for running simulations of quantum systems, measured nowadays in petaflops, quadrillions of floating point operations per second. It's well known that we are still not using all the available computational power. Even now, although together with my colleague Andor Menczer we have, in collaboration with industrial partners and Pacific Northwestern National Laboratory, reported the largest calculation on a single computational node, we are still nowhere if we talk about exascale computing and the possibility of achieving 1,000 petaflops. Now if we put together 40 such machines, we immediately reach the full capacity of the most powerful supercomputer of a decade ago. This is a difficult problem, but the technology is around us, and improvements in mathematics are also around us. Physicists came up with powerful methods, Gero and others are actively working on the mathematical aspects, and there are also some algorithmic ideas that can improve the mathematical scaling. Math and physics, that's not enough alone, you have to include computer science, and if you put everything together, then you can win the game.

Q: How does the prospect of quantum computing fit into this picture?

Legeza: When you focus on how to optimize algorithms on the current, classical hardware, this is a mathematical issue. Thinking about how to implement the algorithms in a different way on different hardware, that's a technical issue. But a third issue is how this connects to quantum computing. All the simulations we are doing are immediately connected to quantum information theory and quantum computing, so it all goes hand in hand.

I think it's safe to say that there is no universal quantum solver. So once quantum computers will work to solve real-life problems, there will be very specialized, specially optimized quantum algorithms for different tasks. In this kind of task, of course, the superiority of the quantum computer is not questionable. On the other hand, we have the classical algorithms, which we can adapt to solve problems over a broad range, and then of course improve step by step. Where is the border, the edge, between the two?

Maybe there's a set of problems that are accessible by quantum computers in a much better way, a set of problems that are still more accessible by classical computers, and a third possibility: creating hybrid algorithms. That is, we could use classical computers to prepare inputs for quantum computers, or to do pre- or post-processing of quantum computer simulations.

Q: Would you like to comment on the role of the TUM-IAS in fostering the kind of collaboration you've been describing?

Friesecke: The TUM-IAS is a rare thing. When we wrote up our proposal, it was seen as an advantage that it connects two fields. There's a big gap in support for this kind of work, because it's high risk but also potentially high reward. Funding agencies all claim they like high-risk/high-reward, but if you look at the decisions, what is the project list? It's almost always on the conservative side. The TUM-IAS should keep it their way, promoting new collaborations between people from different disciplines.

"Math and physics, that's not enough alone, you have to include computer science, and if you put everything together, then you can win the game."

ÖRS LEGEZA

Legeza: The financial support from this program has been very important, and so has the way the TUM-IAS brings people together to exchange ideas. I'm now involved in a number of other collaborations, with other institutions, that were made possible in part by this Fellowship. And because the Fellowship supports a PhD position, that is also a way to ensure knowledge transfer, and this person can go abroad and expand the research network. There is also support for holding workshops, which we did in April 2024, bringing together experts from here and overseas. So the TUM-IAS not only represents a community, but also stimulates further interactions. All these aspects are important: encouraging knowledge exchange and travel, as well as supporting the younger generation. ■

Scientific Reports

When their research projects come to an end, we ask our Fellows to provide a final Scientific Report presenting their achievements. At the same time, true to our philosophy "once a Fellow, always a Fellow," we are happy to welcome them as Alumni Fellows.

Focus Group: Molecular Assemblies and Covalent Nanostructures on Wide-Bandgap Semiconductor Surfaces

Prof. Lifeng Chi (Soochow University), Alumna Hans Fischer Senior Fellow | **Mohammadreza Rostami (TUM),** Doctoral Candidate
Hosts: **Prof. Johannes Barth, Prof. Martin Stutzmann (TUM)**

Prof. Lifeng Chi

Supramolecular engineering on wide-bandgap semiconductors

On-surface reactions provide a general means for constructing defined molecular nanosystems with novel properties. Wide-bandgap semiconductors offer a platform to prevent the quenching of electronic and optical excitations. Our scientific purpose is thus focused on exploring the potential of GaN and TiO_2 single crystals as well as Cu_2N thin films for on-surface reactions.

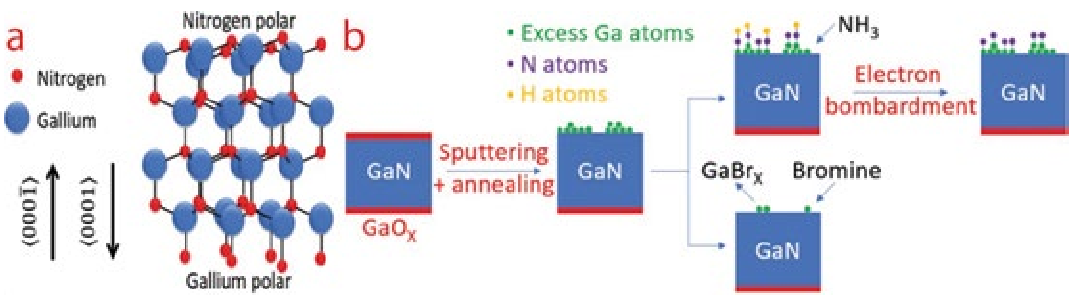


Fig. 1, a) Schematic view of the polar c-plane wurtzite GaN faces and b) our strategy for compensation of preferential removal of nitrogen.

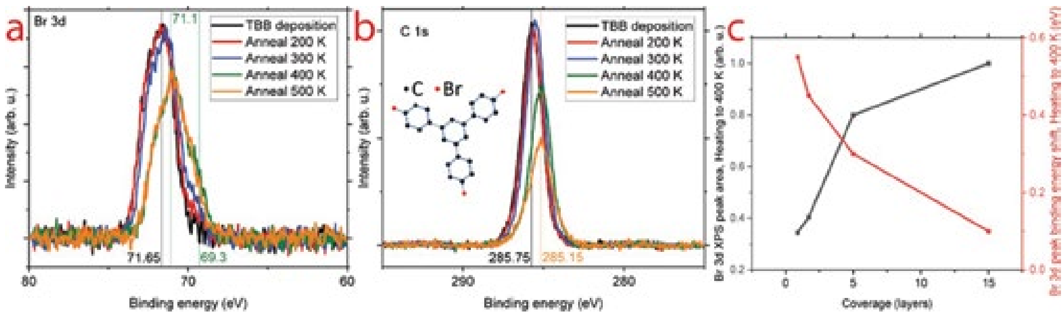


Fig. 2, XPS of (a) Br 3d (coverage ≈ 0.9 monolayer (ML)) and (b) C 1s (coverage ≈ 0.9 ML) regions after deposition of TBB on HVPE Ge-doped GaN (0001) and their evolution upon annealing (inset: schematic structure of a TBB molecule). (c) The Br 3d peak area after debromination by heating to 400 K and bonding Br atoms to the Ga sites on HVPE Ge-doped GaN (0001) surface, normalized by the Br 3d peak area corresponding to 15 layers of TBB on GaN vs. TBB coverage along with peak binding energy shifts of the Br 3d XPS narrow region scan after heating to 400 K vs. TBB coverage is shown in (c).

Gallium nitride (GaN)

GaN, a wide-bandgap semiconductor with absorption and emission in the ultraviolet/visible range, is proposed as an alternative to metallic surfaces for assembling organic molecular structures intended for optoelectronic applications. However, the formation of a persistent surface oxide layer in air considerably limits the use of GaN for well-defined interfaces. We have investigated, characterized, and processed n-type free-standing c-plane hexagonal wurtzite GaN crystals (Fig. 1a) grown by the hydride vapor phase epitaxy and ammonothermal growth methods. Surface cleaning and full removal of the oxide layer on GaN surfaces could be reproducibly achieved via sputtering and annealing cycles, as evidenced by X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). Scanning tunneling microscopy (STM), however, indicated substantial roughening of the GaN surface and the formation of unwanted Ga-rich islands and clusters. Although ammonia (NH3) and bromine (Br) treatments compensated the N/Ga atoms ratio reduced by sputtering (Fig. 1b), the surface morphology remained rough, exhibiting randomly shaped and distributed hillocks. Nevertheless, by introducing 1,3,5-tris(4-bromophenyl) benzene on GaN (Fig. 2), on-surface debromination and polymerization of the molecules upon heating GaN (Fig. 2) and the removal of Ga atoms by Br atoms during the desorption were observed and proven by XPS studies [1]. ►

[1] Rostami (2024a).

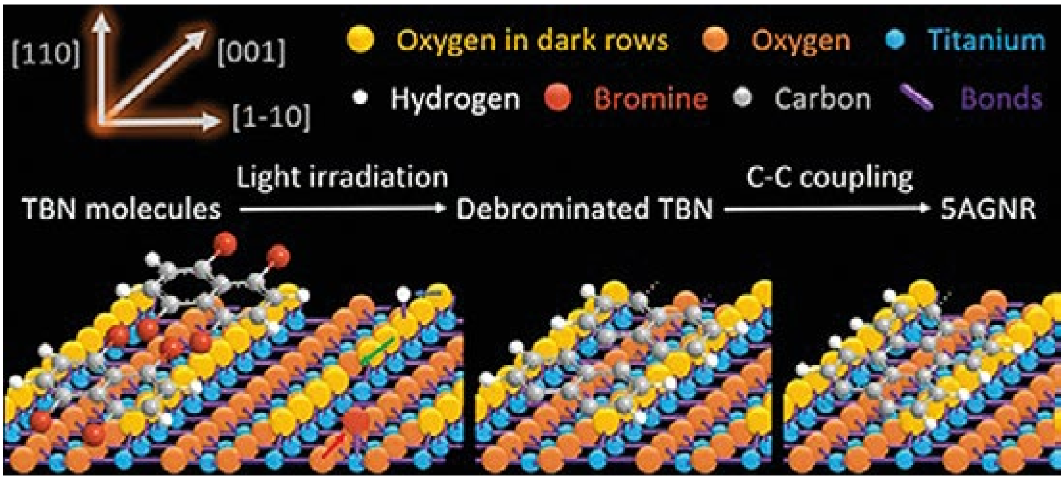


Fig. 3, Schematic view of our strategy for on-surface synthesis of 5AGNRs. Yellow, orange, blue, gray, white, and red spheres correspond to oxygen (O) atoms in the dark rows of STM images, O atoms in the substrate plane, titanium (Ti), carbon (C), hydrogen (H), and bromine (Br) atoms, respectively.

Titanium dioxide (TiO_2)

Although on-surface synthesis provides promising strategies to successfully construct various graphene nanoribbons (GNRs) with precise width control, the use of metal surfaces typically involves the quenching of electronic and optical excitations, thus preventing the study of intrinsic electronic structures and resulting in contradictory reports. Semiconducting titanium dioxide (TiO_2) including rutile TiO_2 (110) and anatase TiO_2 (101) surfaces can be used for photocatalysis of surface-assisted Ullmann coupling. We first systematically studied the influence of light and Fe adatoms on the debromination of 4,4”-dibromo-p-terphenyl precursors affording poly(*para*-phenylene (PPP as the narrowest GNR) wires through the Ullmann coupling reaction on a rutile TiO_2(110) surface by STM and XPS. The temperature threshold for bromine bond cleavage and desorption is reduced upon exposure to UV light (240-395 nm wavelength), but the reaction yield could not be improved. However, in the presence of co-deposited Fe adatoms, precursor debromination occurred even at 77 K, allowing for Ullmann coupling and PPP wire formation at 300-400 K, i.e., at markedly lower temperatures compared to the conditions without Fe adatoms. Furthermore, scanning tunneling spectroscopy data revealed that adsorbed PPP wires feature a HOMO-LUMO gap of ≈ 3.1 eV. [2]. By employing PPP wires with extended length single-molecule conductivity, measurements become possible by lifting the wire using an STM tip, as we demonstrated in related experiments [3].

We furthermore prepared 5AGNRs on semiconducting rutile TiO_2 (110) and anatase TiO_2 (101) surfaces using photocatalysis of surface-assisted Ullmann coupling of 1,4,5,8-tetrabromonaphthalene (TBN) molecules. Although annealing monolayers or multilayers on both rutile and anatase TiO_2 favored the TBN debromination as indicated by XPS, rarely C-C coupling and the formation of 5AGNRs were observed in STM images. On the other hand, the irradiation of the surface by violet or UV light drastically enhanced the formation of 5AGNRs (Fig. 3). Light with a shorter wavelength in the UV range (265 nm) causes more extensive debromination compared to near-violet light (377 nm). Furthermore, STS revealed a HOMO-LUMO gap of about 2.1 eV for 5AGNRs, revealing their semiconducting nature (Fig. 4) [4]. ▸

[2] Rostami (2025).

[3] You (2025).

[4] Rostami (2024b).

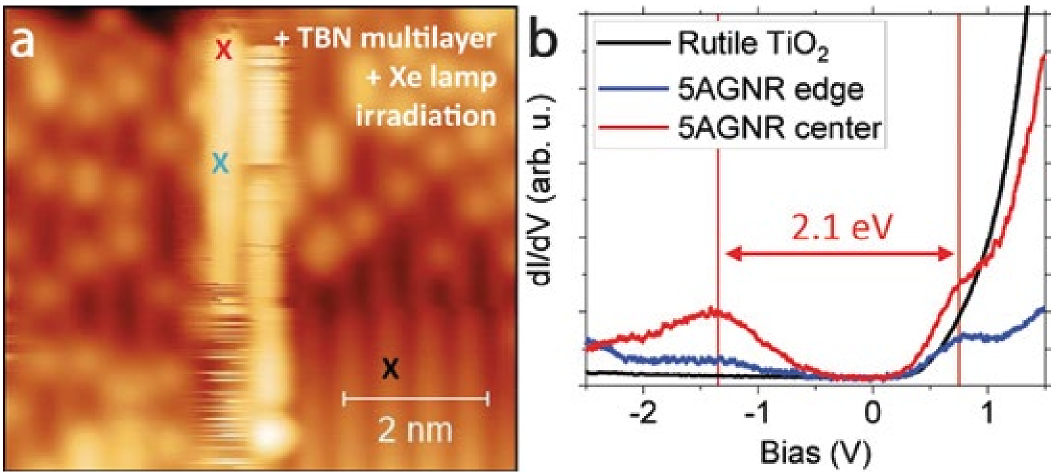


Fig. 4, An STM image of 5AGNRs on a rutile TiO_2 (110) surface after irradiation of a TBN multilayer with a Xe lamp; (a) ≈ 8.7 nm × ≈ 8.7 nm, V_s = 1 V, It = 10 pA, Z-height = 341 pm. (b) STS spectra of the 5AGNRs and rutile TiO_2 shown in (a). STM and STS acquisition temperature: 77 K.

[5] Rostami (manuscripts to be submitted).

Monolayer copper nitride (Cu_2N)

Cu_2N ultrathin films can be realized on atomistically clean copper surfaces and represent a stable and versatile buffer layer in ultrahigh vacuum, bearing promise for decoupling functional structures from the metallic substrate underneath. Although a preparation protocol based on nitrogen ion bombardment has been previously applied for in-situ deposition of Cu_2N monolayers on Cu surfaces, the encountered small domain size limits its application potential. Hence, we developed an alternative approach, growing extended Cu_2N monolayer films on both Cu (111) and (100) surfaces by ammonia-mediated post-annealing of ultrathin copper oxide films. The structure and properties of Cu_2N and copper oxide monolayers were characterized in depth by STM and LEED. The exchange of nitrogen with oxygen elements in the respective Cu_2N and copper oxide layers on Cu (111) surfaces was revealed by XPS. This oxidation-reduction two-step strategy provides a promising new approach to fabricate Cu_2N buffer layers, on which we have studied molecular depositions and assemblies and confirmed their decoupling effect by tunneling spectroscopy and DFT calculations.

We further demonstrated Ullmann coupling of 5,15-(*di*-4-bromophenyl)porphyrin ($(BrP)_2P$) and 4,4”-dibromo-*p*-terphenyl (DBTP) molecules and the formation of PPP wires on Cu_2N, highlighting its role as a sheet material with remarkable decoupling potential. To tackle these issues, tunneling spectroscopy revealed an enlargement of the HOMO-LUMO gap of the decoupled $(BrP)_2P$ molecules and PPP wires on Cu_2N compared to Cu (111) islands, indicating crucial potential for fundamental understanding and transformative insights into the electronic and optical phenomena of surface-confined nanostructures and materials. Moreover, systematic complementary computational modeling studies of these fascinating material platforms have been conducted [5].

Within this project the PhD thesis of M. Rostami was completed in Dec. 2024, also involving an extended research experience in China. Moreover, synergetic scientific achievements have been obtained in cooperation with the Focus Group of TUM-IAS Hans Fischer Senior Fellow Mathias Senge (Trinity College, Dublin). ■

Selected publications

Rostami, M., Yang, B., Haag, F., Allegretti, F., Chi, L., Stutzmann, M. & Barth, J.V. Influencing the surface quality of free-standing wurtzite gallium nitride in ultra-high vacuum: Stoichiometry control by ammonia and bromine adsorption. *Applied Surface Science*, 160880 (2024a).

Rostami, M., Yang, B., Ma, X., You, S., Zhou, J., Zhang, M., Cui, X., Zhang, H., Allegretti, F., Wang, B., Chi, L. & Barth, J.V. Catalytic effects of iron add-atoms and light on poly(para-phenylene) wires on TiO_2 surfaces. *Nanoscale*, accepted (2025).

You, S., Gao, Y., Tang, T., Xu, C., He, J., Li, X., Zhang, H., Du, S. & Ch, L. Identifying carbon-carbon triple bonds from double bonds via single-molecule conductance, *ACS Nano*, accepted (2025).

Rostami, M., Yang, B., Ma, X., You, S., Zhou, J., Zhang, M., Cui, X., Zhang, H., Allegretti, F., Wang, B., Barth, J.V. & Chi, L. Photocatalytic fabrication of 5-armchair graphene nanoribbons on TiO_2 surfaces. Submitted (2024b).

Rostami, M., Yang, B., Seyedmohammadzadeh, M., Kaya, P., Kaderoğlu, C., Olgar, H., Aktürk, E., Chi, L., & Barth, J.V. Post-synthesis of Cu2N monolayers on Cu (111) from copper oxide films and their decoupling effects.; Rostami, M., Kaderoğlu, C., Yang, B., Seyedmohammadzadeh, M., Kaya, P., Olgar, H., Senge, M.O., Aktürk, E., Chi, L., & Barth; Replacement Method Fabrication of Cu_2N on Cu(100): Analysis of Structure and Electronic Properties | manuscripts to be submitted

For a full list of publications, please visit
www.ias.tum.de/ias/chi-lifeng

Focus Group: Light-Induced Molecular Transformations on Cluster-Assembled Materials

Prof. Ib Chorkendorff (Technical University of Denmark), Alumnus Hans Fischer Senior Fellow | **Clara Aletsee, Charitini Panagiotopoulou, Carina Schramm (TUM),** Doctoral Candidates
Hosts: **Prof. Ueli Heiz, Prof. Ian Sharp (TUM)**

Prof. Ib Chorkendorff

Versatile reactors for light-induced molecular transformation

Recent studies in the UHV suggest a new mechanism for the photocatalytic conversion of alcohols on Pt-decorated rutile $TiO_2(110)$ single crystals. To elucidate the transferability of this mechanistic concept, we developed versatile gas and liquid phase photoreactors. The findings we obtained provide understanding that is pivotal for the tailored development of new efficient photocatalysts.

Heterogeneous photocatalytic systems are usually described on the basis of electrochemistry, which most interpretations and strategies for optimizing photocatalysts rely on. Charge carrier dynamics are usually in the spotlight, whereas the surface chemistry of the photocatalyst is neglected. This is unjustified, because studies on alcohol photoreforming on metal-decorated rutile single crystals revealed the electrochemical reaction model not to be generally applicable. Hence, many photocatalytic reactions may proceed in a different manner, and the thermal chemistry needs to be accounted for. Combining a variety of surface science techniques, we found a new surface reaction mechanism, illustrated in Fig. 1. Upon dissociative adsorption of the alcohol, a surface-bond hydrogen and the corresponding alkoxy species are thermally formed. The latter is suggested to interact with the negatively charged defect states of the titania surface [1]. Being the photoactive species, the alkoxy species reacts in a photo-hole mediated step, in which the C-H bond is homolytically cleaved. This forms the corresponding aldehyde or ketone, which thermally desorbs from the surface.

[1] Walenta, C.A. et al. (2019).

The evaluation of this new reaction mechanism under more applied conditions, such as, e.g., ambient pressure or liquid phase, and for materials other the single crystals, has been challenging since fabrication of such model photocatalysts often involves tedious strategies, yielding only low quantities in the μ-gram scale. In addition, these model catalysts ex-

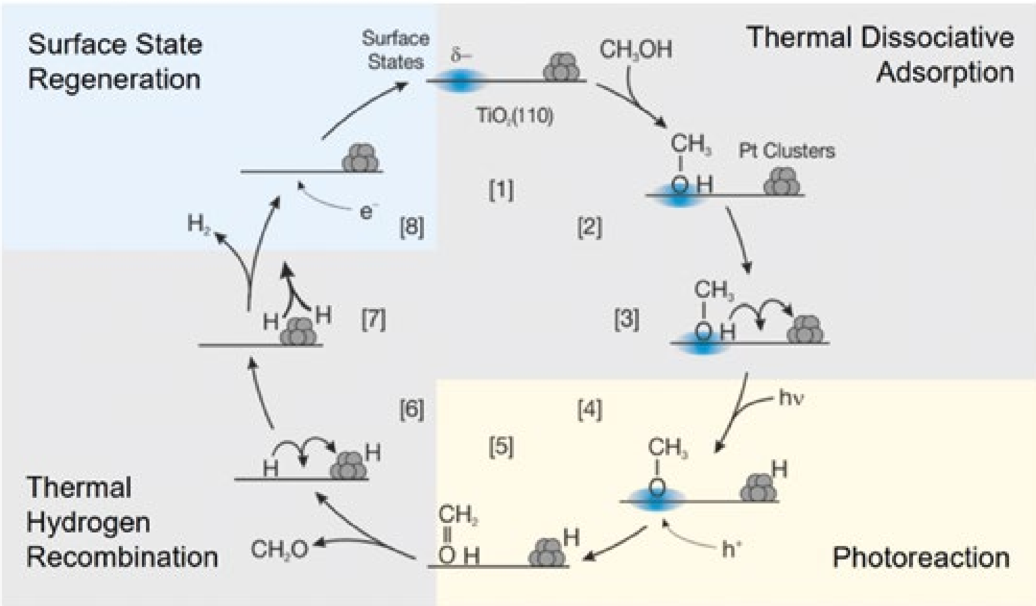


Fig. 1, The catalytic cycle for methanol photoreforming of platinum-loaded TiO_2(110). The overall reaction can be divided into two thermal parts, dissociative adsorption of the alcohol and product desorption (formaldehyde and H_2 after the recombination of hydrogen atoms), and two photochemical ones (hole reaction and surface state refilling). This model considers only one photon for the reaction, which is also reflected experimentally in the order of the reaction with respect to the illumination intensity.

hibit different forms, such as powders or film(-like) structures grown on various supporting materials. Therefore, in the first part of this project, we introduced a new design concept for a gas phase μ-photoreactor [2] as shown in Fig. 2. It is tailored not only to host low catalyst amounts of different shapes, such as in planar form or as powders, but also to be re-openable, which enables a fast sample exchange for screening studies and analysis of the catalyst material after the reaction experiments, mandatory for obtaining details on the reaction mechanism. Briefly, the reactor is based on a fully Pyrex-based lid with an implemented gas flow channel system, which is pressed on the supported catalyst by a polymeric spacer with a circular cutout, creating a reactor chamber volume of only 10.5 μl. The entire gas flow is transmitted by a capillary to a QMS, enabling time-resolved and sensitive reaction monitoring at ambient pressure.

The lid fabrication from two Pyrex wafers by a lithographic and wet-etching approach provides capillaries in the desired, reproducible μm-dimensions. The consecutive fusing strategy allows illumination with an interchangeable light source (λ > 320 nm). ▸

[2] Aletsee, C.C. et al. (2023).

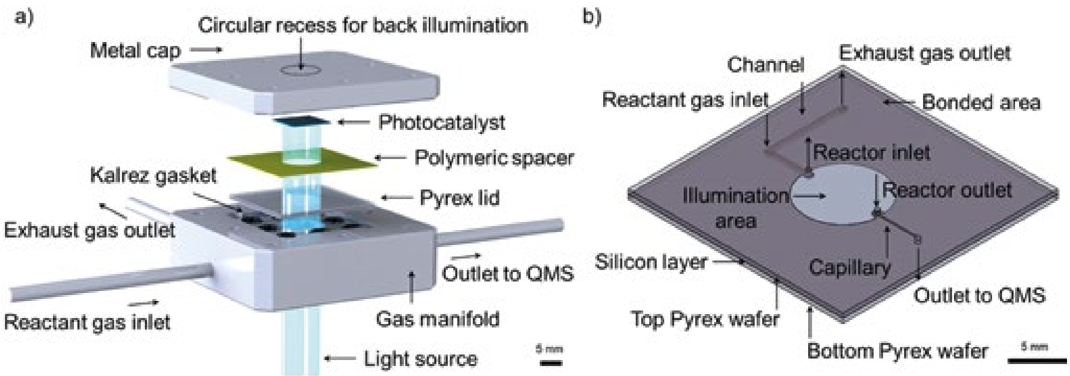


Fig. 2, a) Schematic drawing of the assembled photoreactor with labeled components in explosion view. (b) Top view of the reactor lid consisting of two Pyrex wafers fused together via anodic bonding by a Si layer with a circular recess of Si for illumination. The lid further contains the capillary for the pressure drop toward the QMS and channels for the gas flow.

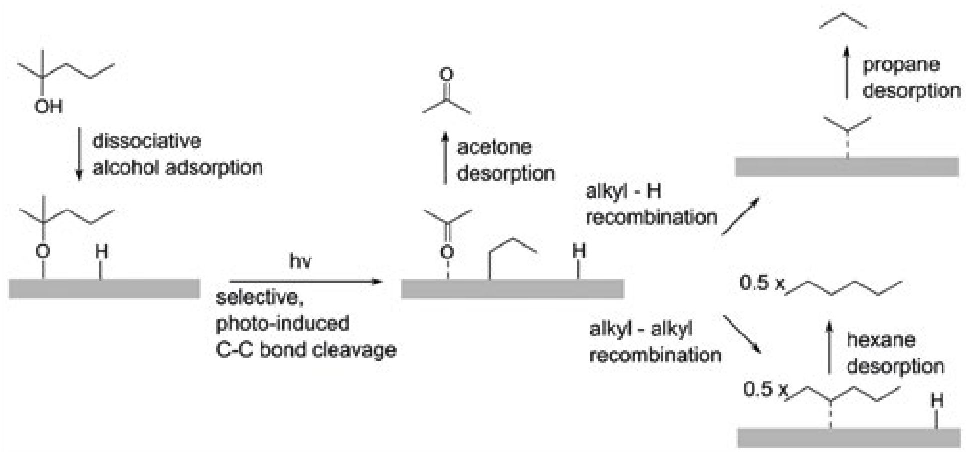


Fig. 3, Photocatalytic reaction mechanism for the conversion of 2-methyl-2-pentanol on TiO_2 P25 involving the steps of dissociative alcohol adsorption, photo-induced C-C bond cleavage and acetone formation, acetone desorption and alkane formation and desorption.

The gas-dependent flow rate through the capillary was determined to be 10^{15}–10^{16} molecules s^{-1}. These values corroborated first estimations using pump speeds and obtained pressures in the QMS.

The functionality of the device was demonstrated by the photooxidative dehydrogenation of ethanol over Pt-loaded TiO_2 (P25) at varying illumination intensities. By means of dark-illumination difference spectra, reaction products were unambiguously identified despite the presence of several overlapping mass peaks in the QMS. A version of this photoreactor was also made that is compatible with a commercial setup for dark electrochemical reactions [3].

For the evaluation of photocatalytic materials in the liquid environment, we also designed a liquid phase reactor. The reactor itself is exchangeable, which allows the characterization of a variety of catalysts with respect to shape (e.g., powder, planar structures) and extends the usability of the setup toward other applications such as electro(-photo)catalysis.

These versatile reactor concepts have been proven to be well suited for screening photocatalytic materials under various chemical environments and with various shapes, which are available only in small amounts due to their time-consuming fabrication. Furthermore, changes resulting in the catalyst during the reaction can be studied by opening the reactor and characterizing the material afterwards. The combination of these properties has proven beneficial to enable studies of photocatalytic reactions or materials.

To illustrate the versatility of these reactors, we investigated the selective photooxidation of tertiary alcohols at ambient conditions (1000 mbar, T = 23°C) in an anaerobic environment on bare TiO_2 P25 upon UV irradiation [4]. Exemplified for 2-methyl-2-pentanol and 2-methyl-2-butanol, the reaction proceeds exclusively via the photo-induced, homolytic cleavage of the long alkyl chain, resulting in the respective ketone and the alkyl-moiety, which predominantly recombines with hydrogen upon alkane formation. Alternatively, the dimerization of two alkyl-radicals occurs as a side reaction and happens on bare TiO_2 at enhanced alcohol surface concentrations. The reaction scheme is shown in Fig. 3. This demonstrates that alkyl-radical chemistry is enabled on bare TiO_2, which is also relevant for other reactions, such as Kolbe-type ones.

These new reactor platforms open an avenue for fast and versatile testing of potential photocatalysts in the search for new processes with high selectivity that is not accessible by conventional thermal processes. ■

[3] Hochfilzer, D. et al. (2024).

[4] Aletsee, C.C. et al. (2025).

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Hochfilzer, D., Aletsee, C.C., Krempl, K., Pedersen, T., Krabbe, A., Tschurl, M., Hansen, O., Vesborg, P.C.K., Kibsgaard, J., Heiz, U. & Chorkendorff, I. Enabling real-time detection of photocatalytic reactions by a re-useable μ-reactor. *Measurement Science and Technology* 35(1), 015903 (2024).

Aletsee, C.C., Neumann, P., Chorkendorff, I., Tschurl, M., & Heiz, U. Tertiary alcohols as mechanistic probes for photocatalysis: the gas phase reaction of 2-pethyl-2-pentanol on Titania P25 in a Micro-Photoreactor, *ACS Catalysis* 15(3), 2584-2594 (2025).

For a full list of publications, please visit
www.ias.tum.de/ias/chorkendorff-ib

Focus Group: Removing Institutional Roadblocks for Inclusion in Science

Prof. Andrea M. Erhardt (University of Kentucky), Alumna Anna Boyksen Fellow (funded as part of the Excellence Strategy of the federal and state governments)
Hosts: **Prof. Martin Elsner, Prof. Rolf Moeckel (TUM)**

Prof. Andrea M. Erhardt

Workshops and evaluation tools to increase gender diversity

Gender diversity in the sciences is a persistent problem, with no easy solutions or regular evaluation of program success. This project took a multifaceted approach, evaluating novel education tactics for both postdoctoral researchers and male faculty. Ongoing work focuses on building a tool to measure changes in coauthorship gender ratios before and after intervention implementation.

Universities across the world have attempted to both recognize and address the lack of gender diversity in the sciences. Challenges with bias, lower collaboration opportunities, and lower-profile speaking engagements persist. During this Fellowship, we took a multipronged approach to addressing and evaluating intervention activities.

This report will outline the four deliverables/actions for this project. These include 1) a workshop for TUM postdoctoral researchers focused on techniques for improving diversity and inclusion as they build their future research groups; 2) the development and execution of the Advocates and Allies Program at TUM; 3) a workshop to highlight female scientists and promote networking opportunities; and 4) an ongoing project to develop a tool to quantify the impact of interventions on female academic success.

Postdoctoral diversity workshop

Postdoctoral researchers represent the future of science. Typically, members of this group both have the most regular contact with graduate students and are developing ideas of their own future research group structure. In June 2023, I gave the two-hour workshop entitled "Be Part of the Solution: Identifying Solutions to Advance Underrepresented Groups in Science."

This workshop focused on understanding the problem ("Why are we here?"), providing action items ("What can we do about it?"), and outlining the path toward executing those objectives ("How do we move forward?"). These modules included interactive sessions and resulted in multiple follow-up conversations with participants. The group in attendance was enthusiastic and engaged. I have offered to repeat the workshop if needed.

Additionally, the outreach I did to gender equity officers and others on campus resulted in collaborations on their future faculty and postdoctoral orientation materials. I reviewed and provided feedback on multiple iterations of unconscious bias training that was in development at TUM and was a resource on diversity materials at TUM.

Andrea Erhardt leading discussion at her sponsored TUM-IAS workshop in April 2024 © TUM-IAS.

Advocates and Allies: Teaching men to be better gender advocates

A hallmark of our efforts was the establishment and execution of the Advocates and Allies Program at TUM. This program takes a unique approach, namely focusing on having men educate other men on gender and equity issues. The general framework of this program has been established at ~15 US universities over the last seven years; significant revisions tailored it to the TUM professoriate.

We ran two workshops, the first focused on TUM faculty and the second for TUM-IAS Fellows. The participants were recruited through gender diversity officers, department listservs, and personal messages from Profs. Elsner and Moeckel. During this workshop, the participants engaged in topics that included gendered language, understanding the impacts of sexism, and the importance of inclusive networking. Overall, the feedback was very positive, with participants saying that they came away with a greater appreciation of both the issues and constructive actions. We have been in discussions to implement this program for a larger university audience.

Isotope science workshop

Increasing the professional networking of women includes raising visibility through invited talks. As I continue to learn about both the impacts and drivers of gender inequity in science, one of the consistent themes is the lower visibility and reduced networking activities for female scientists. With this in mind, Martin Elsner and I originated a two-day workshop gathering the top scientists in our field, isotope chemistry, highlighting top female scientists. More than 50 researchers from Europe, North America, and South America attended, with more than 50% ▸

female participation in a highly masculine field. A lovely introduction from the TUM-IAS Managing Director promoted an environment to discuss gender issues throughout the meeting. We balanced both scientific objectives and gender equity objectives, creating an extremely positive environment to highlight female isotope chemists.

This meeting was an originating event for a larger community push, with a follow-on meeting planned for Prague in July 2025. This future meeting will again have a stated intent to showcase female and diverse researchers. The leadership team is composed of female and diverse scientists, including myself, Dr. Amy Hofmann (Cal Tech/NASA) and Dr. Issaku Kohl (University of Utah). My inclusion directly resulted from my role running the TUM-IAS meeting.

Scientifically, these efforts have resulted in new research directions. The collaborations established with Martin Elsner have resulted in two proposal submissions for an instrument platform. Additionally, Martin Elsner arranged for a visit to the ThermoFisher factory in March 2023, allowing Dr. Erhardt to meet the instrument development team and learn about the latest scientific advances. This networking and our collaboration have opened a new research focus for Dr. Erhardt, a direction that would not have been possible without the TUM-IAS support.

Gender diversity publication metric

Moving forward, I will continue ongoing work on building a tool to measure the impacts of the interventions tested in this program along with larger, nationwide interventions. One of the keys to success in academia is building a large collaboration network, as these collaborations can result in joint proposal submissions, inclusion in publications, and enhancement of the scholar's reputation. Women have been shown to have smaller collaboration networks than men of the same rank and tier institution, likely a result of unconscious bias. This tool will analyse the gender ratio of scholars' publication networks, examining comparable programs where efforts have been undertaken to increase gender equity.

To accomplish this, a researcher's publication history and coauthors are taken from the SCOPUS database for each year. Using a commercially available Gender API, the likelihood of each coauthor to be male or female is determined. The researcher can then be assigned a "gender diversity score" based on the gender distribution of coauthors. This determination can then be done in aggregate to look at trends within institutions or disciplines, or after an intervention program.

While this work is ongoing, Anna Boyksen funds were used to support a part-time computer science student. We hope to test the impact of programs such as Athena Swan (UK) and NSF ADVANCE (USA). I hope to show the early results at the 2025 TUM-IAS General Assembly, with publication following thereafter. ■

Selected publications

Erhardt, G.D., Dziulba, T.D., Moeckel, R., Elsner, M. & Erhardt, A.M. Engaging men in creating a culture for the success and advancement of women in the transportation workforce. Transportation Research Board Annual Meeting. *Poster Presentation* (2024).

Erhardt, A.M. & Erhardt G.D. The impact of male-lead training on changing gender perceptions: Early results from Advocates and Allies training sessions in the USA and Germany. American Geophysical Union. *Poster Presentation* (2023).

Erhardt, A.M. & Erhardt G.D. The impact of male-lead training on changing gender perceptions: Early results from Advocates and Allies training sessions in the USA and Germany. Goldschmidt Geochemistry Conference, *Poster Presentation* (2023).

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For a full list of publications, please visit
www.ias.tum.de/ias/erhardt-andrea-m

Focus Group: Multibody Systems

Prof. Michel Géradin (Université de Liège), Alumnus Hans Fischer Senior Fellow (funded by the Siemens AG) | **Prof. Karin Nachbagauer (University of Applied Sciences Upper Austria),** Alumna Hans Fischer Fellow (funded by the Siemens AG) | Daniel Lichtenecker (TUM), Doctoral Candidate | Dr. Valentin Sonneville (TUM), Postdoctoral Researcher
Host: **Prof. Daniel Rixen (TUM)**

Prof. Michel Géradin

Prof. Karin Nachbagauer

New formulations and methods in flexible multibody dynamics

The Focus Group has achieved significant progress in two directions. A two-field formulation of the floating frame of reference method has been developed with the objectives of improved generality and enhanced numerical performance. Sensibility analysis to design parameters and performance optimization of flexible multibody systems has been performed using the adjoint variable method.

[1] Géradin, M., Rixen, D.J. (2021).

[2] Géradin, M. Dynamics of a flexible body: a two-field formulation. Multibody System Dynamics, 54(1), 1-29 (2022).

[3] Géradin, M., Sonneville, V. (2024).

Enhanced formulations for flexible multibody dynamics

The first and essential objective of this part of the project was to develop a fresh and more general approach to model reduction methods for flexible multibody dynamics, taking account of second-order effects in a simple and effective manner. For that purpose, the two-field formulation of the floating frame of reference method has been developed to construct reduced structural models [1,2]. It consists in a separate interpolation of the displacement and velocity fields, which leads to drastic simplification of the system kinetic energy. The adoption of a natural strain measure makes it possible to properly include geometric stiffening, even for reduced finite element models of flexible components.

The two-field model concept has been implemented in a rather general numerical environment (JuDyn) using the open-source programming language Julia, taking advantage of its unique features (e.g., modularity, strong variable typing, function polymorphism, JIT compilation).

The two-field approach has been generalized to the dynamics of flexible multibody systems in a non-inertial frame [3], making it possible to address problems of rotor dynamics arising in mechanical and aerospace engineering (Fig. 1).

The method has also been extended to describe the inertial forces in nonlinear structural models such as beams [4] and shells [5] described in a geometrically exact manner [6].

A large variety of numerical tests have been performed to verify the concepts, validate the JuDyn code, and evaluate its computing performance. The most significant test consisted in simulating the deployment in space of a polymer reflector prototype stowed inside a CubeSat [7] (Fig. 2). This benchmark required specific developments such as modeling of unilateral contact and extension of the shell model to viscoelasticity. The main outcomes of this part of the project are:

1) a set of papers published in peer-reviewed journals describing the theoretical concepts,

2) their implementation in the JuDyn package (https://github.com/michelg45/JuDyn.jl). The modularity of JuDyn makes it easily extensible for research and teaching purposes. ►

[4] Sonneville, V., Géradin, M. (2022).

[5] Sonneville, V. A geometric local frame approach for flexible multibody systems. PhD thesis, University of Liège. (2015).

[6] Simo, J.C., Fox, D.D., Rifai, M.S. On a stress resultant geometrically exact shell model. Part I: Formulation and optimal parametrization. CMAME 72(3), 267–304 (1989).

[7] Nielsen, C.J.G. et al. Actively Controlled Deployable Polymer Reflectors for Small Satellite Applications. 75th Int. Astronautical Congress (IAC) (2024).

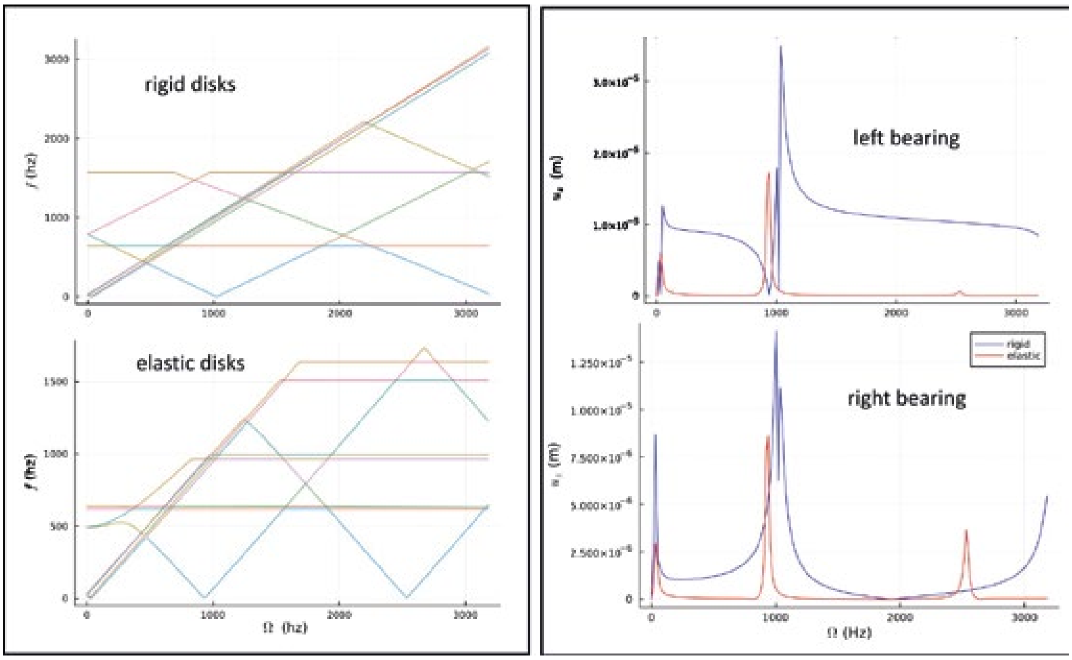

Fig. 1, Comparison of dynamic behavior of a twin-disk elastic rotor equipped with rigid or flexible disks. Left: change in rotor vibration frequencies vs. rotation speed (Campbell diagrams) due to disk flexibility. Right: displacement amplitude reduction at bearings due to disk flexibility.

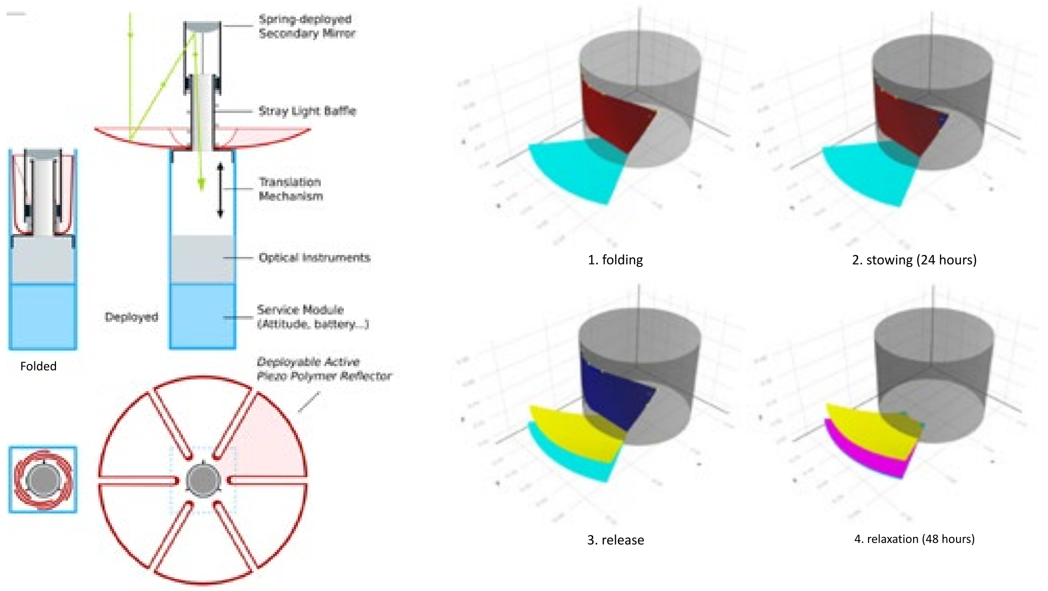

Fig. 2, Left: concept of deployment in space of a polymer reflector from a CubeSat. Right: simulation of the successive deployment phases: folding, 24 hours stowing, release, 48 hours relaxation.

[8] Lichtenecker, D., Rixen, D., Eichmeir, P. & Nachbagauer, K. (2023).

[9] Lichtenecker, D. & Nachbagauer, K. (2024).

Optimal control strategies for robotic systems

This part of the project has focused on a digital twin for flexible robots, for intelligent and efficient control of robots for future scenarios of, e.g., human-robot interaction or surgery robots.

For this purpose, a method for smart control of the robot has been developed to meet various optimization goals, such as, e.g., to minimize the occurring joint forces or tension in flexible materials.

From the mathematical point of view, this task includes the solution of an optimization problem in multibody dynamics using the adjoint method. Since multibody dynamics systems often include highly nonlinear equations to describe also stiff problems, an efficient gradient strategy must be chosen for the optimization procedure to guarantee a fast but accurate update of the optimization variables. Therefore, adjoint gradients have been developed, with great success in both time-optimal and energy-optimal scenarios as compared to standard optimization strategies using numerical gradients. A comparison in function evaluations [8] has shown the superiority of the proposed adjoint gradients.
Moreover, in case future robots will include flexible components made, e.g., from composite or bio-inspired materials, the inverse dynamics problem will lead to the need for extensions of the gradients to account for elastic deformation as well as strain limits. Hence, a new adjoint gradient approach in flexible dynamics has been published recently and tested

in a time-optimal two-arm flexible robot, as well as in an energy-optimal nonlinear pendulum [9]. Moreover, a discrete adjoint method for variational integration for optimal control of geometrically exact beam dynamics has been developed for constrained multibody systems [10].
The major outcomes of this part of the project are

1) a set of papers published in peer-reviewed journals describing the theoretical concepts for efficient optimal control in multibody dynamics,

2) their application for innovative flexible robotic systems, such as soft robotic fingers for reliable grasping (together with UC Berkeley [11]),

3) the spreading of the application of the method in the international multibody community through the organization of an IUTAM Symposium on the research topic of the Focus Group.

A follow-up MIRMI project on the combined optimal design and control of flexible multibody systems focuses on the application of our results for flexible robotic systems for modern medical robots, as in rehabilitation or prosthetic applications. Moreover, we have extended the methods for an application in medical tumor drug dosage using the optimal control with adjoint gradients [12]. Furthermore, another follow-up project on collaborative robotics will use the developed methods for safer, more reliable, and time-efficient human-robot-collaboration. ■

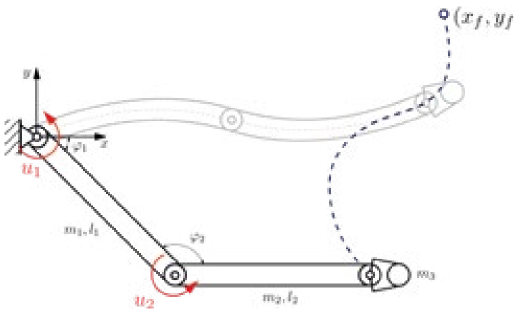

Fig. 3, Optimal control of a flexible two-arm robot following a given trajectory.

[10] Schubert, M., Sato Martin de Almagro, R.T., Nachbagauer, K., Ober-Blöbaum, S. & Leyendecker, S. Discrete Adjoint Method for Variational Integration of Constrained ODEs and Optimal Control of Geometrically Exact Beam Dynamics, *Multibody System Dynamics* (2023).

[11] Lichtenecker, D., Yang, W.T., Nachbagauer, K., Tomizuka, M. Synchronization of Soft Pneumatic Actuators for Reliable Grasping, *Proc. of the 7th IMSD*, Madison, Wisconsin, USA (2024).

[12] Eichmeir, P., Steiner, W. & Nachbagauer, K. The Use of Slack Variables in the Adjoint Method Handling Inequality Constraints in Optimal Control and the Application to Tumor Drug Dosage. *Computational & Nonlinear Dynamics*, 20(2): 021004(2025).

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Lichtenecker, D. & Nachbagauer, K. A discrete adjoint gradient approach for equality and inequality constraints in dynamics. *Multibody System Dynamics*, 61(1), 103–130 (2024).

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For a full list of publications, please visit
www.ias.tum.de/ias/geradin-michel
www.ias.tum.de/ias/nachbagauer-karin

Focus Group: Quantum Logic and the Second Quantum Revolution

Prof. Roberto Giuntini (University of Cagliari), Alumnus Philosopher in Residence (funded by the TÜV SÜD Foundation and as part of the Excellence Strategy of the federal and state governments)
Hosts: **Prof. Hans Bungartz, Prof. Stefania Centrone, Prof. Klaus Mainzer (TUM)**

Prof. Roberto Giuntini

Bridging quantum logic, artificial intelligence, and quantum computation

The "second quantum revolution" was central to the Fellowship, focusing on quantum logic's impact across disciplines. The research bridged quantum physics with machine learning, AI, cognitive science, and biomedical diagnostics. Key outcomes included new algorithms, quantum computer benchmarking, and interdisciplinary dialogue through seminars and collaboration with the Leibniz Supercomputing Centre.

Scientific concept and goals

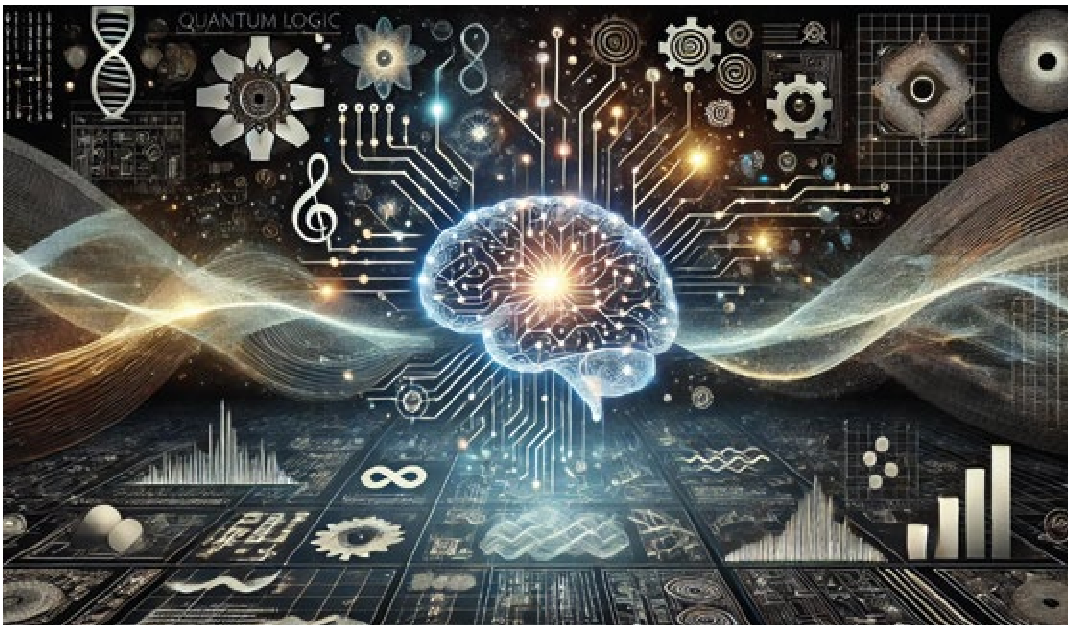
Over the course of six visits to the TUM-IAS, spanning more than six months in total, I investigated the concept of "quantumness," a defining feature of quantum systems characterized by phenomena such as superposition, entanglement, non-locality and contextuality. The project aimed to apply quantum logic to disciplines beyond physics, including machine learning, data science, and biomedical diagnostics. The research expanded to include the intersection of artificial intelligence (AI) and quantum sciences. This included exploring how large language models (LLMs) could benefit from quantum principles, providing a framework for advancing quantum-inspired computational tools.

Summary of the work carried out

Seminar series highlights

The seminar series (Quantumness: From Logic to Engineering and Back), organized with my Hosts, was a cornerstone of the Fellowship, fostering rich interdisciplinary dialogue. The proceedings of these seminars will be published, edited by H. Bungartz, S. Centrone, R. Giuntini, M. Molls and K. Mainzer, in the prestigious "Synthese Library" series under the title Quantum Logic and Beyond.
Key seminars included:

First Quantum Afternoon (December 6, 2023): Prof. Giuseppe Sergioli presented "Quantum State Discrimination for Supervised Classification," showcasing quantum logic's appli-



cation in machine learning. Prof. Christian Mendl provided insights into quantum simulations for analyzing complex systems.

Computing Systems: Mathematical Entities or Physical Objects? (March 15, 2024): Prof. Marco Giunti explored the dual nature of computational systems and its philosophical implications for quantum research.

Second Quantum Afternoon (May 16, 2024): Profs. Robert Wille and Klaus Mainzer examined automation in quantum computing design and the interplay between AI and quantum technologies.

Quantum Logic as a Logic (May 21, 2024): My lecture traced the evolution of quantum logical frameworks, complemented by Prof. Francesco Paoli's analysis of contradictions within quantum logic.

From Known Knowns to Unknown Unknowns in AI: Historical and Technical Issues (June 5, 2024): Prof. Fabio Roli explored AI's shift from solving well-defined problems to addressing adversarial challenges, emphasizing adversarial machine learning's role in enhancing safety and tackling security threats. ▸

Leibniz Quantum and Beyond (September 9, 2024): This seminar explored the intersection of philosophy, medicine, and contemporary physics, highlighting contributions from Leibniz's theoretical frameworks to contemporary advancements in science and technology.

Collaboration with Leibniz Supercomputing Centre (LRZ)

The collaboration with LRZ was instrumental in achieving the Fellowship's goals. The Quantum Cagliari QExa20 project, initiated during this period, focused on benchmarking quantum processors and noise characterization. These efforts addressed critical challenges in quantum device certification and reliability.

Conference: With Novel Nuclear Technologies Towards a Greenhouse Gas-Free Basic Energy Supply

I participated in the Working Group IV, Energy Economics and Society, as part of the conference With Novel Nuclear Technologies Towards a Greenhouse Gas-Free Basic Energy Supply, held at the TUM Science and Study Center Raitenhaslach from June 13 to 15, 2024. This event was organized by the TUM Senior Excellence Faculty under the patronage of Bavarian State Minister Dr. Florian Herrmann. During this conference, I also contributed a paper titled "Categorizing the Risks" (see the publication list).

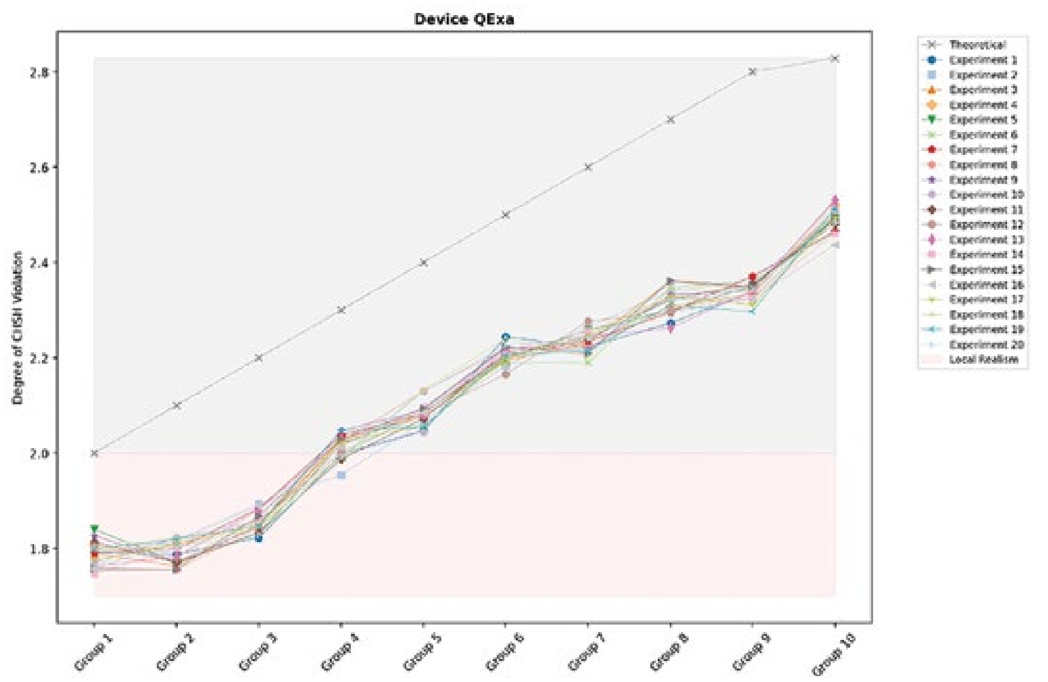


Fig. 1, Local realism and non-locality: Testing quantum properties. The violation of the Clauser-Horne-Shimony-Holt (CHSH) inequality was tested on the IQM quantum computer at the Leibniz Supercomputing Centre using quantum states randomly generated by a universal set of quantum gates ("Clifford gates + T-gate"). Experimental results for states strongly violating local realism are promising, supporting the potential role of non-locality in achieving quantum advantage. Extending this approach to more qubits will require applying different inequalities.

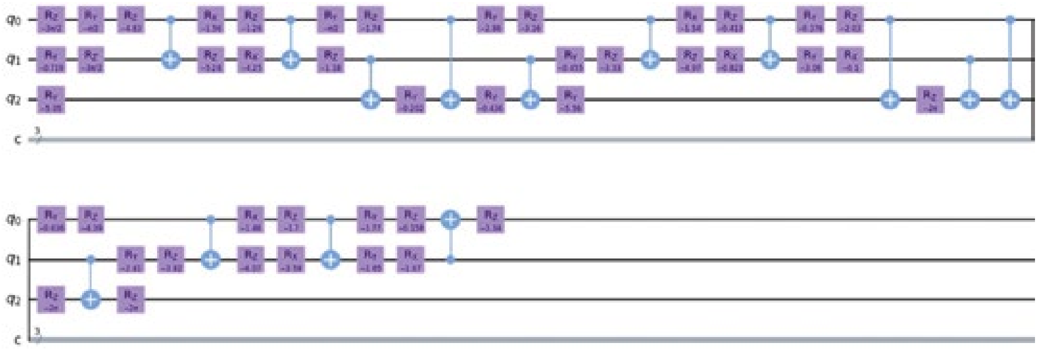


Fig. 2, Quantum circuit implementing the pretty-good measurement (PGM) classifier applied to an artificial dataset on the IBM-Q simulator. The circuit consists of controlled-NOT (CNOT) gates, represented by the standard symbols, and rotation gates $R_i(n)$ along a given direction i (x,y or z) of a given angle n.

Educational initiatives

With Prof. Giuseppe Sergioli, I designed the course Quantum Information Meets Artificial Intelligence, subsequently taught at TUM by Prof. Sergioli as part of the courses offered by the Chair of Philosophy and Theory of Science of Prof. Stefania Centrone. The course introduced students to interdisciplinary concepts, bridging quantum sciences and AI, and underscored the Fellowship's commitment to fostering the next generation of researchers.

Major outcomes and significance

Applications of quantumness and contributions to quantum computing

This research, originally grounded in foundational and philosophical inquiry, has led to significant advancements with direct applications to quantum benchmarking and computing. The work has demonstrated that theoretical principles of quantum logic and fundamental physics are not only conceptually profound but also essential for evaluating the performance of near-term quantum processors. Our results have laid the groundwork for assessing the ability of quantum computers to achieve the so-called quantum supremacy, a crucial milestone in the field. The developed methodologies provide essential tools for benchmarking quantum hardware, ensuring their reliability, and optimizing their computational potential. In particular, the research efforts during the Fellowship led to significant advancements in the following areas:

Classification of Quantum Correlations (Fig. 1), including the entanglement of pure and mixed states in near-term quantum computers. This work involved collaboration with the research group of Dr. Luigi Iapichino (Leibniz Supercomputing Center) and with Carla Rieger (TUM, CERN);

improved understanding of quantum non-locality and its role in enhancing computational efficiency and scalability [1];

non-locality benchmarking for certification: developed a certification protocol based on non-locality benchmarking techniques to evaluate quantum processors' ability to generate genuine multipartite non-local states; ►

[1] Granda Arango, A. C., Holik, H. F., Sergioli, G., Giuntini R. & Freytes H. Geometrical aspects of resources distribution in quantum random circuits. (arXiv.2405.01650); Sergioli, G., Granda Arango, A. C., Cuccu C., Centrone S., Rieger C. & Giuntini R. Classification of quantum correlations via quantum-inspired machine learning. (Submitted to Quantum Machine Intelligence).

[2] Sergioli, G. et al. A quantum-inspired classifier for clonogenic assay evaluations. *Scientific Reports* 11 (2021) (DOI: http://doi.org/10.1038/s41598-021-82085-8).

integration with quantum random circuits: created a software tool for generating quantum random circuits, supporting benchmarking and analysis of resources such as entanglement and quantum magic across various quantum processors.

Quantum-inspired machine learning

framework for quantum multi-class classifiers leveraging quantum state discrimination techniques. This research demonstrated that these classifiers can be implemented on near-term quantum computers after the classification functions are "distilled" on classical platforms from the quantum-encoded training data (Fig. 2);

development of Python packages aimed at optimizing algorithms for quantum-inspired machine learning. This work involved collaboration with David Schneller and Carlo Cuccu: algorithms, bridging theoretical innovation with practical applications. This software will be published on GitHub;

biomedical microscopy imaging: the application of quantum-inspired methods in microscopy imaging has led to significant advancements in image recognition and analysis. Building upon the work presented [2], new algorithms were implemented to extract and classify complex patterns in microscopic clonogenic assay evaluation. This important technique quantifies the survival rate of in vitro cell cultures based on the ability of a single cell to grow (cell proliferation) and form a colony. It is used to determine the number and size of cell colonies in vitro after irradiation or drug administration.

Integration with artificial intelligence∫: in the last part of the research period, we started a research line aiming at integrating quantum principles with artificial intelligence, particularly focusing on quantum data processing and natural language understanding.

Quantum logic as a logic

Building on foundational discussions, this research examined also the emergence of contradictions in the logic of quantum systems mathematically interpreted according to the rules of the so-called “unsharp approach to quantum mechanics.” The transition from sharp to unsharp logic emphasizes the necessity of accommodating contradictory information within quantum mechanics. The results hold both philosophical and computational significance, opening pathways for developing advanced (holistic) logical systems to manage quantum complexities.

Philosophical leadership

My election as Corresponding Member of the Académie Internationale de Philosophie des Sciences (AIPS) and Ordinary Member of the European Academy of Sciences and Arts reflects the Fellowship’s recognition in global academic circles and underscores the integration of philosophical inquiry with cutting-edge science.

Future directions

Short-term goals

Organizing a summer school on Quantum and AI with Prof. Stefania Centrone and Deutsches Museum.

Hosting a TUM-IAS/University of Cagliari meeting in April 2025 to strengthen the collaborations between the University of Cagliari, the TUM-IAS, and TUM.

Deepening ties with TUM researchers involved in quantum sciences.

Long-term goals

Expanding research on quantum machine learning, quantum cognition, and AI.

Leveraging quantum technologies for sustainable solutions to global challenges.

Conclusion

The TUM-IAS Philosopher in Residence Fellowship provided a unique platform to bridge philosophical inquiry and cutting-edge science, resulting in significant advancements in quantum logic, computation, and AI. These outcomes underline the transformative potential of interdisciplinary research in addressing contemporary scientific and societal challenges.

This research was carried out with the collaboration of: Prof. Maria Luisa Dalla Chiara (University of Florence), expert in quantum logic and philosophy of science; Prof. Giuseppe Sergioli (University of Cagliari), specializing in quantum information and machine learning; Prof. Fabio Roli (University of Genoa), expert in adversarial machine learning; Prof. Federico Holik (University of La Plata), specializing in quantum correlations; David Schneller, who contributed to the development of Python packages for quantum-inspired machine learning; Carlo Cuccu, focused on optimizing machine learning algorithms at TUM; Carla Rieger, expert in the classification of quantum correlations and entanglement. ■

Selected publications

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Dalla Chiara, M. L., Giuntini, R. & Sergioli, G. A Quantum approach to pattern recognition and machine learning. Part I. *International Journal of Theoretical Physics*. 63(55) (2024) (DOI: http://doi.org/10.1007/s10773-024-05566-2).

Dalla Chiara, M. L., Giuntini, R. & Sergioli, G. A Quantum approach to pattern recognition and machine learning. Part II. *International Journal of Theoretical Physics*. 63(55) (2024) (DOI: http://doi.org/10.1007/s10773-024-05566-2).

Giuntini, R., Ledda A. & Vergottini G. Generalizing orthomodularity to unsharp contexts: properties, blocks, residuation. *Logic Journal of the IGPL.* jzae076 (2024) (DOI: https://doi.org/10.1093/jigpal/jzae076).

Giuntini, R. & Sergioli G. Categorizing Perceptions of Dangers and Risks: A Philosophical Perspective (to be published in the Proceedings of the Conference *With Novel Nuclear Technologies Towards a Greenhouse Gas-Free Basic Energy Supply)*.

For a full list of publications, please visit
www.ias.tum.de/ias/giuntini-roberto

Focus Group: Boundary Situations and Spiritual Care

PD Dr. Rico Gutschmidt (University of Konstanz / ETH Zurich), Alumnus Philosopher in Residence (funded by the TÜV SÜD Foundation and as part of the Excellence Strategy of the federal and state governments)
Host: **Prof. Eckhard Frick (TUM)**

PD Dr. Rico Gutschmidt

Patients as experts: Philosophizing in healthcare

Severe physical or emotional suffering or confrontation with their own death can lead patients to experience their situation as a boundary situation in the sense defined by Karl Jaspers. In a qualitative study, we investigated how patients and caregivers perceive such situations. The study showed that acknowledging the philosophical dimension of boundary situations can be supportive for patients.

The term "boundary situation" was defined by the German psychiatrist and philosopher Karl Jaspers (1883–1969) and refers to the limits of action and life, such as struggle, guilt, suffering, and death. Human life always moves within these boundaries, but this is experienced especially in particular situations [1]. Such situations include severe physical and emotional suffering and the direct confrontation with one's death, e.g., due to a terminal illness.

In this research project, we investigated how patients experience boundary situations and how caregivers in medicine, psychotherapy, nursing, and social work perceive the boundary situations of their patients. The aim of the study is to gain a better understanding of the experience of boundary situations. How does it feel for people to experience a boundary situation, and how does their own experience of boundary situations or their professional dealing with boundary situations change their view of themselves and the world?

A unique feature of this research project was that patients were interviewed as experts in boundary situations. Philosophers can think a great deal about boundary situations, but patients in boundary situations have immediate access. The philosophical interest of this project was the question of what we can learn about life from patients in boundary situations.

Patients and caregivers were interviewed as part of a qualitative interview study. As this project was mainly concerned with an analysis of lived experience, a hermeneutic-phenomenological method was chosen: interpretative phenomenological analysis [2]. It combines

[1] Jaspers, K. *Philosophie*. Bd. II, Berlin, Göttingen, Heidelberg: Springer (1932/1973).

[2] Smith, J. A., Flowers, P. & Larkin, M. X. *Interpretative Phenomenological Analysis. Theory, Method and Research,* London: Sage (2009).

philosophical hermeneutics, i.e., the study of understanding, with the philosophical school of phenomenology, which is concerned with describing experiences.

Implementation

Following preparatory observations and participation in ward rounds, interviews were conducted with eight patients and eight caregivers. Various wards of the Department of Psychosomatic Medicine and Psychotherapy (day-clinic and inpatient treatment, palliative ward) and other areas of the TUM University Hospital rechts der Isar (neuro-oncology, radio-oncology) were involved. The response was excellent, the cooperation with the responsible persons worked very well, and there was a considerable interest in the topic.

The interviews lasted 20 to 30 minutes. All interviews were digitally recorded and transcribed verbatim. The transcripts were analyzed inductively according to the principles of interpretative phenomenological analysis. An overarching understanding of the entire data set was developed from an analysis of the individual interviews in defined individual steps. Finally, the research questions were approached with the help of broader concepts from philosophy and spiritual care.

Methodological challenges

People in boundary situations are particularly vulnerable and often cannot be interviewed directly about their situation. Although qualitative studies have been conducted in the health sector for a long time, there still ►

Public lecture on the boundary situation of death by Thomas Fuchs, Karl-Jaspers-Professor for Philosophical Foundations of Psychiatry and Psychotherapy (Heidelberg), as part of the project's dissemination program.

needs to be an established method for qualitative studies on boundary situations due to this particular difficulty [3]. This project was, therefore, methodologically explorative. For example, it became apparent during implementation that open questions are insufficient in this context, which is why a philosophical conversation was initiated in some cases.

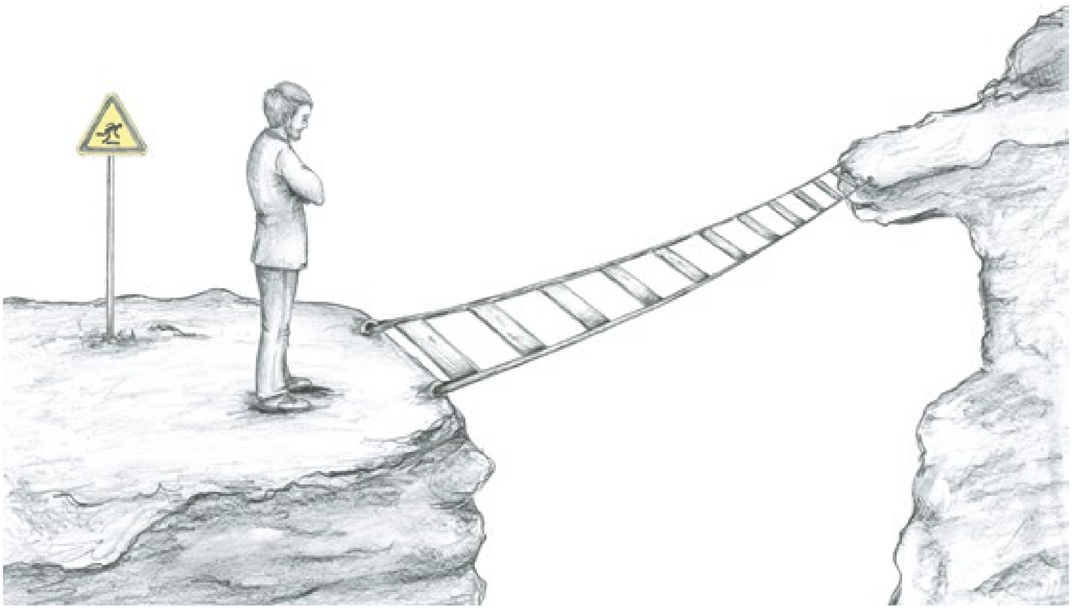
Another challenge was that the experience of a boundary situation is often unspeakable: It frequently leaves you at a loss for words and involves insights that are very difficult to put into words [4]. This unspeakability was frequently present in the conversations as a feeling: It was often impossible to talk directly about the respective boundary situation, especially about death. For this reason, notes were also taken on non-verbal expressions, emotional states, and personal feelings. In addition, it was often necessary to search together for words that could express the experience.

Results

Some significant results were obtained on the experience of boundary situations. Patients often perceive themselves as being outside of normality and feel alienated. Correspondingly, there is a better connection to patients in boundary situations when caregivers have experienced boundary situations themselves.

[3] Cf. Feith, D., Peter, C., Rehbock, T. & Tiesmeyer, K. Grenzsituationen. Qualitative Forschung zu existenziellen Krankheitserfahrungen und Therapieentscheidungen. In: Netzwerk Qualitative Gesundheitsforschung (Hrsg.): *Perspektiven qualitativer Gesundheitsforschung,* Weinheim: Beltz Juventa Verlag, 216–269 (2020).

[4] Cf. Gutschmidt, R. Grenze und Transformation. Philosophische Erfahrung als nichtpropositionale Einsicht. *Deutsche Zeitschrift für Philosophie* 70 (5), 781–794 (2022).



Confronting boundary situations can lead to a new perspective on life. However, while we cannot avoid boundary situations, we can avoid confronting them.

Intuition and sensing also play a crucial role in dealing with patients in boundary situations.

From a philosophical point of view, it is interesting that patients and caregivers have altered perspectives on things that seem to be taken for granted. From the perspective of boundary situations, things we normally rely on are experienced as small miracles. Patients and caregivers also speak of a new attitude toward life, which can be described with serenity, gratitude, and appreciation. And there have been many reports of particular insights. For example, people have always been aware of their own mortality but understand it in a new and more profound way in boundary situations.

Applications, transfer, and further research

The study has shown that acknowledging the philosophical dimension of boundary situations by caregivers can be supportive. Philosophical conversations about the general situation in which they find themselves can be relieving for patients in boundary situations. Some patients have explicitly emphasized the importance of philosophical reflection in dealing with their situation.

The findings are to be made available to those responsible in the healthcare sector, thus contributing to better support for patients in boundary situations. The findings could be used to design training courses to sensitize caregivers to patients in boundary situations. Last but not least, verifying and expanding the results obtained in a quantitative study would be important. ■

Selected publications

Frick, E. & Gutschmidt, R. Wir werden mit dem Geheimnis der Existenz nie fertig. *Spiritual Care* 12 (4), 371–374 (2023).

Gutschmidt, R. Grenzsituationen im Gesundheitsbereich. *Spiritual Care* 13 (2), 191–194 (2024).

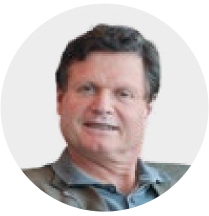
Frick, E. & Gutschmidt, R. (Eds.) *Existential Elucidation. Jaspers, Boundary Situations, and Spiritual Care*. De Gruyter (forthcoming).

For a full list of publications, please visit
www.ias.tum.de/ias/gutschmidt-rico

Focus Group: Sustainable Photocatalysis Using Plasmons and 2-D Materials

Prof. Naomi J. Halas (Rice University), Alumna Hans Fischer Senior Fellow (funded by Cluster of Excellence e-conversion) | **Prof. Peter Nordlander (Rice University),** Alumnus Hans Fischer Senior Fellow (funded by Cluster of Excellence e-conversion) | **Dr. Olivier Henrotte (LMU),** Postdoctoral Researcher | **Jan Schabesberger (TUM),** Doctoral Candidate
Hosts: **Prof. Jonathan Finley, Prof. Ian Sharp (TUM), Prof. Emiliano Cortés (LMU)**

Prof. Naomi J. Halas



Prof. Peter Nordlander

Plasmonic and 2-D materials for sunlight-to-chemical energy conversion

Plasmonic and 2-D materials are revolutionizing the quest for sustainable energy, merging cutting-edge science with environmental impact. Plasmonic materials amplify energy transfer using localized surface plasmon resonances, while 2-D materials offer unmatched surface area and exceptional electronic properties. By joining forces, these innovative materials unlock new possibilities for solar-driven chemical transformations, paving the way toagreener future by reducing dependence on fossil fuels and powering next-generation green energy solutions.

Overall scientific concepts and goals

The urgent need for sustainable energy solutions has driven significant interest in photocatalysis, a process that utilizes light to drive chemical reactions, offering a pathway to clean energy production and environmental remediation. Conventional photocatalysts often suffer from low efficiency due to limited light absorption and charge recombination. To address these challenges, this project focuses on integrating plasmonic and two-dimensional (2-D) materials to advance photocatalytic systems.

Plasmonic materials, such as noble metal nanoparticles, exhibit localized surface plasmon resonances (LSPRs) that enable efficient light harvesting and energy transfer. When coupled with 2-D materials such as graphene, transition metal dichalcogenides (TMDs), or hexagonal boron nitride, the combined system benefits from enhanced charge separation, large surface areas, and tunable electronic properties. Together, these materials hold the potential to significantly boost the efficiency and sustainability of photocatalytic reactions.

The primary goal of this project is to understand the fundamental mechanisms of photocatalysis and light-to-chemical energy conversion on plasmonic materials and 2-D materials. By advancing the fundamental understanding of light-matter interactions and charge dynamics in these systems, this research aims to bridge critical gaps in the field and provide scalable solutions for global energy and environmental challenges.

This work is situated at the intersection of materials science, nanotechnology, and energy research, addressing pressing issues of energy security and environmental sustainability. The outcomes will not only advance photocatalytic technologies but also contribute to broader efforts in sustainable energy and green chemistry.

Summary of research work carried out and outcomes

The Focus Group Sustainable Photocatalysis Using Plasmons and 2-D Materials focused on two fundamental areas for sustainable photocatalysis: plasmon-driven energy transfer and 2-D materials for light-to-chemical energy conversion.

Plasmon-driven energy transfer and operando spectroscopy

Understanding the mechanisms of metal-molecule energy transfer in plasmonic materials is critical for advancing sustainable photocatalysis. Plasmonic materials, such as gold and silver nanoparticles, exhibit unique optical properties that allow them to harvest light efficiently through localized surface plasmon resonances (LSPRs). When light interacts with these materials, it excites electrons, creating high-energy carriers that can transfer energy to nearby molecules. This energy transfer is the foundation of plasmon-driven photocatalysis, enabling reactions such as water splitting for hydrogen production and carbon dioxide reduction into valuable fuels.

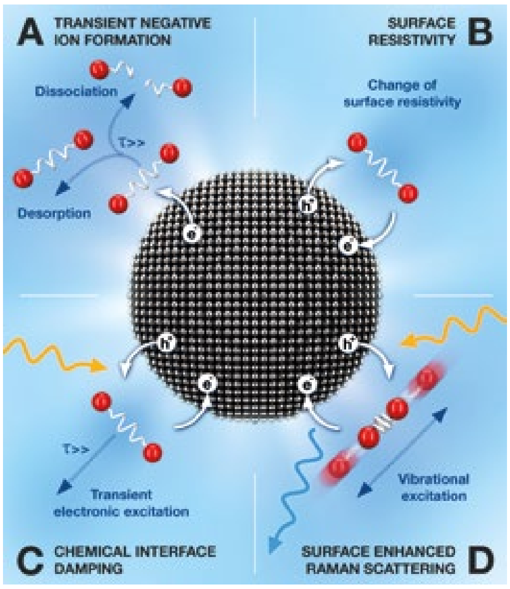


Fig. 1, Four different phenomena arising at the metal-molecule interface due to electron scattering. Each phenomenon has a different impact on adsorbed molecules, from electronic or vibrational excitation to desorption or molecular dissociation, and results in an electron-hole pair excitation in the substrate. © Stefancu, A., Halas, J.N., Nordlander, P. & Cortes, E. Electronic excitations at the plasmon–molecule interface. *Nat. Physics* 20, 1065–1077 (2024).

However, the efficiency of these processes depends on precise control of energy transfer pathways, including hot electron injection, Förster resonance energy transfer, and thermal effects. Therefore, during the ▸

Fellowship we published a review focused on the mechanisms of plasmon-driven chemical reactions (see Fig. 1). We have shown that several mechanisms that involve energy transfer or exchange between an electron, a nanoparticle, and an adsorbed molecule can be rationalized under the same fundamental framework of resonance and non-resonance electron transfer. Thus this work bridges the field of plasmon-driven photocatalysis with the more classical field of surface science, enabling the design of more efficient plasmonic catalysts.

This work led us to the idea that there is an underlying connection between the effect of adsorbed molecules on the electrical and optical properties of metallic nanostructures, a work which is in preparation for publication. The basic idea is that adsorbed molecules on metal surfaces disrupt the flow of electrons, increasing the electrical resistance of the metal. This effect is physically similar to the case when metal electrons are excited through light and can transfer energy to adsorbed molecules. Therefore, our work advanced the understanding of the interaction between plasmonic materials and adsorbed molecules, with the end goal of using plasmonic materials for industrially relevant processes such as clean hydrogen production.

A big challenge in developing more efficient plasmonic photocatalysts is monitoring their activity during the photocatalytic process, i.e., *operando*. A very powerful tool for tracking plasmon-driven chemical reactions in operando conditions is surface-enhanced Raman spectroscopy (SERS). This method uses light to investigate the chemical composition of molecules and can therefore be used to track every step of a photocatalytic reaction. During our research work, we reviewed the use of SERS in all areas of catalysis and energy conversion, from photocatalysis to battery development (see Fig. 2). Therefore,

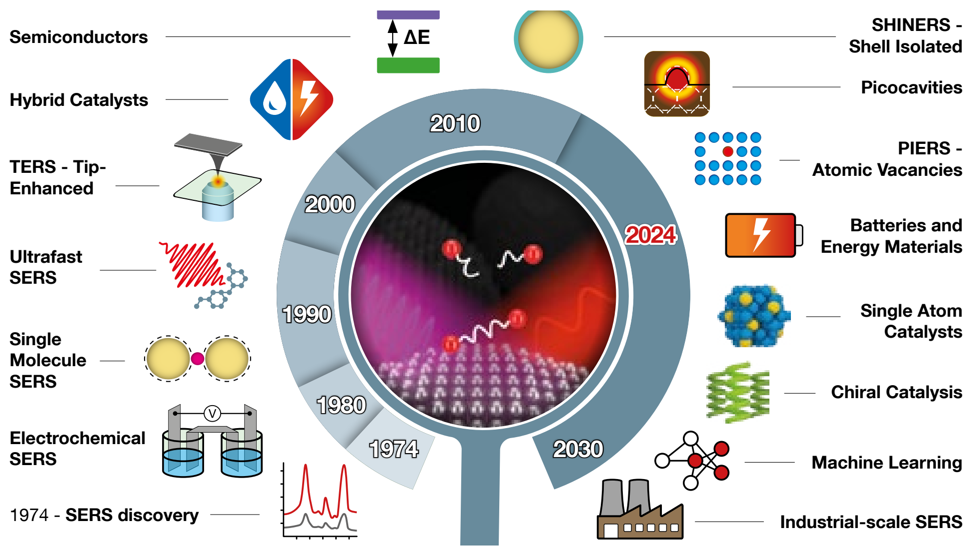


Fig. 2, Progress of surface-enhanced Raman spectroscopy for monitoring catalytic processes. Since the discovery of SERS in 1974, numerous important techniques and materials have been developed for its application in catalysis. Notably, the past 20 years have witnessed rapid advancements in the field, with many emerging areas and topics promising further advancements in the integration of SERS for real -time monitoring of energy conversion processes. In this figure, we summarize a selection of the most important milestones and developments of SERS in the field of catalysis over the last 50 years. © Stefancu, A. et al. Impact of surface enhanced raman spectroscopy in catalysis. *ACS Nano* 18, 43, 29337–29379 (2024).

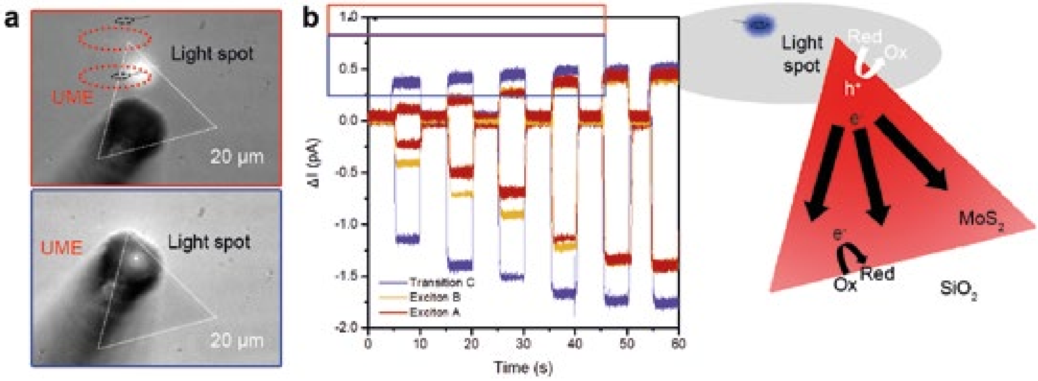


Fig. 3, Aligned-unaligned excitation-detection experiments in monolayer MoS2. a, Optical image of a monolayer (ML-) MoS2 flake (white dashed triangle) showing the position of the light excitation spot (black dashed circle) and the ultramicroelectrode (UME) position (red dashed circle) for unaligned (red box) and aligned measurements (blue box). b, Photoactivity (ΔI) measured far from the light excitation spot (red box), and aligned with the light excitation spot (blue box), while the ML-MoS_2 was excited under chopped light (5 s; increased light power at every pulse; transition C, 455 nm, purple; exciton B, 595 nm, yellow; exciton A, 660 nm, dark red). The probe positions for the red and blue boxes correspond to the respective optical images in (a). c, Scheme representing the spatial distribution of the photo-redox process detected at the UME in ML-MoS2 when excited at a fixed position, with the corresponding photogenerated charge carriers (oxidation: holes, blue region; reduction: electrons, red region).
© Henrotte, O. et al. Spatially resolved photocatalytic reactive sites and quantum efficiency in a 2D Semiconductor. *Submitted*, 2025.

this work provides an exhaustive view of *operando* monitoring of catalytic materials and chemical processes and highlights future areas of interest in energy conversion, such as using artificial intelligence (AI) to accelerate material discovery.

Monitoring the photochemical reactivity of 2-D materials

Two-dimensional transition metal dichalcogenides (2-D TMDs) are promising material platforms for optoelectronics, sensing, and quantum information technologies, showing significant potential for groundbreaking applications. They also hold immense potential for photocatalysis, due to their earth-abundance, strong light-matter interaction, and high surface-to-volume ratio, which means they can host many active sites for chemical reactions. However, progress has been limited due to an incomplete understanding of their photocatalytic reactive sites and their reactivity. Therefore, it is essential to identify active chemical sites and monitor their reactivity under appropriate *operando* conditions, using advanced approaches that can probe these aspects. Employing this unique, performance-oriented feedback, the material synthesis can be optimized regarding morphology, dopants, and other defects. This will provide a deeper understanding that will lead to novel photocatalyst design, fully leveraging the tunability of 2-D TMDs to develop next-generation materials and set new benchmarks in efficiency and sustainability.

To accomplish this goal, we developed a novel *operando* imaging method capable of identifying the spatial distribution of reactive sites for oxidation and reduction on a 2-D TMD: an MoS_2 monolayer (ML), using light as the sole external driving force (see Fig. 3). We observed the effects of the electronic properties of the material, electron/hole transport, and lateral confinement of photocarriers ►

on chemical reactivity. Unlike other imaging techniques that have been recently utilized to study photocatalytic systems, this new imaging method enables the direct mapping of efficiency with high spatial resolution (~200 nm) and allows the local measurements of hydrogen generation under light excitation for the first time.

The separation and transport of charge carriers during photocatalysis are also critical factors in solar-driven devices. Building on insights from our study, we explored strategies to enhance charge carrier mobility on 2-D platforms. We observed a significant improvement in the efficiency of MoS_2 under visible light, with charge extraction increasing by 5 to 30 when connected to a conductive material. Notably, this enhanced performance extended over distances of several hundred micrometers from the connection point.

These findings offer a clear path toward designing highly efficient sunlight-powered devices by improving charge transport over long distances and optimizing photocatalytic performance. Such advancements could significantly impact solar energy conversion technologies, hydrogen production, and sustainable energy systems.

Synthesis of 2-D materials for photocatalysis

Using this insight into the photocatalytic activity at the microscopic level, the epitaxial growth of the 2-D material can be tuned for increased catalytic performance. As line or point defects can trap photoexcited charge carriers and act as reactive sites, material parameters such as morphology, layer number, or dopants will greatly influence the overall performance. We worked on understanding the epitaxial growth of different 2-D materials using chemical vapor deposition (MoS_2) and molecular beam epitaxy (InSe, GaSe) as better alternatives to the dry stamping transfer technique, aiming at crystals of more reproducible interface quality due to the controlled deposition process. Connected to the MBE system, we developed an all-in ultrahigh-vacuum optical (Raman, photoluminescence, differential reflectance) analytic setup to characterize 2-D material properties in pristine conditions. As a next step, we will use this capability to analyze MBE-grown layers on top of plasmonically active structures and test the electronic properties of the heterostructures, all crucial for photocatalytic applications. A challenge in this respect is optimizing growth recipes for substrates that can yield high-quality crystals but are also suitable for plasmonic applications.

Future related research

In summary, our research project achieved its initial goal of understanding better light-to-chemical energy conversion in plasmonic systems and in 2-D materials, specifically MoS_2. These advances will allow us to translate plasmonic and 2-D materials into practical applications for clean hydrogen generation or CO_2 reduction. One promising approach based on our results is to combine plasmonic and 2-D materials, forming hybrid reactors that would combine the ability of plasmonic nanoparticles to absorb light and the reactive sites of the 2-D material.

In close collaboration with Dr. Andrei Stefancu (LMU). ■

Selected publications

Stefancu, A., Halas, J.N., Nordlander, P. & Cortes, E. Electronic excitations at the plasmon–molecule interface. *Nat. Physics* 20, 1065–1077 (2024).

Stefancu, A. et al. Impact of surface enhanced raman spectroscopy in catalysis. *ACS Nano* 18, 43, 29337–29379 (2024).

Henrotte, O. et al. Spatially resolved photocatalytic reactive sites and quantum efficiency in a 2D Semiconductor. *Submitted*, 2025.

Stefancu, A. et al. Optical and electrical probing of plasmonic metal-molecule interactions. *To be submitted*, 2025

Henrotte, O. et al. Optimizing charge transport in a 2D Semiconductor for enhanced photocatalysis. *In preparation*, 2025.

For a full list of publications, please visit
www.ias.tum.de/ias/halas-naomi-j
www.ias.tum.de/ias/nordlander-peter

Focus Group: Machine Learning

Prof. Reinhard Heckel (TUM), Alumnus Rudolf Mößbauer Tenure Track Assistant Professor

Prof. Reinhard Heckel

Data-driven algorithms for signal and information processing

The past decade has seen remarkable advances in information and signal processing technologies by building data-driven solutions, even for problems that are traditionally solved without any data. The Professorship for Machine Learning develops such data-driven algorithms and corresponding mathematical performance guarantees.

Deep learning for imaging and signal processing

An important problem in signal processing and imaging is to reconstruct a signal or image from few and noisy measurements. Until recently, the best methods for image reconstruction measurements were designed by experts on the basis of the physics of the measurement process alone, without using data.

Today, deep neural networks trained on example images perform best for many applications. For example, the newest magnetic resonance imaging scanners and the iPhone use deep networks to reconstruct high-quality images.

However, deep networks often rely on large amounts of clean data, lack theory, and can be sensitive to perturbations. To address those challenges, we develop robust algorithms and theory for deep learning-based imaging and signal reconstruction, as well as for classical signal reconstruction.

Untrained neural networks for imaging:
We developed the deep decoder, a neural network that reconstructs images from noisy measurements with excellent performance and without data beyond a single measurement.

For accelerated magnetic resonance imaging (MRI), the deep decoder significantly improves on classical sparsity-based methods, and its performance even approaches that of neural networks trained on large datasets (see Fig. 1).

The deep decoder and, more broadly, self-supervised networks, are applicable to a variety of image reconstruction problems. For example, they enable high-quality phase microscopy.

Moreover, unlike competing neural network-based methods, the deep decoder comes with rigorous performance guarantees: We developed mathematical denoising and signal reconstruction guarantees.

Foundations for neural networks trained end-to-end for signal reconstruction:

In our current work, we focus on neural networks trained on example images, as they give state-of-the-art image quality and are very fast.

We are particularly focused on developing foundations and theory. For example, we derived denoising rates for neural network-based denoising and quantified the benefits of scaling (increasing) training data and of using large transformer-based models.

Robustness:

We were developing methods that would be robust to perturbations and distribution shifts.

We demonstrated that distribution shifts, such as training on data from one hospital and testing on data from another hospital, lead to a significant degradation of performance in practice.

Motivated by this finding, we developed a new fine-tuning method that is, for the first time, robust to such distribution shifts. We also proposed data-centric approaches for improving robustness to distribution shifts and derived theoretical results for worst-case robustness. ▸

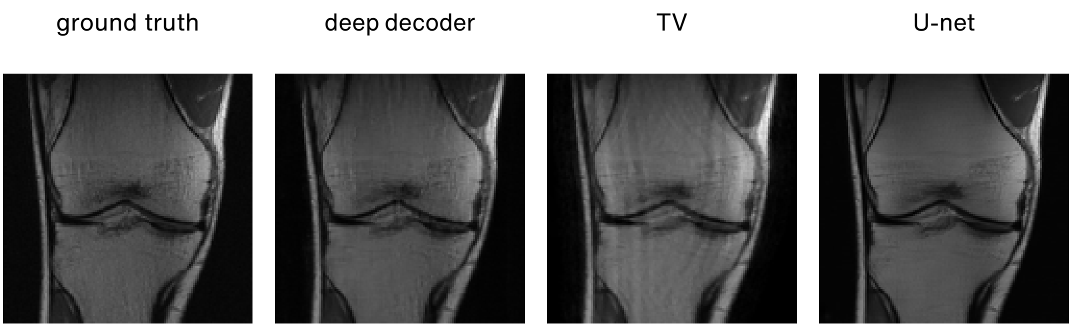


Fig. 1, Sample accelerated MRI reconstructions for the un-trained deep decoder, a classical method (TV), and a trained baseline method (U-net). The deep decoder enables excellent reconstructions.

Foundations and methods for machine learning

We developed methods for and foundations of machine learning, in particular for adaptive machine learning, statistical learning, theory for neural networks, and robust machine learning.

Adaptive machine learning:
An important challenge in machine learning is to learn from data adaptively and continuously.

We developed methods and theory for active learning. In particular, by developing theory for continual learning, we contributed to learning from data continuously without forgetting previously learned tasks.

Theory for deep learning:
Neural networks perform very well in practice, but many aspects such as common training practices and architectural choices are not well understood. We contributed to the theoretical understanding of neural networks. For example, we have shown why early cessation of the training of overparameterized neural networks can be very effective.

Robustness and uncertainty quantification:
Neural networks often perform significantly worse under distribution shifts, i.e., slight differences in training and testing data. We developed methods to improve robustness under distribution shift and are working on better understanding distribution shifts. For example, we have recently shown that for a large class of distribution shifts and models, there is a monotone relation of in- and out-of-distribution performance.

DNA data storage

Due to its longevity and enormous information density, DNA is an attractive storage medium. However, practical constraints on reading and writing DNA require the data to be stored on several short DNA fragments that cannot be ordered spatially.

We developed coding and error-correction schemes for this unique setup. With our collaborators we showed, with accelerated aging experiments, that digital information could be stored on DNA and perfectly retrieved after thousands of years.

Subsequently, we built information theoretic foundations for future DNA storage systems by characterizing the number of bits that can be stored per amount of DNA, and we are building empirical foundations by characterizing the error probabilities in practice.

We also used our system for the first commercial application of DNA storage, namely for storing Massive Attack's music on DNA, mixed into spray paint, and subsequently to store a TV series commercially for Netflix (see Fig. 2). ■

Fig. 2, The first two commercial applications of the coding scheme, storing music and storing a show for Netflix.

Selected publications

R. Heckel, Deep Learning for computational imaging, Oxford University Press, 2025.

T. Klug, K. Wang, S. Ruschke, and R. Heckel, MotionTTT: 2D Test-time-training motion estimation for 3D motion corrected MRI, NeurIPS 2024.

Simon Wiedemann and R. Heckel, A deep learning method for simultaneous denoising and missing wedge reconstruction in cryogenic electron tomography, Nature Communications, 2024.

M. Zalbagi Darestani, A. Chaudhari, and R. Heckel, Measuring robustness in deep learning based compressive sensing, ICML 2021 (long talk, top 3 % of submissions).

P. L. Antkowiak, J. Lietard, M. Zalbagi Darestani, M. Somoza, W. J. Stark, R. Heckel, R. N. Grass*, Low cost DNA data storage using photolithographic synthesis and advanced information reconstruction and error correction, Nature Communications, 2020, featured as Editor's highlight.

For a full list of publications, please visit
www.ias.tum.de/ias/heckel-reinhard-1

Focus Group: Molecular Imaging of Cellular Metabolism

Prof. Ron M. A. Heeren (University of Maastricht), Alumnus Hans Fischer Senior Fellow | **Sutirtha Chattopadhyay (TUM University Hospital Klinikum rechts der Isar),** Doctoral Candidate
Hosts: **Prof. Thomas F. Hofmann (TUM), Prof. Percy A. Knolle (TUM University Hospital Klinikum rechts der Isar)**

Prof. Ron M. A. Heeren

Innovative molecular imaging reveals cellular metabolism

Cellular metabolism is defined by a complex interplay between molecules, molecular signals, and a dynamic environment. The detailed study of local metabolism provided insight into the heterogeneity of living systems from plant to human cells. Innovative single-cell imaging of complex surfaces, combined with advanced "omics" approaches, is employed to chart living systems in unique detail.

The objective of the Focus Group was threefold. First to establish a close collaboration between the labs of Ron Heeren at the University of Maastricht and the research labs at TUM. The second, more scientific aim was to employ these technologies to characterize the metabolic profile of key immune cells and their interaction with mammalian cells. The third objective was to explore the tissue microenvironment in the direct vicinity of individual immune cells in liver and other tissues. Multimodal molecular imaging combined with spatial "omics" was the main technology used for the research conducted in this collaboration.

While in the early years of the Fellowship Covid-19 made certain topics more difficult to pursue, a new collaborative infrastructure for interdisciplinary research based on mass spectrometry imaging was established early on at TUM. This facilitated the scientific research the Focus Group aimed for. Several programs were set up to train TUM researchers at the Maastricht facilities, enabling the direct knowledge transfer needed to conduct research at TUM.

Initial research was aimed at establishing metabolic images of isolated primary immune cells with MALDI-MSI. In particular, we implemented and optimized post-ionization by MALDI-2 to overcome the effects of ion suppression and increase sensitivity. The increased sensitivity resulted in the improved spatial resolution required for single-cell metabolic imaging. This approach spawned an exciting new area of research for investigating the molecular causes and effects of cellular interactions. This was successfully realized and resulted in high-content, high-resolution images such as the molecular image of hepatocytes shown in Figure 1. ▸

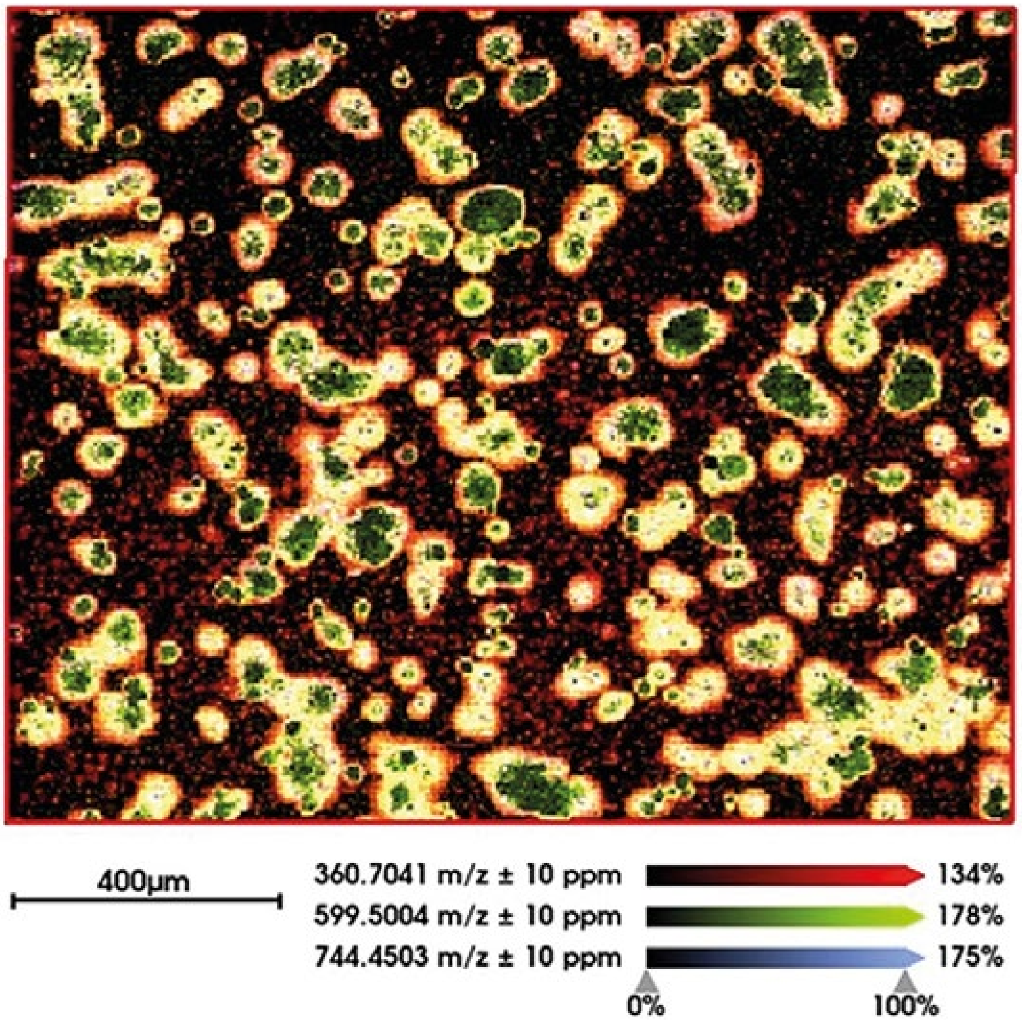


Fig. 1, Multicolor mass spectrometry image of the metabolism of isolated hepatocytes imaged with single-cell resolution measure at 5um using an optimized MALDI-MSI protocol.

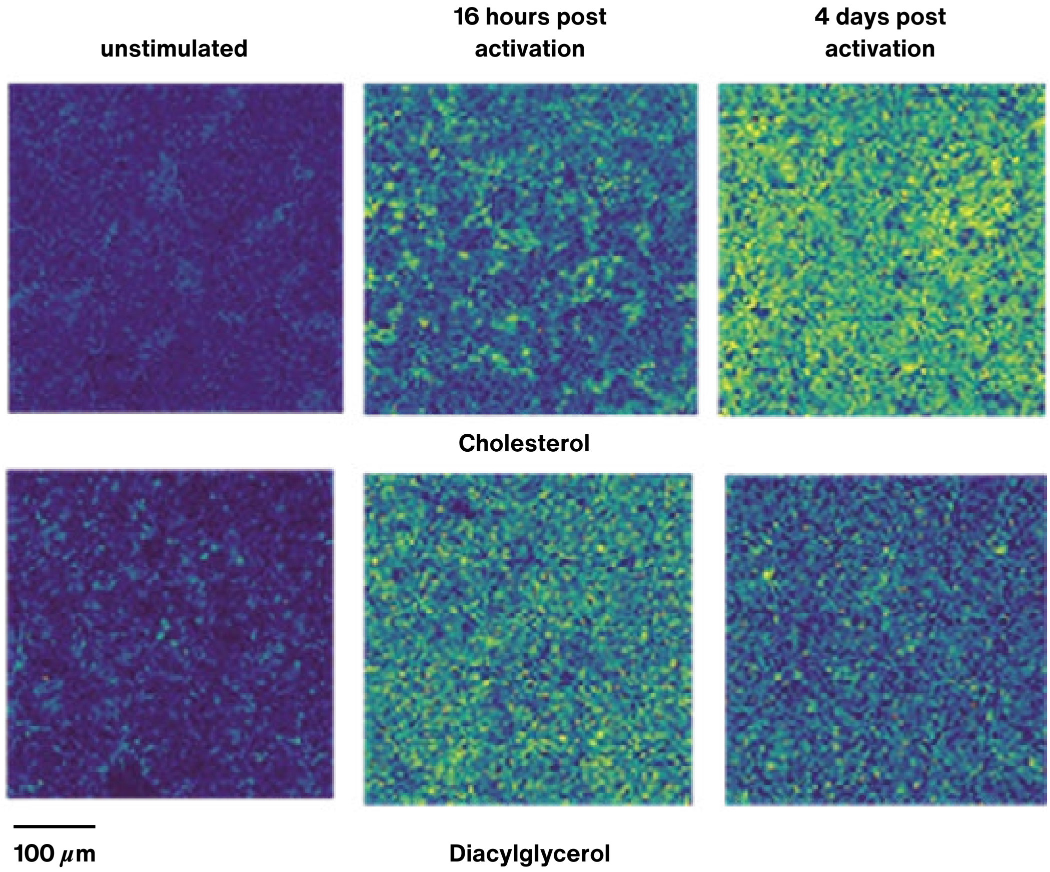


Fig. 2, Dynamics of diacylglycerol and cholesterol signature visualized with MALDI-MSI in T cells following activation (unpublished results).

One of the experiments employed anti-CD3 activated CD8 T cells, the changing metabolic signature of which was determined through multimodal molecular imaging post-activation. The results demonstrated the feasibility of this approach to use this metabolic profile to determine the metabolic age of activated CD8 T cells (Figure 2). This identified metabolites and lipids as local mediators of cell-cell communication, a finding impossible to obtain with protein-based technologies. This formed the basis of several grant proposals submitted and the basis of future work on cell-cell communication. Moreover, the research combined targeted and untargeted approaches to build cell type-specific metabolome and lipidome signatures characteristic for specific functional states of immune cell populations in tissues. Machine learning-based analysis of the cell-cell communication between liver tissue cells and immune cells detected in situ are targeted to provide a new level of understanding of how immune responses are fine-tuned to the tissue microenvironment. This information has been demonstrated to be crucial in the understanding of virus-specific CD8 T cells in the liver. In a study published in Nature (2024), it was demonstrated that a liver immune rheostat renders these CD8 T cells refractory to activation and leads to their loss of effector functions.

Additional collaborative studies were conducted in close collaboration with Corinna Dawid on the spatial distribution of food- and flavor-related compounds in mushrooms and plant-based alternative meat products. The studies were based on a new protocol developed to generate metabolic images of plant-based samples and demonstrated the use of molecular imaging technologies in food and ingredient classification and authentication.

A close collaboration between Bastian Hoechst and the imaging team of M4i resulted in a better morphological understanding of breast cancer-isolated extracellular vesicles and their role in cell-cell communication. The work has been submitted for publication and is under review.

The findings of these and several other projects were used as the basis of a joint ERC-synergy application, in close collaboration with the Helmholtz Institute, with the target to establish a synergistic European research program in cell-cell communication in the immune system. Unfortunately, the program was not funded after the interview stage, but it did form the basis for future collaborations and proposals that take advantage of established network. TUM is a collaborator in a Dutch large-scale research infrastructure grant, BioBeyond_NL, and Ron Heeren is proposed as a Mercator Fellow in a DFG Collaborative Research Center, Dynamics and Determinants of Tissue Immunity, in which imaging MS will play a central role. Future research will entail the integration of spatial transcriptomics and spatial metabolomics using technologies under development at Maastricht University. Ron Heeren was named TUM Ambassador at the end of this Hans Fischer Senior Fellowship, which will facilitate strengthening the future collaborations on research and education in immune metabolism and molecular imaging. ■

Selected publications

Vats, M., Flinders, B., Visvikis, T., Dawid, C., Hofmann, T. F., Cuypers, E. & Heeren, R. M. A. Mass spectrometry imaging for spatial ingredient classification in plant-based food. *J. Am. Soc. Mass Spec.*, 36, 100-107 (2025).

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Dudek, M., Pfister, D., Donakonda, S., Filpe, P., Schneider, A. et al. Auto-aggressive CXCR6+ CD8 T cells cause liver immune pathology in NASH. *Nature*, 592, 444-449 (2021).

For a full list of publications, please visit
www.ias.tum.de/ias/heeren-ron-ma

Focus Group: Gene-Regulatory Mechanisms

Dr. Lothar Hennighausen (NIDDK, National Institutes of Health, USA), Alumnus Hans Fischer Senior Fellow, **Prof. Priscilla Furth (Georgetown University, USA),** Anna Boyksen Fellow | **Dr. Markus Hoffmann (TUM, *now NIDDK, National Institutes of Health, USA*),** Doctoral Candidate, *now Postdoctoral Fellow*
Host: **Prof. Markus List (TUM)**

Dr. Lothar Hennighausen

Discovering networks in multiple layers of gene regulation

Prof. Priscilla Furth

This project explored gene-regulatory networks across different molecular levels. We have developed several computational tools to facilitate the analysis of biological data, enabling the generation of new hypotheses for experimental validation. Our primary objective is to support researchers in analyzing their data more effectively and understanding how biological processes are regulated.

Focus Group goal and effort rationale

Multicellular organisms, such as humans for example, comprise a vast number of individual cells. Although each cell contains almost identical DNA, they develop into at least 200 different types, each with its own shape and function. This process relies on various regulatory mechanisms that work at multiple molecular levels. These include genomics (the DNA sequence itself), epigenomics (the structural changes in DNA that control its accessibility), and transcriptomics (the production of RNA from DNA). Controlled adjustments to such regulations are essential for normal processes responding to stimuli, such as pregnancy or immune response to a virus. However, studies have shown that disruptions can lead to diseases such as Alzheimer's, diabetes, cancer, and autoimmune disorders. In our project, we created new computational tools to investigate these regulatory mechanisms, aiming to support researchers to improve our understanding of how disruptions can cause disease.

NIDDK, National Institutes of Health, and TUM-IAS collaborative research highlights

Inspired by the above goals, our collaboration involving NIDDK, National Institutes of Health, USA, and the TUM-IAS has focused on the following areas:

Regulation in genomics

In our study on regulatory networks in genomics, we developed a network-based approach to uncover interactions between single nucleotide genetic variations on the DNA (also called SNPs) that individually have

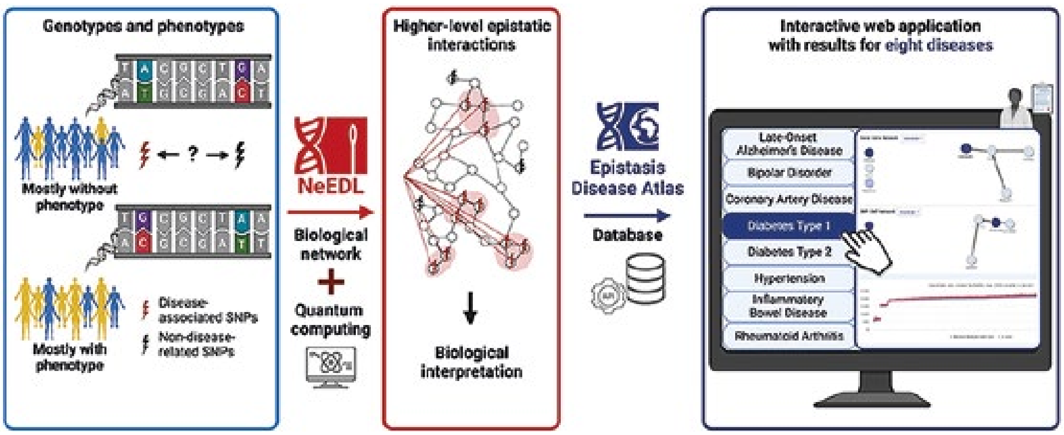

Fig. 1, Graphical abstract of our manuscript *"Network medicine-based epistasis detection in complex diseases: ready for quantum computing."* (Hoffmann, M. et al. (2024))

little or no effect but together could contribute to complex diseases. Our tool, NeEDL (network-based epistasis detection via local search), identifies sets of SNPs that could interact with each other and may have an impact on disease risk. Since we know of millions of SNPs, this represents a difficult task. Hence, to make our approach faster, we also explored quantum computing. When tested on diseases, NeEDL showed more robust performance than existing methods, offering new insights into how a combination of genetic interactions may drive disease.

Regulation in epigenomics

To investigate regulatory networks at the epigenomic level, we developed TF-Prioritizer, which identifies proteins called transcription factors (TFs) controlling the production of RNA from the DNA in specific biological conditions. TF-Prioritizer combines data on RNA expression and DNA accessibility to pinpoint TFs that might be important for different physiological conditions. We analyzed gene regulation during pregnancy and lactation in mice, identifying known and new transcription factors that may play important roles in this process. We showed that TF-Prioritizer streamlines complex data analysis, helping researchers better understand the regulation of RNA expression and its links to disease.

Regulation in transcriptomics

We developed two tools to explore how regulatory networks operate within the transcriptomics layer. At this regulatory level, small molecules called microRNAs (miRNAs) help control protein expression by binding to other RNA ▸

Fig. 2, Genetoberfest logo.

molecules and degrading them. A single miRNA can interact with many different RNAs, creating a network of connections between them. For instance, if one RNA is very abundant and binds many miRNAs, it can prevent those miRNAs from interacting with other RNAs that they typically regulate. To investigate this network and identify such upregulated RNA-miRNA relationships that could disrupt this regulatory mechanism, we developed the tool spongEffects. We showed that this tool is particularly useful in cancer research, enabling us to detect RNA interactions unique to different breast cancer subtypes and supporting personalized treatment approaches. Building on this, we created circRNA-sponging to examine circularRNAs, which have been shown to accumulate in a cell over time and could, hence, bind many miRNAs, thereby deregulating the network.

Synergistic activities across disciplines during our self-organized international conference: Genetoberfest – crossing bridges between bioinformatics and clinical research (TUM-IAS 2023)

During the Hans Fischer Senior Fellowship, we organized the Genetoberfest conference from October 16 to 19, 2023, at the TUM-IAS building in Garching. The conference drew the attention of 90 participants from all over Europe, the USA, Canada, Qatar, and South Korea. We offered keynote talks, plenary talks, and a wrap-up talk by undergraduate students. We further picked flash talks and two poster sessions from submitted abstracts. During these sessions, we discussed subjects that mattered most for clinical researchers but also for bioinformaticians. Subjects included: (i) the transformative impact of large-scale projects fostering open science, such as The Cancer Genome Atlas or the International Human Epigenome Consortium, (ii) opportunities for using AI in biomedical and clinical research, (iii) limitations in open data sharing and strategies to overcome them, (iv) how high-quality science could and should be incentivized, (v) how software development in biomedical science could be funded, and (vi) what science could learn from applications of AI in industry. The overall goal of our conference was to find common ground between the various disciplines, to determine how we can bridge them, and finally, to advance science.

TUM-IAS doctoral candidate research stay with Dr. Lothar Hennighausen's group at NIDDK, National Institutes of Health (2023)

In January 2023, the TUM-IAS supported a research visit for its doctoral candidate, Markus Hoffmann, to work with Dr. Lothar Hennighausen's research group at the NIH's NIDDK in the USA, fostering international collaboration through in-person research. The aim was for Markus Hoffmann to gain direct experience with benchwork methods to better understand the data underlying his biomedical software tool. The visit was so fruitful that Markus Hoffmann chose to stay on as a postdoctoral fellow in Dr. Hennighausen's lab, enabling him to deepen his biochemical expertise further and apply these insights to his software development. ■

Selected publications

Hoffmann, M. et al. Network medicine-based epistasis detection in complex diseases: ready for quantum computing. *Nucleic Acids Research* 52(17), 10144–10160 (2024).

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Hoffmann, M. et al. spongEffects: ceRNA modules offer patient-specific insights into the miRNA regulatory landscape. *Bioinformatics* 39(5) (2023).

Hoffmann, M. et al. circRNA-sponging: a pipeline for extensive analysis of circRNA expression and their role in miRNA sponging. *Bioinformatics Advances* 3(1), vbad093 (2023).

For a full list of publications, please visit
www.ias.tum.de/ias/hennighausen-lothar

Focus Group: Optoelectronic Properties of Perovskite Semiconductors

Prof. Laura Herz (University of Oxford), Alumna Hans Fischer Senior Fellow (funded by Cluster of Excellence e-conversion) | **Dr. Sebastián Caicedo-Dávila (TUM),** Postdoctoral Researcher
Hosts: **Prof. David Egger (TUM), Prof. Thomas Bein (LMU)**

Prof. Laura Herz

Next-generation semiconductors for solar energy harvesting

Solar cells offer a promising approach to carbon-free energy generation, but a wider catalogue of light-absorbing materials is required for higher energy returns. This Focus Group investigated novel metal halide perovskite semiconductors, combining optical spectroscopy, microscopic theory, and material synthesis to examine electric and ionic charge transport as well as optical and vibrational properties that affect performance.

[1] NREL Best Research-Cell Efficiency Chart, www.nrel.gov/pv/cell-efficiency.html, accessed 11 Nov 2024

Climate change and energy security are among the greatest challenges for the coming century, leading to renewed research on exploiting the energy of sunlight as a clean and sustainable solution. While single-junction silicon devices are currently the dominant market player, their power conversion efficiency is fundamentally limited to ~30%. Moving to higher efficiencies will require the stacking of semiconductor layers with different bandgaps, in so-called multi-junction solar cells. As a result, intense activity has focused on creating a new diverse catalogue of inorganic (or hybrid organic-inorganic) semiconductors. These materials have been targeted to enable low embodied energy of production, i.e., low energy payback time for fabricating the light-harvesting device, for example by material deposition from solution or low-temperature vapor deposition. Lead halide perovskites are a prominent example for this class, having shown power conversion efficiencies, in research cells, of more than 26% in single-junction devices and more than 34% in tandem with silicon photovoltaics [1]. Intriguingly, this materials class has been found to straddle the boundaries of traditional "hard" inorganic semiconductors (such as bulk silicon) and classic "soft" molecular solids, opening up a complex array of exciting new fundamental science.

This Focus Group has investigated the complex physical and chemical phenomena that underlie the spectacular optoelectronic properties of such perovskite solar absorber materials, with a particular focus on elucidating the effects of material softness. The Focus Group has also explored a range of novel perovskite-like material compositions that show improved properties, with a focus on reduced toxicity and elimination of lead. The Focus Group encompassed a team of complementary experts combining a variety of tools from optical spectroscopy (Herz), microscopic theory (Egger, Caicedo-Dávila), and material synthesis (Bein).

Scientific progress of the Focus Group

Effects of lattice softness and anharmonicity in lead halide perovskites

Halide perovskites show great optoelectronic performance, but their softness results in unusually strong lattice anharmonicity, which leads to novel lattice dynamics that can be hard to capture through traditional computational methods. Understanding such lattice dynamics is critical to photovoltaic material performance, as they govern dynamic disorder, hot-carrier cooling, charge-carrier recombination, and transport. The Focus Group examined such effects through a combination of cutting-edge experimental and theoretical approaches.

In one study (*Nature Communications* 2024), work by the Focus Group examined the effect of electron lone pairs on anharmonic effects in lead halide perovskites. It was shown that the ns2 electron configuration of octahedral cations is not, as had been previously proposed, a prerequisite for the strong anharmonicity and low-energy lattice dynamics encountered in these materials. The lattice dynamics of $CsSrBr_3$ and $CsPbBr_3$ were compared, i.e., two compounds that are structurally similar but with the former lacking ns^2 cations with the propensity to form electron lone pairs. Low-frequency diffusive Raman scattering revealed that low-frequency tilting occurs irrespective of octahedral cation electron configuration, thus ruling out a significant role of lone-pair formation on anharmonicity in lead halide perovskites.

A further study (*ACS Energy Letters* 2024) examined the ultralow-frequency Raman and infrared terahertz time domain for a wide range of metal halide semiconductors to elucidate the origin of their unusually broad low-frequency Raman response, whose origin is still much debated. Extrinsic defects, octahedral tilting, and “liquid-like” boson peaks were ruled out as causes of the central Raman peak, which was shown to originate from significant broadening of Raman-active, low-energy phonon modes that reflect strong lattice anharmonicity.

Novel low-toxicity, lead-free metal halide semiconductors

The highest-efficiency perovskite solar cells are currently based around materials incorporating toxic lead. The Focus Group therefore explored a range of novel bismuth-based metal halide semiconductors, which offer lower toxicity.

In one study, the Focus Group explored the interplay between charge-carrier localization and material alloying, examining $Cs_2AgSb_xBi_{1-x}Br_6$ double perovskite thin films (*J. Phys. Chem. Lett.* 2023, Fig. 1). While initially delocalized charge carriers were found to experience electronic bands formed upon alloying, subsequently self-localized charge carriers probe the energetic landscape more locally. Therefore, the alloy’s low-energy sites (e.g., Sb sites) turn into traps, which dramatically deteriorates transport properties, ►

highlighting the inherent limitations of alloying strategies in materials that spontaneously form self-trapped charges.

A second study (*Advanced Optical Materials* 2022) explored two-dimensional (2-D) hybrid double perovskites, a class of materials featuring superior intrinsic and extrinsic stability. The Ruddlesden-Popper phases $(4FPEA)_4AgBiX_8$ (X = Cl, Br, I) forming double perovskites with different halides and the organic spacer cation 4-fluorophenethylammonium (4FPEA) were examined. Highly oriented thin films were fabricated and investigated spectroscopically, revealing that these systems are dominated by phonon-coupled and defect-mediated polaronic states.

These outcomes inspired further work (*JACS* 2024) in which electroactive organic cations were combined with inorganic halide perovskites to form layered two-dimensional hybrid materials. By introducing naphthalene and pyrene moieties into Ag–Bi–I and Cu–Bi–I double perovskite lattices, intrinsic electronic challenges of double perovskites were addressed and the electronic anisotropy of 2-D perovskites modulated. Based on the findings, an oriented thin film of $(POE)_4AgBiI_8$ was integrated into a device to construct the first pure n = 1 Ruddlesden-Popper 2-D double perovskite solar cell.

Workshop on “Understanding ion migration in solid-state materials for energy applications”

The Focus Group held a workshop at the TUM-IAS in September 2024, which cut across a multitude of scientific disciplines, bringing together leading experimental and theoretical international experts (Fig. 2) working on electronic and ionic transport in solids with relevance to energy applications. A particular focus was on the interplay between light-induced effects and ionic motion, which is still insufficiently understood. Research spanned light-induced ionic motion in photovoltaic materials such as metal halide perovskites and opto-ionic and ionic transport effects in materials for photocatalysis and batteries. A lively, interactive program of 18 keynote talks and discussions provided fertile ground for exchanging ideas and exploring future collaborations among the participants. ■

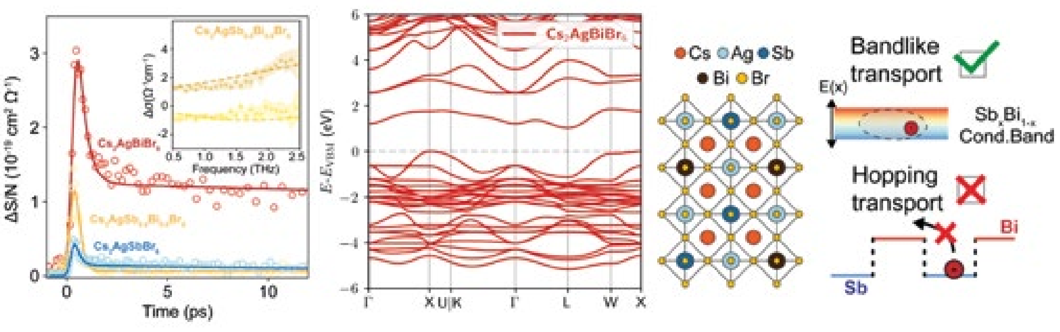

Fig. 1, Graphic showing time-resolved THz photoconductivity and band structure of charge carriers in $Cs_2AgSb_xBi_1$–xBr_6 double perovskite (reproduced from *J. Phys. Chem. Lett.* 14, 10340–10347 (2023), under CC-BY 4.0 creative commons license).

Fig. 2, Participants in the workshop Understanding Ion Migration in Solid-State Materials for Energy Applications, held at the TUM-IAS in September 2024 (© TUM-IAS).

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Caicedo-Dávila, S., Cohen, A., Motti, S. G., Isobe, M., McCall, K., Grumet, M., Kovalenko, M. V., Yaffe, O., Herz, L. M., Fabini, D. H. & Egger, D. A. Disentangling the effects of structure and lone-pair electrons in the lattice dynamics of halide perovskites. *Nature Communications* 15(1), 4184 (2024).

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For a full list of publications, please visit
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Focus Group: Responsible Innovation Communication

Prof. Maja Horst (Aarhus University), Alumna Hans Fischer Senior Fellow |
Dominic Lammar (TUM), Doctoral Candidate
Host: **Prof. Ruth Müller (TUM)**

Prof. Maja Horst

Working toward responsibility in innovation communication

This Focus Group investigated the role of communication in shaping public perceptions of and research on artificial intelligence (AI) in Germany. Through a media analysis, expert interviews, and an interdisciplinary workshop, it approached the question of what responsible innovation communication might look like in a charged communication environment that is marked by strong hopes but also fears.

Communication plays a key role in in the development and implementation of emerging technologies in society [1]. It is not only necessary to generate resources because researchers need to “sell their ideas” to generate funding, gain institutional support, and attract partners for collaboration. Communication is also crucial to the way in which society and citizens make sense of, and react to, new technologies. For instance, public narratives around nuclear power, genetic technology, and artificial intelligence are crucial for the social acceptance of – or opposition to – such technologies. However, while there is a vast literature regarding matters of responsible research and innovation (RRI), it has tended to under-emphasize the role of communication.

Since its founding in 2021, this Focus Group has taken public communication around artificial intelligence (AI) in Germany as an empirical field to investigate what responsible innovation *communication* might mean. Public expectations and debates around AI are a particularly pertinent place to trace questions around responsibility, because they are marked by high levels of hope as well as fear. At the same time, TUM constitutes an excellent place for such investigations because of the breadth of AI research(ers) it is home to.

[1] Davies, S. R. & Horst, M. : Science communication as culture: a framework for analysis. Bucchi, M. & Trench, R. (Eds.): *Handbook of public communication of science and technology. Routledge (2021).*

Empirical work

In a first step, we conducted a media analysis to identify the broader themes and concerns present in German public debates around AI. We consciously decided against further defining what AI is or is not, because we were precisely interested in how news articles understand and describe this phenomenon. In our analysis, we identify two distinct discourses around AI. We show that AI is often either described in a highly abstract fashion ("AI will cause a technological revolution") or a highly contextual manner ("researcher X uses model Y to solve problem Z"), and we trace how technology hype around AI emerges in the interaction between these two ways of describing AI. The manuscript resulting from this work package is currently under review.

Drawing on these findings, we then engaged in interviews with AI experts themselves. In these semi-structured interviews, we trace how experts perceive the wider debates around their field of investigation and how they engage with public concerns as well as hopes. Our interest here lies in understanding how narratives around an emerging technology like AI can affect scholars' everyday research and communication practices. A manuscript currently in progress will foreground the communication practices our interviewees identify as effectively "selling" their work to funders, policy makers, and the wider public without engaging in what they consider over-extrapolations of limited findings. ►

Workshop on Responsible Innovation Communication using Lego Serious Play Methodology.

Keynote lecture on responsible innovation communication by Maja Horst.

We complemented these interviews by conducting a workshop in which participants of diverse backgrounds (public relations practitioners, scientific experts developing medical AI systems, social scientists working on public communication) explicitly discussed what it might mean to communicate responsibly around AI. The workshop was facilitated by an external moderator using Lego Serious Play Methodology as a way to engage all participants in an open and constructive exchange.

Public and interdisciplinary outreach

At the same time, the different members of the Focus Group have presented and discussed their work in a variety of other settings, thus making their findings available to relevant groups of stakeholders across and beyond leading academic institutions. For instance, Maja Horst has spoken on the importance of responsible innovation communication as part of her Linde Lecture at the TUM-IAS General Assembly (2022) and during her keynote lecture at the EuroTech Alliance's Tech4Society anniversary celebration in Brussels. Her Host Ruth Müller engaged with the topic of innovation communication during a panel event at the Tandon School of Engineering in New York.

To mark the end of the Focus Group at TUM itself, we organized a panel discussion on responsible innovation communication to foster discussion among different stakeholders across this university. The event was kicked off by a keynote by Maja Horst and followed by a discussion between the panelists featuring, among others, Ulrich Marsch, managing director of TUM-IAS, and Jeanne Rubner, TUM Vice President for Global Communication and Public Engagement.

Future research

In the long run, the findings from this Focus Group will inform Maja Horst's further work on a broad theoretical framework for understanding *innovation communication* as a crucial dimension of RRI. At the same time, the results from our interviews and the workshop on responsible innovation communication build a basis for further engagement with the topic, for instance in the form of developing communication guidelines for responsible communication at TUM itself. ■

Selected publications

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Krarup, T. & Horst, M. European Artificial Intelligence Policy as Digital Single Market Making. *Big Data & Society* 10(1) (2023).

Horst, M. Science Communication as a Boundary Space: An interactive installation about the social responsibility of science. *Science, Technology and Human Values* 47(3), 459–482 (2022).

Lammar, D., Horst, M. & Müller, R. AI in the German Media: Narratives of AI-in-Particular and AI-in-General in German Media Reporting about Artificial Intelligence. *Digital Journalism, special Issue Covering AI amidst the Hype* (forthcoming).

Holohan, M. & Müller, R. "Beyond humanism: telling response-able stories about significant otherness in human–chatbot relations." *Frontiers in Psychology* 15 (2024).

For a full list of publications, please visit
www.ias.tum.de/ias/horst-maja

Focus Group: Novel Tensor Network Methods for Strongly Correlated Quantum Systems

Prof. Örs Legeza (Wigner Research Centre for Physics), Alumnus Hans Fischer Senior Fellow | **Elizabeth Adomako Boamah (TUM),** Doctoral Candidate
Host: **Prof. Gero Friesecke (TUM)**

Prof. Örs Legeza

Novel tensor network methods for correlated quantum systems

The main research interests of the Focus Group were in the mathematical aspects of novel tensor network state (TNS) methods and their application to strongly correlated quantum many-body systems. These methods can be used to simulate and study magnetic properties in solid states, exotic quantum phases, complex molecular clusters, ultracold atomic systems, and nuclear structures on high-performance computing infrastructures.

For the method development, we combined established methods for simple networks with concepts from quantum information theory, computational mathematics, and high-performance computing to push the current frontier of moderate system sizes to much larger and more complex systems. By performing, for example, electronic structure calculations via our state-of-the-art TNS code, we achieved a quarter petaflops performance on a single DGXH100 GPU accelerated hardware platform for the active compounds of the FeMoco and cytochrome P450 (CYP) enzymes with complete active space (CAS) sizes of up to 113 electrons in 76 orbitals [CAS(113, 76)] and 63 electrons in 58 orbitals [CAS(63, 58)], respectively. This incredible computational power has the potential to pave the way for simulation of challenging multi-reference problems in chemistry or highly correlated materials science, i.e., to perform large-scale, high-accuracy ab initio computations routinely on a daily basis for a broad range of disciplines.

Altogether, during the three-year time period of the Fellowship, our research work resulted in 27 publications in high-quality journals including *Phys. Rev. Lett, Phys. Rev. B, Phys. Rev. Research, Phys. Let. B, J. Chem. Theory Comput., J. Math. Chem., J. Chem. Phys*, and *npj Computational Materials* among many others, each indicating the support provided by the TUM-IAS. Fundamental results have been achieved in condensed matter physics focusing on new exotic quantum phases of matter, such as Wigner necklace in carbon nanotubes, Z4 parafermions, hadron formation in repulsive Hubbard Models, and formation of chemically stable spin qubits in hexagonal boron nitride. Extensions to time-dependent phenomena and dissipat-

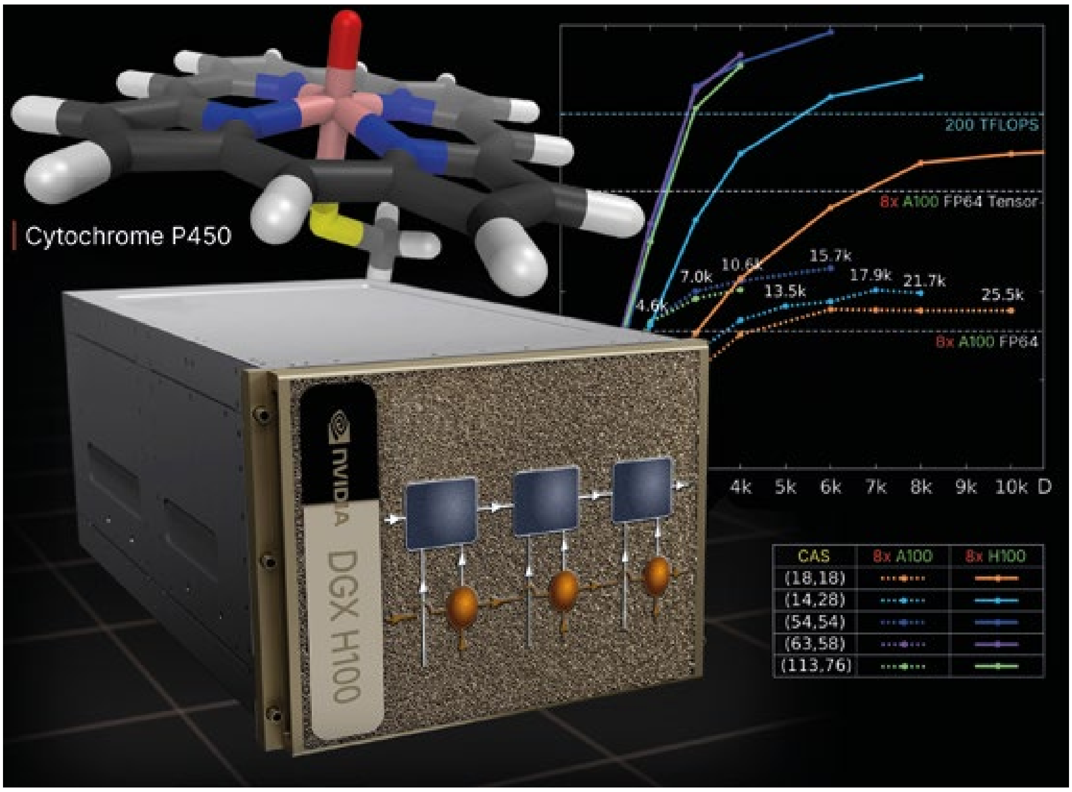

Fig. 1, Application of the massively parallel Density Matrix Renormalization Group algorithm to cytochrome P450 (CYP) enzymes achieving a quarter petaFLOPS performance on a state-of-the-art single DGX-H100 GPU node.

ing quantum systems have also been part of our research. We have also introduced novel methods to locate and characterize quantum phase transitions, focusing on the most difficult infinite order Kosterlizt-Thouless phase transition and on Mott-Hubbard transition in model systems without upklapp scatterings.

In nuclear structure theory, we have opened a new research direction via tensor network state methods by studying neutron- and proton-rich heavy isotopes, also bringing into the field concepts of quantum information theory and entanglement-based analysis tools. From a method development point of view, we have combined the in-medium similarity renormalization group (ISMRG) approach with the density matrix renormalization group (DMRG) method and demonstrated the very stable and robust convergence of the new method (VS-DMRG) on hard problems that are beyond the scope of conventional algorithms. ▸

In quantum chemistry, we have studied convergence of a fully correlated wave function in the infinite basis limit via a rigorous mathematical framework based on matrix product state representation. We have also introduced novel methods by combining the density matrix renormalization group (DMRG) method with the concept of restricted active space (RAS) and have shown that the new method has the potential to outperform conventional methods such as coupled cluster (CC) and multi-reference configuration interaction (MRCI). In addition, on the basis of rigorous scaling analysis, we have developed a new extrapolation approach (DMRG-RAS-X) to predict full-CI (exact) energies of large chemical systems. We studied several strongly correlated (multi-reference) molecular systems, also from the point of view of quantum information theory.

By combining our complementary expertise, we aimed to find an optimal representation of a quantum many-body wave function, i.e., a parametrization with the minimum number of parameters for a given error margin, which is a task of the utmost importance in modern quantum physics and chemistry. To this end, we have developed novel algorithmic solutions to further boost the performance of tensor network state methods based on global fermionic mode optimization. This new approach has the potential to revolutionize simulations on two and higher dimensional quantum lattice models, demonstrated via large-scale numerical simulations, especially when massively parallel computations are performed on high-performance computing infrastructures.

We have also developed a new code base to carry out proof-of-principle calculations to study the effect of tensor network topologies when one or several loops are introduced. Various interpolations between limiting cases have been determined, and our preliminary results indicate lower numerical errors for a broad parameter regime. This project also formed the basis of the HFSF PhD program, and the related doctoral degree of our PhD candidate is anticipated in the near future.

We have further developed our software package exploiting the enormous computational power offered by high-performance computing centers, and we initiated various collaborations with industrial partners, including NVIDIA, AMD, SandboxAQ (Google startup), Furukawa Electronic Institute of Technology, RiverLane Ltd, FACCTS GMBH (spin-off of the Max Planck Society). Moreover, our DMRG code has been used by some 30 research groups worldwide in condensed matter and nuclear physics and in quantum chemistry.

We have organized three international workshops. The one at TUM-IAS took place in April 2024, bringing together condensed matter physicists, mathematicians, and theoretical chemists to continue the exploration of tensor network state methods and to stimulate further developments. Numerous prominent scientists from the field were invited as speakers for the workshop, and young researchers also attended and contributed to the workshop with talks and posters. The focus of the workshop was on innovative ideas for moving beyond the current limits of quantum many-body simulations despite the major challenges of high dimensionality and accuracy.

During the past three-year time period, we have presented our research results via close to 45 international conferences, workshops, and seminar talks. We have had active collaborations with some ten universities and research institutes in Germany. Among others, follow-up collaborations have also been established recently by CERN, the Parmenides Foundation, and Argonne National Laboratory. ■

Selected publications

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Menczer A., Kapás, K, Werner, M. A. & Legeza, Ö. Two dimensional quantum lattice models via mode optimized hybrid CPU-GPU density matrix renormalization group method, *Phys. Rev.* B 109, 195148 (2024).

Friesecke G., Barcza G. & Legeza Ö. Predicting the FCI energy of large systems to chemical accuracy from restricted active space density matrix renormalization group calculations, *J. Chem. Theory Comput.,* 20, 1, 87–102 (2024).

Friesecke, G. Graswald, B. R., & Legeza, Ö. Exact matrix product state representation and convergence of a fully correlated electronic wavefunction in the infinite-basis limit. *Physical Review* B 105, 16, 165144 (2022).

For a full list of publications, please visit
www.ias.tum.de/ias/legeza-oers

Focus Group: Data-driven Dynamical Systems Analysis in Fluid Mechanics

Prof. Luca Magri (Imperial College London, The Alan Turing Institute, Politecnico di Torino), Alumnus Hans Fischer Fellow | **Dr. Nguyen Anh Khoa Doan (TUM, *now Assistant Professor Delft University of Technology*),** Postdoctoral Researcher
Host: **Prof. Wolfgang Polifke (TUM)**

Prof. Luca Magri

Predicting extreme events before they occur with scientific machine learning

Many turbulent flows exhibit extreme events — large, transient deviations from their normal states. Examples include severe atmospheric phenomena, rogue waves in the ocean, and flashback events in hydrogen-powered combustors. During this Fellowship, we developed advanced scientific machine learning tools to investigate and predict these extreme events, laying the groundwork for their prevention.

Context and overall goal

Climate change and the push to decarbonize society are making extreme events in fluids more common. These events are rare instances where the flow suddenly shifts to extreme states, far from its usual behavior. Such events can occur in various flow systems, including the atmosphere, where atmospheric blocking leads to severe heat waves; the oceans, where rogue waves (extremely large waves) can capsize ships; and in engineering systems such as hydrogen-based clean combustors, where flashback occurs and the flame unexpectedly moves back into the injection system.

At present, accurately predicting these extreme events is challenging due to several obstacles. First, the chaotic nature of turbulent flows makes them difficult to forecast; even the smallest disturbance can cause radically different outcomes (the butterfly effect). Second, extreme events result from complex nonlinear interactions, which differ across systems with varying physical mechanisms, making it hard to apply insights from one system to another. Third, there is a lack of sufficient data on these events.

To revolutionize our approach to extreme events, our Focus Group aims to develop an advanced scientific machine learning framework that synergistically combines deep learning with physics-based methods, thereby enabling the prediction of extreme events in turbulent flows. Such a hybrid physics/machine learning-based framework will overcome the normally data-hungry nature of machine learning tools in the context of the rarity of extreme events in any dataset. ▸

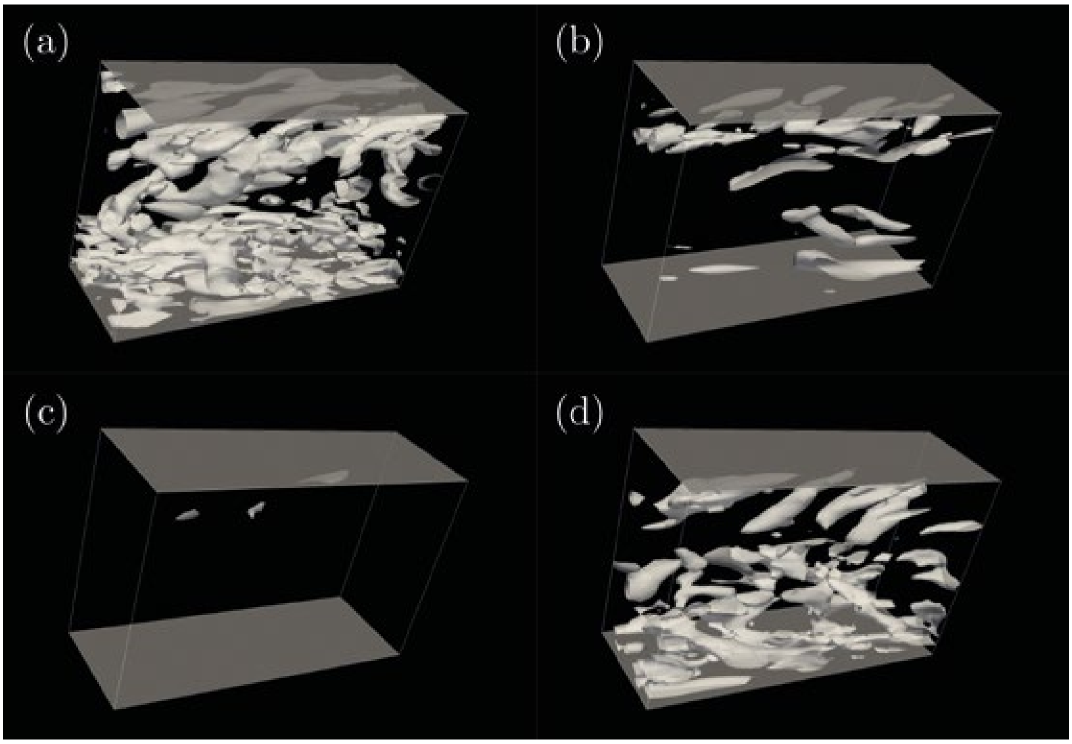

Fig. 1, Snapshots during the extreme events occurring in a channel flow. Isosurface represents vortical structures. The extreme event consists in the sudden collapse and disappearance of these vortical structures. (a) Normal state of the channel flow, (b) start of the extreme events with disappearance of the vortical structures, (c) peak of the extreme event with no vortical structures, (d) recovery of the flow after the extreme events.

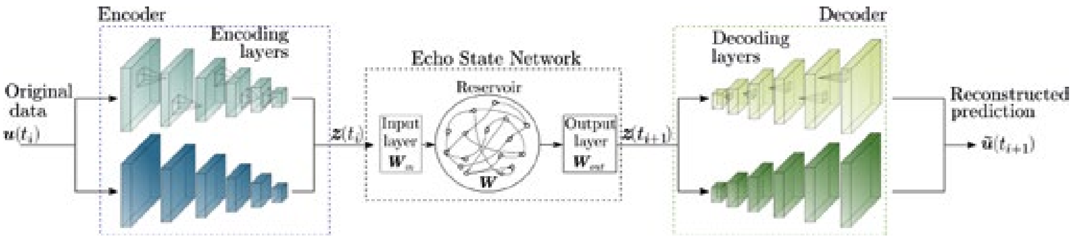

Fig. 2, Autoencoded reservoir computer proposed to learn the dynamics of complex high dimensional turbulent flows and their extreme events.

Summary of work and major outcomes

During this TUM-IAS Fellowship, we pioneered the development of physics-informed reservoir computer methods for the time-accurate prediction of extreme events in turbulent flows. We showed that a combination of physical knowledge with a specific type of reservoir computer, called an echo state network, could provide a longer time horizon in the prediction of extreme events in turbulent flows [1]. Furthermore, to handle high-dimensional flows, we developed a new deep learning architecture that combined a convolutional autoencoder with an echo state network to learn and predict the dynamics of turbulent flows (see Fig. 2) [2].

In parallel to those activities dedicated to the prediction of extreme events, we also developed data-driven techniques and applied them to reacting flows (i.e., flows where chemical reactions play an important role, such as in gas turbines). Deep learning techniques were developed to learn the dynamics of reacting flows, in the context of thermoacoustic instabilities prevention. We showed that neural networks could learn the essential dynamics of a flame and be embedded in a reduced-order acoustic model of the combustor to accurately predict the onset of thermoacoustic instabilities when design changes to the combustor are performed [3]. Furthermore, we also developed data assimilation techniques to improve the accuracy of coarse simulations, demonstrating how a judicious choice of assimilated quantities from high-fidelity simulations could enable coarse ones to accurately predict ignition kernels.[4]

To provide a platform for the dissemination of our results and create opportunities for research cross-fertilization, our Focus Group organized SoTiC 2021 – *Symposium on Thermoacoustics in Combustion: Industry meets Academia* in September 2021. This was a five-day symposium, held online due to Covid, with five keynote presentations from both industry and academia and 64 other presentations. Selected papers from the symposium were published in a special issue of the *International Journal of Spray and Combustion Dynamics*.

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[2] Doan, N.A.K., Polifke, W., & Magri, L. *Lecture Notes in Computer Science* (2021).

[3] Tathawadekar, N., Doan, N.A.K., Silva, C. & Thuerey, N. Modeling of the nonlinear flame response of a Bunsen-type flame via multi-layer perceptron. *Proceedings of the Combustion Institute,* 38 (4), 6261–6269 (2021).

[4] Magri, L. & Doan, N.A.K. (2020).

Future research

The research achieved during this TUM-IAS Fellowship is paving the way for the future control and prevention of extreme events in turbulent flows in engineering applications. Building on the ability to predict their occurrence, further research will be devoted to developing machine learning-based techniques to identify optimal control strategies that can effectively mitigate these extreme events in practical engineering applications, such as the prevention of flashback in hydrogen-powered gas turbines, and to improve prediction of extreme climate events in weather forecasting.

In close collaboration with Prof. Thomas F. Sattelmayer (TUM) and Prof. Mirko R. Bothien (Zurich University of Applied Sciences, Alumnus Rudolf Diesel Industry Fellow). ■

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Doan, N.A.K., Polifke, W. & Magri, L. Short- and long-term predictions of chaotic flows and extreme events: a physics-constrained reservoir computing approach. *Proceedings of the Royal Society of London A,* 477, 20210135 (2021).

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For a full list of publications, please visit
www.ias.tum.de/ias/magri-luca

Focus Group: Drought Mitigation Through Ecosystem Restoration: Challenges and Opportunities

Dr. Anastassia Makarieva (Petersburg Nuclear Physics Institute), Alumna Anna Boyksen Fellow (funded as part of the Excellence Strategy of the federal and state governments)
Host: **Prof. Anja Rammig (TUM)**

Dr. Anastassia Makarieva

Quantifying how natural ecosystems stabilize the water cycle

How ecosystem restoration affects the water cycle, particularly river runoff and atmospheric moisture convergence, is an important and controversial issue in environmental science. We show that ecosystem effects can depend on air humidity. Under wet (dry) conditions, additional transpiration increases (decreases) river runoff, indicating a vegetation-related tipping point in atmospheric dynamics.

The project was implemented within the framework of the biotic pump concept, which states that by moistening the atmosphere, forest transpiration creates conditions that facilitate the transport of atmospheric moisture from the ocean to land. At steady state, the atmospheric moisture convergence (net import) equals the river runoff (net export) of liquid water from an ecosystem. While the biotic pump concept predicts increased river runoff with increased transpiration, there is mixed evidence showing opposite responses in the water cycle, with more trees sometimes associated with less river runoff. One of the project goals was to clarify and resolve this issue.

Based on the data analysis of precipitation and atmospheric moisture content in several regions in Brazil (where there is the world's largest intact forest) and China (where the Loess plateau is home to one of the world's largest ecological restoration projects), we found that precipitation does not increase with increasing atmospheric moisture content in a dry atmosphere, whereas it increases sharply in humid conditions. Combining these results with the biotic pump propositions allowed us to propose a solution to the problem of the dual response of runoff to increased transpiration.

The physical mechanism of the biotic pump is based on the condensation of water vapor, which results in non-equilibrium pressure gradients that cause air to move. However, if the atmosphere is very dry, condensation cannot occur, even if a little extra moisture is added. Thus, when transpiration increases the moisture content of a very dry atmosphere, condensation and the associated convergence of air will not occur. The evaporated moisture will be carried away by the winds, and river runoff will decrease. Conversely, additional transpiration in a humid atmosphere enhances condensation, which in turn increases moisture convergence and river runoff [1].

Recognizing the transition between dry and wet regimes is critical to assessing the impacts of deforestation and to motivating and guiding ecological restoration. In many cases, ecological restoration is planned in areas of water scarcity that it is intended to mitigate. Our work shows that while river runoff may be reduced in the initial stages of ecological restoration, which may temporarily exacerbate water scarcity due to competition for water between plants and people, this negative effect may be temporary and resolve as ecosystems progressively recover and the atmosphere becomes more humid.

Planning for the initial decline in runoff, and for possible extra measures like irrigation to facilitate early ecosystem recovery, can help ecological restoration projects run more smoothly and be better understood and supported by the local stakeholders. In principle, it is also possible to avoid an initial decline in runoff by choosing the starting points for ecological restoration in the local maxima of humidity ("the wetspots"), where increased transpiration from added vegetation will immediately begin to increase moisture convergence. Rigorous interdisciplinary scientific planning, merging ecology and atmospheric science, is required to achieve this. ►

[1] Makarieva, A. M. et al. The role of ecosystem transpiration in creating alternate moisture regimes by influencing atmospheric moisture convergence. *Global Change Biology* 29, 2536–2556 (2023).

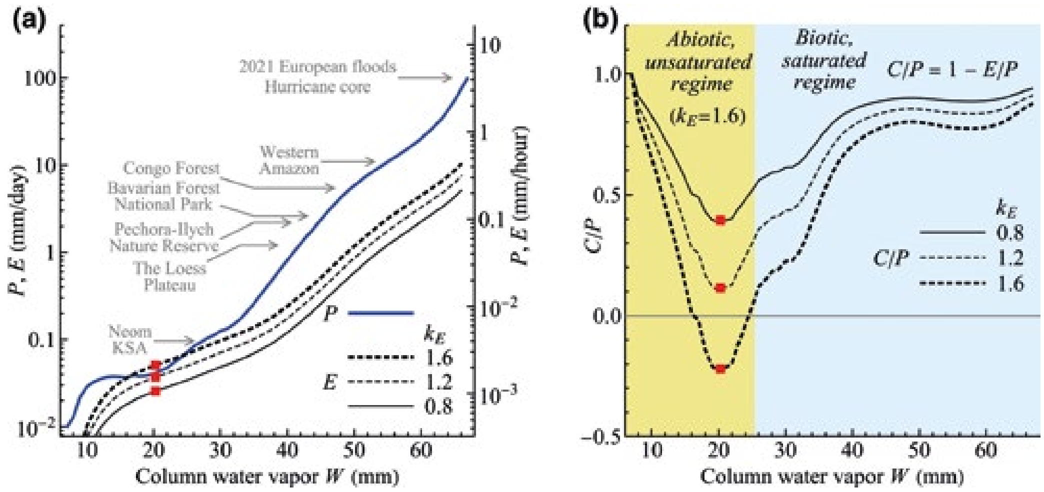

Fig. 1, Atmospheric moisture budget terms *P* (precipitation), *E* (evapotranspiration), *C* (atmospheric moisture convergence) as dependent on the atmospheric moisture content *W* for the Brazilian region studied. In (a), local hourly precipitation data are shown. Arrows indicate characteristic precipitation rates in different locations in the world. Coefficient k_E reflects different assumptions about the strength of the *E(W)* dependence. Red squares indicate the point where the moisture convergence (and steady-state river runoff) are minimal but begin to grow with increasing *E* at larger *W* (transition from the dry to wet regime).

In addition to its effect on atmospheric moisture transport, forest transpiration has an important impact on global surface temperatures. We showed in a theoretical analysis supported by data that reduced transpiration due to historical deforestation can lead to considerable temperature changes that should be expressed as an increase in the vertical air temperature lapse rate [2].

Over the past two years, our planet has experienced dramatic warming that has challenged climate science. The global mean surface temperature rose by about 0.2 degrees Celsius in just one year – a tenfold acceleration compared to the mean warming trend of 1–2 degrees per century. The biotic carbon sink that has been removing about one-third of anthropogenic carbon emissions ceased to function, presumably due to the drought in the Amazon and fires in the Canadian forests. Causes of the extraordinary warming are still unclear, but it can probably have to do with “intricate, long-distance links – known as teleconnections – fueled by sea and atmospheric currents [3]”. If the warming is due to changes in oceanic and atmospheric circulation, and if there is a positive feedback between evapotranspiration and atmospheric moisture convergence, then any large-scale disruption of vegetation functioning, such as the biotic pump outage in the Amazon, could be responsible for the warming. Our results indicate that the protection of the remaining natural forests can become an immediately effective measure against further abrupt destabilization of climate.

To disseminate the project results, an international workshop “Embracing Nature’s Complexity” was organized at the TUM-IAS in April 2024. The workshop assembled more than 70 participants from Europe, China, and North and South America representing science, business, and media. The results of the project were also presented in a plenary talk by Anastassia Makarieva at the Ecosummit “Eco-civilization for a sustainable and desirable future” in December 2024 in Zhengzhou, China [4].

In close collaboration with Dr. Andrei Nefiodov (Petersburg Nuclear Physics Institute). ■

[2] Makarieva, A. M., Nefiodov, A. V., Rammig, A. & Nobre, A. D. Re-appraisal of the global climatic role of natural forests for improved climate projections and policies. *Frontiers in Forests and Global Change* 6, 1150191 (2023).

[3] Schmidt, G. Climate models can’t explain 2023’s huge heat anomaly — we could be in uncharted territory. *Nature* 627 (2024).

[4] www.bioticregulation.ru/ecosummit2024

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Makarieva, A. M. et al. Vegetation Impact on Atmospheric Moisture Transport under Increasing Land-Ocean Temperature Contrasts. *Helyion* 8(10), e11173 (2022).

For a full list of publications, please visit
www.ias.tum.de/ias/makarieva-anastassia-m

Focus Group: Diversity in Information Technology

Prof. Andreea Molnar (Swinburne University of Technology), Alumna Anna Boyksen Fellow (funded as part of the Excellence Strategy of the federal and state governments)
Host: **Prof. Anne Brüggemann-Klein (TUM)**

Prof. Andreea Molnar

Factors influencing women's participation in IT degrees

Through interviews with IT students, we found that women's decisions to enroll in IT degree programs are influenced by individual factors (e.g., family, friends, teachers) and environmental factors (e.g., economic aspects, culture, availability of IT courses in high school, work-life balance). Once enrolled, women found personal characteristics such as confidence, self-determination, and the ability to stand for themselves useful throughout the degree program. In addition, some women reported finding mentorship, role models, and a sense of belonging in the Women in CS group.

[1] NSF Science and Engineering Indicators. National Science Foundation (2018). Retrieved 15 December 2024 from https://nsf.gov/statistics/2018/nsb20181/report

[2] Fatourou, P., Papageorgiou, Y. & Petousi, V. Women are needed in STEM: European policies and incentives. *Communications of the ACM*, 62(4), 52-52 (2019).

Motivation

Despite increasing awareness and efforts to attract women to computing, they are still poorly represented in information technology (IT) careers [1]. The number of females graduating with an IT degree has consistently declined since 1984, when women were 34% of computer science graduates; women currently account for less than 20% of IT graduates in many countries [2]. In Germany, the percentage of women who graduate with a bachelor's degree in ICT was 19.6% in 2018 [3], an increase from 10% in 2000 [4] – however, this number is still low.

This lack of diversity in IT has repercussions for organizations and society. IT companies struggle to find a sufficiently skilled workforce, and increasing women's participation is a focus of attention [5]. While many approaches have been tried, progress has been slow.

This project aimed to identify and characterize initiatives that promote IT among female school students in Germany. It also aimed to take into account personal factors of influence, such as values, identity, and life mission.

Findings

During the project, we conducted interviews with students enrolled in IT degrees at TUM [6, 7]. Our research revealed that early exposure to IT can spark initial interest. This could be through exposure to programming in high school or different initiatives. In particular, among the programs run by TUM, women mentioned StudiumMINT (https://www.tum.de/en/studies/degree-programs/detail/studium-mint-certificate-zertifikat) in interviews as one of their early exposures to IT and as a motivation to enroll, as the quote below highlights:

"I did the StudiumMINT here at home just to get an overview of the possibilities, and I saw there were lectures that we could attend on games engineering, and that was the first time I even considered computer science."

However, apart from initiatives, a combination of other factors can influence women's decisions, including financial incentives for the foreseen jobs, perceived work-life balance, and social support. The role of family, friends, and IT high school teachers cannot be overstated. Additionally, personal attributes such as resilience empower women to overcome challenges and pursue their IT aspirations.

After they enroll in IT degrees at TUM, women credit the Women in CS group for helping them find a supportive community, a sense of belonging, and role models. Women also credit personal characteristics ▸

[3] Catalyst Women in Science, Technology, Engineering, and Mathematics (STEM): Quick Take (2020). Retrieved 8 November 2020 from www.catalyst.org/research/women-in-science-technology-engineering-and-mathematics-stem

[4] UNESCO. UNESCO science report: towards 2030 (2015). Retrieved 8 November 2020 from https://unesdoc.unesco.org/ark:/48223/pf0000235406

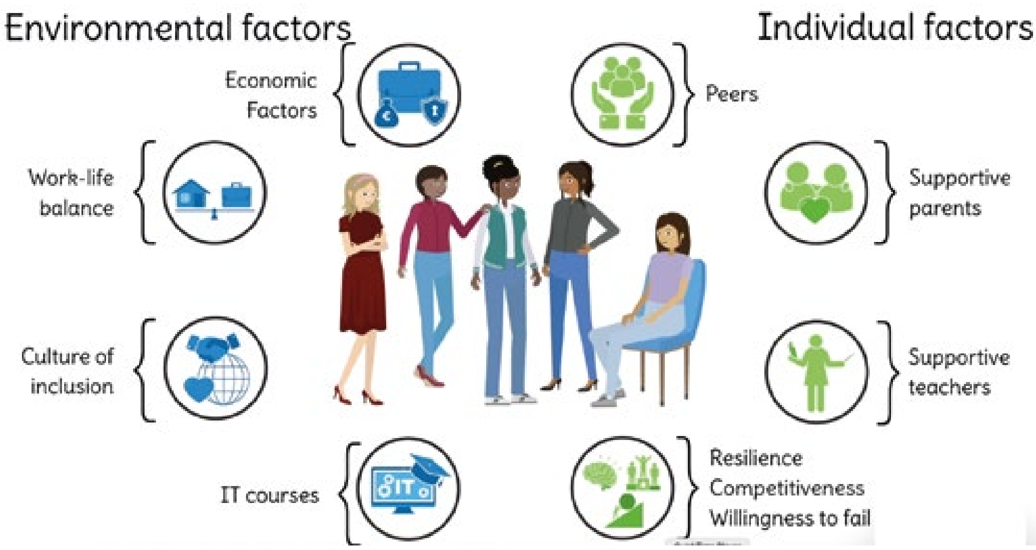

Fig. 1, Results summary.

such as confidence, self-determination, and assertiveness as being important for succeeding in their degrees.

Recommendations

On the basis of the results, we provided the following recommendations:

Information about courses should be easily accessible – we found out that some women only discover their interest in the field upon learning more about specific programs. This information can be disseminated through university websites, initiatives aiming to promote IT for high school students or as a career, and IT teachers.

Initiatives should prioritize programming experiences and opportunities to interact with university faculty. In addition, recognizing the crucial role parents play in shaping their children's career paths, involving parents in these initiatives could be beneficial for attracting more women to the field. After women enroll in the courses, initiatives that could help them find a supportive community and that introduce them to role models are useful for retention.

IT courses available in high school or earlier familiarize women with the field and might demystify some of the views of the IT field. However, when these courses are running, it is important to address unconscious biases among teachers, through training. In addition, care should be taken to ensure that these courses will not be a further alienating experience for women due to the low number of women attending.

Plans and suggestions for future research

The study was conducted with a limited sample of participants from TUM, and a larger sample is needed before the findings can be generalized. We are currently collecting data to compare the findings with UK and Bangladesh.

In close collaboration with Julia Pühl and Carine Khalil (TUM). ■

[5] Kiely, G. L., Heavin, C. & Lynch, P. Building a shared understanding of female participation in IT through collaboration: A shared mental model approach. *Journal of the Midwest Association for Information Systems*, Vol. 1, (2019).

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[7] Molnar, A. & Brüggemann-Klein, A. (2024).

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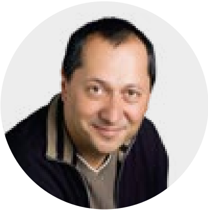
Molnar, A. & Stoilescu, D. Diversity initiatives for woman in IT: friends or enemies? *IEEE Technology and Society Magazine* 42 (3), 33-36 (2024).

For a full list of publications, please visit
www.ias.tum.de/ias/molnar-andreea-1

Focus Group: Machine Learning for Energy Analysis

Dr. Sani Nassif (Radyalis LLC), Alumnus Rudolf Diesel Industry Fellow |
Philipp Fengler (TUM), Doctoral Candidate
Host: **Prof. Ulf Schlichtmann (TUM)**



Dr. Sani Nassif

How can we model a circuit's power without knowing its structure?

Energy is crucial in integrated circuits and is determined by their implementation. Missing information in early design stages or for external designs limits the achievable accuracy of power models. We studied efficient data generation and precise machine learning methods to overcome this gap, and we identified the low variance of graph neural networks and the high accuracy of linear models for circuits. The results show potential for early power estimation.

Integrated circuits (ICs) are an integral part of our lives today. Used as microcontrollers in small household devices, as well as for high-performance computing clusters, the design of the circuits faces challenges including minimization of costs as well as safety and security requirements. Estimating the power dissipation of the final design is required to control many of these challenges. Power dissipation not only correlates directly with the operating costs of the IC, but also influences the optimality of the design due to safety margins. These margins are necessary to prevent damage and to maintain the correct functionality of the circuit. Power estimation is most accurate with resource-expensive methods in the late design stages. But modifications of the circuit at this stage are much more costly and negatively impact time to market. Therefore, precise power estimation at early design stages is of great importance.

Hierarchical IC design and limitations for power estimation

Due to the miniaturization of the fundamental element of digital ICs, the transistor, it is common to have circuits with billions of devices. Handling such complexity requires a high degree of automation and the reuse of existing components, and it mandates the use of a hierarchical approach. Fig. 1 shows an example of such a hierarchy for a smartphone on the left-hand side. Various functional blocks of the phone are packed into one integrated circuit, the system-on-chip, but need not be re-designed for every phone model and are often reused from a library of intellectual property (IP) blocks or sourced from external vendors. For example, the smartphone's central processing unit (CPU) may be obtained from a specialist for this circuit type, while a custom circuit to accelerate machine learning (ML) applications is designed in-house. Therefore, depending on the design stage of the circuit (block) and the information provided by external vendors, an IP block's actual structure and implementation may not be available and can be described as a black box.

Power dissipation of ICs has different sources. One dominant kind is dynamic power dissipation. It happens while charging and discharging capacitances within the circuit. Therefore, it is closely related to the change of signal values within the circuit, described by switching activity. While the functionality of the circuit (e.g., logic functions) already gives a basis for estimating the switching activity of an IC design, it may differ significantly from the final switching activity of a circuit. Due to the circuit's structure, signals can have different latencies, leading to switching events not captured by the functionality alone. Obtaining the switching activity of an IP block for its final stage is required to enable highly accurate dynamic power estimates.

Fig. 1 on the right-hand side qualitatively shows the limitations of power estimation accuracy on black-box designs. The missing information on the circuit structure in early design stages or for IP blocks from external providers also limits the achievable accuracy. Our Focus Group investigated the opportunities that data-driven approaches such as ML provide to overcome the lack of information here. Recent research has also focused on power dissipation becoming more influential not only for small battery-based devices, but also in large server clusters. In addition, ma-

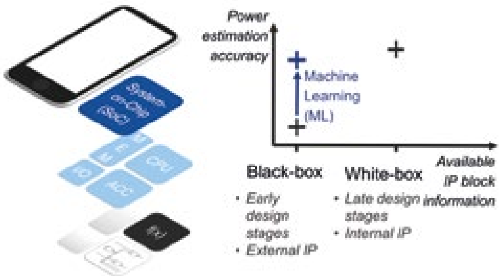


Fig. 1, Hierarchical integrated circuit design and influence on power estimation accuracy.

chine learning, such as graph neural networks (GNN), shows promising results. For example, GRANNITE [1] shows that a data-driven switching activity model can be applied to various circuit types. However, it is based on detailed information about the structure of the circuit and hence is not applicable to our use case.

Data-driven power modeling for black-box circuits

As diverse as the applications of ICs are today, the approaches to performing power estimation are just as diverse. For ML-based methods, existing circuit designs must be characterized by their power dissipation behavior. Measurements, simulation, and statistical methods have been used here [2]. At the beginning of the Fellowship program of our Focus Group, we identified suitable available circuit designs and power estimation frameworks to generate data. As researchers have investigated the power consumption of ICs for decades, we first focused on using available domain knowledge on power dissipation to ►

[1] Zhang, Y., Ren, H. & Khailany, B. GRANNITE: Graph neural network inference for transferable power estimation. *2020 57th ACM/IEEE Design Automation Conference (DAC)*, 1–6 (2020).

[2] Nasser, Y., Lorandel, J., Prévotet, J. C. & Hélard, M.. RTL to transistor level power modeling and estimation techniques for FPGA and ASIC: A survey. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems* 40(3), 479–493 (2020).

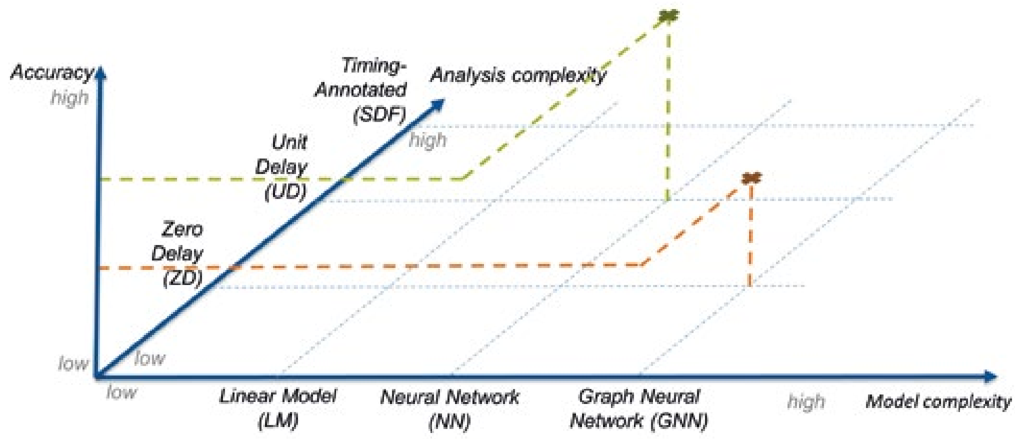


Fig. 2, Qualitative overview of circuit analysis and power modeling complexity space.

[3] Willard, J., Jia, X., Xu, S., Steinbach, M. & Kumar, V. Integrating physics-based modeling with machine learning: A survey. *arXiv preprint arXiv:2003.04919* 1(1), 1–34 (2020).

develop suitable modeling methods. This fusion is often referred to as physics-based or -informed ML [3]. We investigated the design of neural network-based modeling using the theoretic knowledge of power dissipation of ICs. However, due to limited knowledge of the circuit design in our black-box scenario, such a physics-based, i.e., in our case, circuit structure-based, approach is barely applicable.

Therefore, we moved our focus to identifying the most suitable data-driven approach for early-stage and black-box circuit designs. Modern integrated circuits can contain billions of transistors. Therefore, the modeling approach has to be suitable for dealing with very many circuit signals. This results in a decision for the modeling method and how to obtain the data to fit the model. Fig. 2 shows this decision space qualitatively. Circuit analysis by simulation can be done using different timing models (where “zero delay” means, for example, that circuit propagation delays are not considered). On the other hand, different modeling approaches will result in different obtainable accuracies. If both dimensions are combined, the actual accuracy of a modeling framework can be assessed. Within this project, we have set up the framework to investigate the different choices for precise power estimation. This research has shown that a simpler timing model for circuit analysis, such as unit delay, can also provide high accuracy in early design stages. Furthermore, for many circuit designs, a simple linear regression shows accuracy comparable to more complex approaches under the assumption of limited structural information about the circuit. However, overall, the variance of accuracy was smaller for a more complex graph neural network. We presented these results at the ISQED conference and received the Best Paper Award for this work.

Solving the puzzle of transferable power dissipation modeling

Based on these results, we have identified further research questions. The GNN results also show that transferability (i.e., one model for different circuits) can be achievable for black-box circuits. This results in the need for a large number of diverse circuit designs. For research purposes, the number of available circuits is limited. Here, the automatic generation of artificial circuit designs is suitable. We have developed a concept to generate circuit designs with diverse power dissipation behavior to enable the development of transferable ML-based models. Furthermore, the designs must be simulated with diverse workloads to obtain sufficient switching activity data. The unit delay timing model has shown potential here but needs an efficient simulation tool. With bachelor's and master's degree students, we investigated the opportunities to develop a simple yet fast unit delay simulator using graph processing units. In addition, our project has shown that simple linear regression is helpful for power estimation in early design stages. Therefore, we are investigating hybrid models for simple yet transferable power estimation.

While the Rudolf Diesel Industry Fellowship of Sani Nassif at TUM-IAS is finished, the members of our Focus Group continue to work on these still open research questions to obtain highly accurate power estimation of digital ICs under limitations such as unknown circuit structure. ■

Selected publications

Fengler, P., Nassif, S. & Schlichtmann, U. Toward Early Stage Dynamic Power Estimation: Exploring Alternative Machine Learning Methods and Simulation Schemes. *2024 25th International Symposium on Quality Electronic Design (ISQED)*, pp. 1–8 (2024).

Fengler, P., Chen, J. Nassif, S. & Schlichtmann, U. Enabling Machine Learning for Power Modeling via Artificial Netlist Generation. *Accepted by: 2025 IEEE International Symposium on Circuits and Systems (ISCAS).*

For a full list of publications, please visit
www.ias.tum.de/ias/nassif-sani

Focus Group: Scientific Machine Learning

Prof. Wil Schilders (Eindhoven University of Technology), Alumnus Hans Fischer Senior Fellow (funded by the Siemens AG) | **Chinmay Datar (TUM),** Doctoral Candidate
Host: **Prof. Hans-Joachim Bungartz (TUM)**

Prof. Wil Schilders

Training neural networks without back-propagation

Finding neural network architectures and training networks pose big challenges in machine learning. We unravel novel architectures and propose new algorithms for training our neural networks. Particularly, our training algorithms do not rely upon gradient-based iterative optimization. We focus on solving time-dependent differential equations, both linear and nonlinear, using our neural networks.

Motivation and focus of the work:

Differential equations model diverse phenomena, from quantum systems to celestial motion, making the approximation of partial differential equations (PDEs) central to computational science. Traditional mesh-based methods such as finite differences, volumes, and elements are well established but face challenges with complex domains and high-dimensional problems. Artificial neural networks offer a promising, mesh-free alternative with high expressivity, the ability to handle high dimensions, and advanced tools for automatic differentiation. Yet significant challenges remain:

1) Finding appropriate neural network architecture: This typically involves extensive experimentation with a lot of trial and error and dealing with a high-dimensional hyper-parameter space, which can often entail significant computational costs.

2) Difficulties in training neural networks: The most pressing challenges in training neural networks are vanishing and exploding gradients, long training times, low accuracy, and inability to capture high-frequency temporal dynamics in the functions to be approximated.

The focus of our work has been on dealing with the two challenges outlined above.

Summary of the work carried out:

We categorize our work in three primary directions – (1) systematic construction of continuous-time neural networks, (2) sampling weights of deep neural networks, and (3) solving partial differential equations with sampled neural networks. Next, we summarize our contributions in each direction.

Systematic construction of continuous-time neural networks:
We developed a systematic method to design neural architectures for linear time-invariant (LTI) systems. [1] Using a variant of continuous-time neural networks, where neuron outputs evolve as solutions of first- or second-order ODEs, we introduced a gradient-free algorithm to compute sparse architectures and parameters directly from the LTI system. Our novel design features “horizontal hidden layers," in contrast to conventional "vertical” architectures, which may be less effective. We derived an upper bound for numerical errors and showcased the superior accuracy of our networks on various examples, including the 2-D diffusion equation (see Figs. 1 and 2).

Sampling weights of deep neural networks (supervised learning):
In this direction, we first developed an algorithm for constructing neural network parameters by sampling them from certain data-driven distributions so that iterative updates are no longer necessary to obtain a trained network. [2] We demonstrated that the sampled networks achieve accuracy comparable to iteratively trained ones but can be constructed orders of magnitude more rapidly.

Solving partial differential equations with sampled neural networks (self-supervised learning):
We extended our work on sampling network parameters to the setting of self-supervised machine learning problems in which one seeks to solve partial differential equations using neural network ansatz. [3] In this project, we addressed the challenges in training neural-PDE solvers and presented an approach to constructing special neural architectures and training our networks without back-propagation by integrating two key ideas: separation of space and time variables and random sampling of weights and biases of the hidden layers. We reformulate the ▸

[1] Datar, C., Datar, A., Dietrich, F., & Schilders, W. (2024a); Datar, C., Datar, A., Dietrich, F. & Schilders, W. (2024b).

[2] Bolager, E. L., Burak, I., Datar, C., Sun, Q., & Dietrich, F. (2023).

[3] Datar et al. (2024).

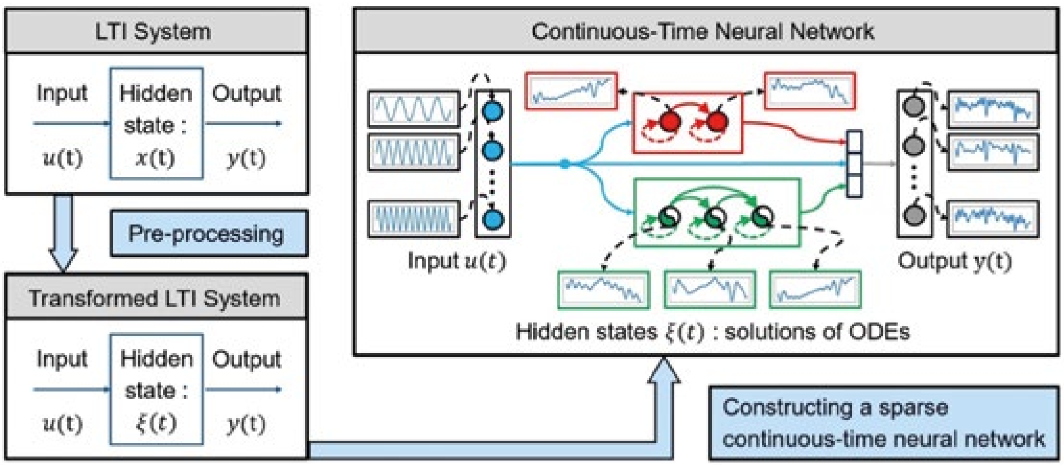


Fig. 1, Illustration of the systematic construction of continuous-time neural networks from linear time-invariant (LTI) systems: We also show the architecture of our continuous-time neural network with two horizontal hidden layers (marked in red and green). The states of neurons in the hidden layers are solutions of either first-order ODEs (red solid balls) or second-order ODEs (green yin-yang balls) (from Datar, C., Datar, A., Dietrich, F., & Schilders, W. 2024a).

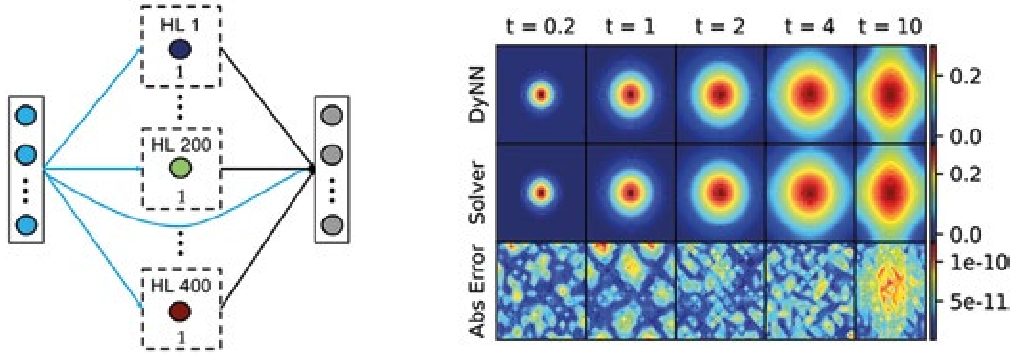


Fig. 2, Left: DyNN architecture. Right: Diffusion equation: DyNN solution (top panel), numerical solution (middle panel), absolute error between the two solutions at five different time instants (bottom panel) (from Datar, C., Datar, A., Dietrich, F., & Schilders, W. 2024a).

[4] Rahma, A., Datar, C. & Dietrich, F. (2024).

[5] Datar, C., Datar, A., Dietrich, F., & Schilders, W. (2024a); Datar, C., Datar, A., Dietrich, F. & Schilders, W. (2024b).

[6] Datar et al. (2024); Rahma, A., Datar, C. & Dietrich, F. (2024).

PDE as an ordinary differential equation (ODE) using a neural network ansatz, construct neural basis functions only in the spatial domain, and solve the ODE leveraging classical ODE solvers from scientific computing. See Fig. 3 for an illustration of our approach. We later extended this work and used neural network ansatz to parameterize Hamiltonian functions of energy-conserving systems [4].

Impact of the project:
Our work with continuous-time neural networks streamlines neural architecture design, reducing trial-and-error and cutting computational costs. These ideas can extend to embedding physics, such as two-body problem solutions, for approximating gravitational N-body systems. Sparse architectures are crucial for fast inference in edge computing, low-energy hardware, and real-time applications.

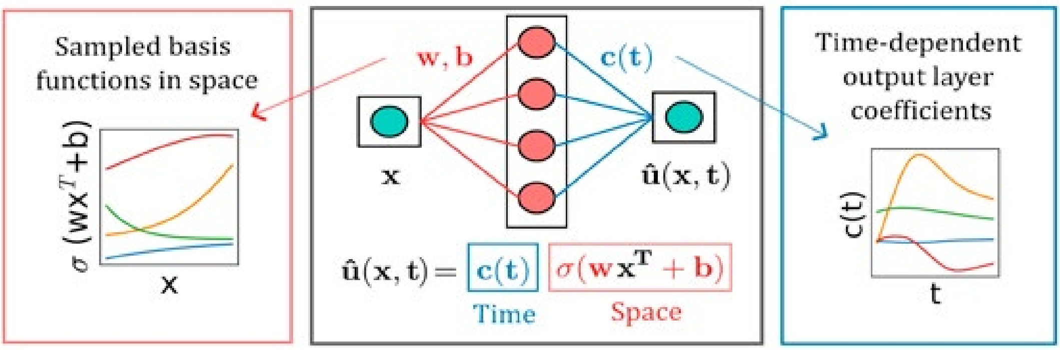


Fig. 3, Solving a time-dependent PDE with a neural network ansatz: We sample hidden-layer parameters (w,b) and fix the neural spatial basis functions (left). The PDE is reformulated as an ODE in terms of the time-dependent output layer coefficients c(t) (right), obtained by solving the ODE and computing the solution û (x,t) (from Bolager, E. L., Burak, I., Datar, C., Sun, Q., & Dietrich, F. 2023).

Our back-propagation-free algorithm outperforms gradient-based optimization in physics-informed neural networks, achieving faster training and greater accuracy – by up to five orders of magnitude. This enables neural PDE solvers to tackle complex real-world problems, overcoming challenges of limited accuracy and lengthy training times.

Future work:

The final outcomes of the project will serve as stepping-stones for multiple research directions in the future. We intend to extend our work with systematic construction of neural architectures [5] for more challenging classes of dynamical systems such as linear parameter-varying (LPV) systems, classes of parabolic PDEs with quadratic nonlinearities such as Burgers' equation, and, ultimately, more involved nonlinear dynamical systems. We intend to extend our work in the direction of back-propagation-free neural PDE [6] solvers to gray-box settings and inverse problems, where parts of the PDE must be estimated, and high-dimensional problems with complicated solutions. We already have promising initial results in both directions and intend to publish these results in the coming months.

Final workshop

To mark the end of the Fellowship, a workshop was organized by Wil Schilders and Dirk Hartmann (Siemens): "Advancing scientific machine learning in industry." The workshop was very well attended (> 120 participants), a considerable number from industry. The two-day workshop also had a panel discussion with panel members from different industries, and a working dinner to discuss a number of challenges faced in the area of scientific machine learning. This has led to a white paper that has been distributed to all participants and can serve as a starting point for further collaborations in the field of scientific machine learning.

In close collaboration with Prof. Felix Dietrich (TUM) and Dr. Dirk Hartmann (Siemens AG). ■

Selected publications

Datar, C., Datar, A., Dietrich, F., & Schilders, W. Systematic construction of continuous-time neural networks for linear dynamical systems. *arXiv preprint arXiv:2403.16215* (2024a) (Accepted: SIAM Journal of Scientific Computing (SISC)).

Datar, C., Datar, A., Dietrich, F. & Schilders, W. Continuous-time neural networks for modeling linear dynamical systems. In *ICLR 2024 Workshop on AI4DifferentialEquations In Science*. (2024b).

Bolager, E. L., Burak, I., Datar, C., Sun, Q., & Dietrich, F. Sampling weights of deep neural networks. *Advances in Neural Information Processing Systems* 36 (2023): 63075-63116.

Datar et al. Solving partial differential equations with sampled neural networks. *arXiv preprint arXiv:2405.20836* (2024). (Under review: International Conference of Learning Representations (ICLR)).

Rahma, A., Datar, C. & Dietrich, F. Training Hamiltonian neural networks without backpropagation. *arXiv preprint arXiv:2411.17511* (2024) (Accepted: Machine Learning and the Physical Sciences Workshop at NeurIPS 2024).

For a full list of publications, please visit
www.ias.tum.de/ias/schilderswil

Focus Group: Photophysics and Electronic Structure of Metal-Organic Frameworks

Prof. Natalia Shustova (University of South Carolina), Alumna Hans Fischer Fellow |
Johanna Haimerl (TUM), Doctoral Candidate
Host: **Prof. Roland Fischer (TUM)**

Prof. Natalia Shustova

Photophysics and electronics of hybrid materials for energy-related applications

The TUM-IAS Fischer Fellowship allows for building a multidisciplinary energy-related program between the Shustova (USA) and Fischer (TUM) groups, resulting in 24 publications in the top chemistry journals, including Nature Communications and Nature Chemistry. As a result of productive collaboration, Prof. Shustova was selected as a recipient of the Bessel Research Award from the Humboldt Foundation.

Breakthroughs in hybrid material performance for energy-related applications

Outcomes of the fruitful interdisciplinary program between the Fischer and Shustova research groups built due to the TUM-IAS Hans Fischer Fellowship resulted in 24 publications, as well as the mentorship of the graduate student Johanna Haimerl, whose graduation is expected in 2025. The results acquired due to the TUM-IAS Fellowship laid the groundwork for Prof. Shustova receiving the following awards during the Fellowship period: the competitive Friedrich Wilhelm Bessel Research Award from the Alexander von Humboldt Foundation and the Russell Research Award.

Development of on-demand-activated drug delivery platforms, photochromic heterogeneous catalysts, molecular motors, recyclable and healable materials, artificial muscles, multilevel anticounterfeiting and information encryp-

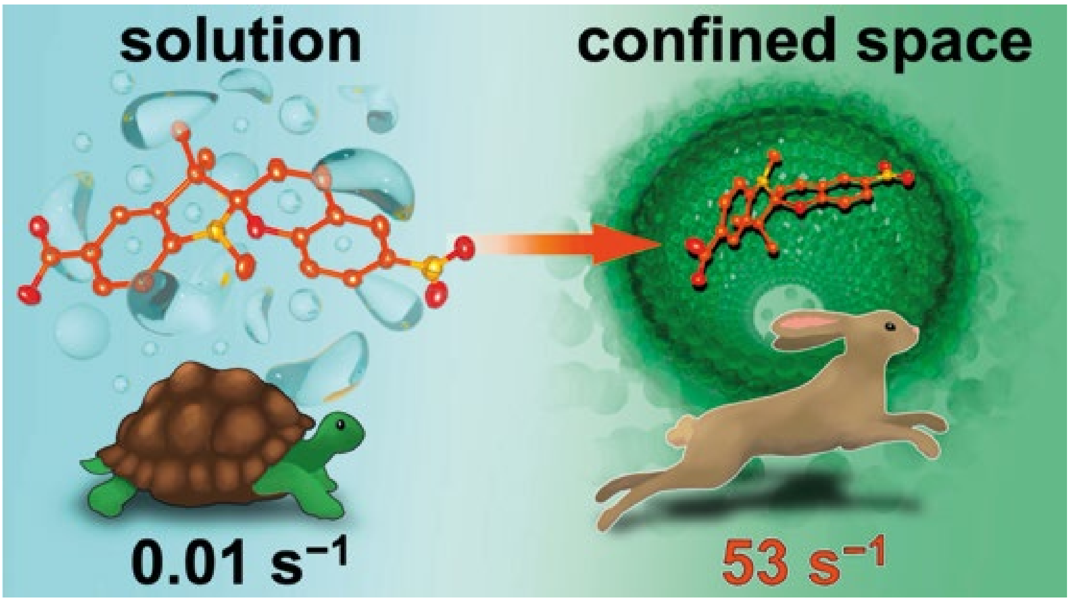


Fig. 1, A schematic representation of the fundamental concept demonstrating ~5,000-fold enhancement in the photoisomerization rate through confined evacuated space of the porous matrix (i.e., metal-organic framework).

tion systems, and tailorable supercapacitors fully relies on fast changes between distinct states occurring in the solid state. Therefore, as a part of the Fellowship, we studied rapid switching between two (or more) discrete states in the solid state, which is a cornerstone for the technological development of devices based on stimuli-responsive materials. It could be anticipated that the forthcoming breakthroughs in artificial muscles, supercapacitors, and especially optoelectronics would critically hinge on substantial improvements in existing switching rates of stimuli-responsive building blocks. However, even in solution, where the molecules exhibit more degrees of freedom in comparison with the solid state, the rates of such processes are typically varied from 10^{-5} to 10^{0} s^{-1} using light as an external stimulus. By utilizing solvent polarity and viscosity as variables, the speed of the photoisomerization process can be enhanced, but typically within one order of magnitude. In the solid state, ▸

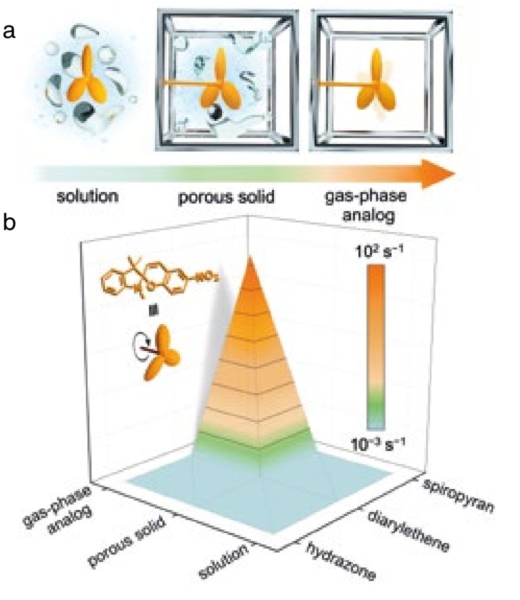


Fig. 2, Breakthrough in the photoisomerization speed limit, a critical aspect in the material design, achieved through the integration of a photochromic molecule (orange propeller) within the evacuated porous hybrid materials (a), a novel concept developed due to the Shustova-Fischer collaboration. (b) Comparison of the achieved isomerization rate constants (depicted by the orange color) with the values previously reported in the literature (shown in blue and green colors).

switching between distinct states is usually further constrained compared to solutions due to close packing, π-π stacking, or hydrogen-bonding interactions, especially for molecules for which isomerization is accompanied by large structural transformations or formation of zwitterionic species (e.g., spiropyran).

Due to fruitful collaborations between the Shustova and Fischer groups, we were able to report a breakthrough in the isomerization speed limit of photochromic molecules on the example of sterically-demanding spiropyran derivatives, achieved through the employment of a conceptually novel strategy, allowing for not only precise control of photoswitch environment (e.g., solvent-free) but also environment tunability due to matrix modularity (Figs. 1 and 2). Furthermore, this approach led to a drastic enhancement of photoswitch isomerization ability in the solid state, addressing challenges associated with limited photoisomerization due to strong intermolecular interactions typically pronounced in the solid state and impeding the development of stimuli-responsive materials.

To the best of our knowledge, such a rapid response observed in the solid state, through the integration of spiropyran derivatives into the confined solvent-free space of rigid frameworks, has no analogs for these classes of photoswitches either in solution or in the solid state. While slight enhancements in photoisomerization rate could be anticipated and achieved using organic solvent as a parameter, the presented conceptually different approach, realized through construction of the spiropyran environment, results in ~1,000 times switching enhancement even in the solid state compared to its behavior in solution, setting a record in the field of photochromic compounds (Fig. 1). Using spectroscopic analysis in combination with photophysical measurements and theoretical modeling, we shed light on the mechanism of possible rapid photoisomerization. Thus, the strategic design of light-responsive materials has resulted in rate enhancement that surpasses the preconceived “speed limit” for the commonly used classes of photoswitches, including but not limited to spiropyran-, diarylethene-, and hydrazone-based photochromic derivatives (Fig. 2). Furthermore, the approach we developed allows for the integration of more than one type of photochromic molecule within the same platform, providing access to the development of solid-state materials with a very broad dynamic range of photoisomerization rates (Fig. 3).

To summarize one of the outcomes achieved during the Fellowship period, the presented conceptual approach, realized through the construction of the spiropyran environment, sets the record in the field of photochromic materials. Moreover, the integration of two distinct photochromic moieties in the same framework provided access to a dynamic range of rates as well as complementary switching in the material's optical profile, uncovering a previously inaccessible pathway for interstate rapid photoisomerization. This concept is a critical component for the development of a forthcoming generation of materials, including recyclable and healable systems, artificial muscles, photochromic heterogeneous catalysts, and tailorable supercapacitors that all rely on the fundamental concept of rapid switching between two or more discrete forms in the solid state. ■

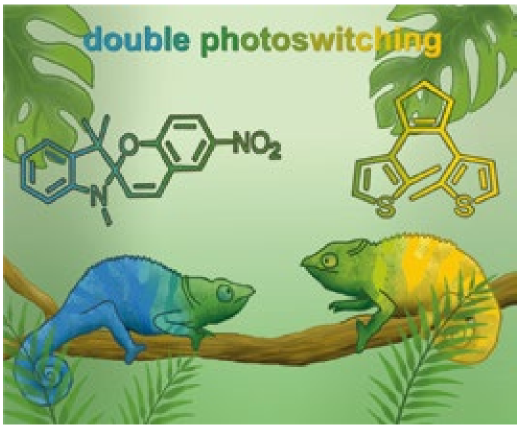


Fig. 3, Like two color-changing chameleons coming face to face, the integration of two distinct stimuli-responsive moieties within the same metal-organic material results in the synergistic behavior of two spiropyran and diarylethene derivatives (both structures are highlighted). Perturbation of the chameleons' environment upon a different external stimulus breaks the synergy, promoting their orthogonal behavior, a concept developed due to the Shustova-Fischer collaboration, highlighted on the example of a novel hierarchical photo-thermo-responsive metal-organic framework.

Selected publications

Stanley, P. M., Haimerl, J., Shustova, N. B., Fischer, R. A. & Warnan, J. Merging Molecular Catalysts and Metal-Organic Frameworks for Photocatalytic Fuel Production. *Nat. Chem.* 14, 1342–1356 (2022).

Thaggard, G. C. et al. Breaking the Photoswitch Speed Limit. *Nat. Commun.* 14, 7556 (2023).

Wilson, G. R. et al. Cooperative and Orthogonal Switching in the Solid State Enabled by Metal-Organic Framework Confinement Leading to a Thermo-Photochromic Platform. *Angew. Chem. Int. Ed.* 62, e202308715 (2023).

Thaggard, G. C. et al. Metal-Photoswitch Friendship: From Photochromic Complexes to Functional Materials. *J. Am. Chem. Soc.* 144, 23249–23263 (2022).

Thaggard, G. C., Haimerl, J., Fischer, R. A., Park, K. C. & Shustova, N. B. Traffic Lights for Catalysis: Stimuli-Responsive Molecular and Extended Catalytic Systems. *Angew. Chem. Int. Ed.* 62, e202302859 (2023).

For a full list of publications, please visit
www.ias.tum.de/ias/shustova-natalia-b

Focus Group: Human-in-the-loop Ocean Robotics

Prof. Leila Takayama (University of California, Santa Cruz, *now Hoku Labs and Robust.AI*), Alumna Hans Fischer Fellow (funded by the Siemens AG) |
Srini Lakshminarayanan (TUM), Doctoral Candidate
Host: **Prof. Sami Haddadin (TUM, *now Mohamed bin Zayed University of Artificial Intelligence*)**

Prof. Leila Takayama

Enabling more people to teleoperate ocean robots

Our Focus Group tackled the design challenges of enabling remote robot operations on land and at sea, using a multidisciplinary approach of robotic controls and human-robot interaction. We developed ways to reduce the cost and improve access to robot teleoperation interfaces, enabling very remote operators to perceive visual, auditory, and force-feedback information from robotic manipulators.

The problem:

Our understanding of the oceans has long been limited by our ability to access ocean depths, which are extremely dangerous for human bodies. There are some oceanographic institutes that can afford to deploy research vessels with ocean robot technologies, but they are few and far between. Performing deep sea navigation and manipulation tasks with these remotely operated vehicles (ROVs) is cognitively extremely demanding, even for the most talented pilots. Ocean science missions are incredibly diverse, e.g., producing 3-D maps of the sea floors, gathering geological samples, recording video of ocean creatures rarely or never before seen, and delicately sampling living creatures from the midwater.

Research goals:

These challenges inspired our Focus Group's research program. How might we make it easier for ROV pilots to perform their remote manipulation tasks, expanding the pool of future robot operators? Even better, what if we could also make this possible for ocean robots operated without tethers, enabling people to fly ROVs more freely and possibly even from shore?

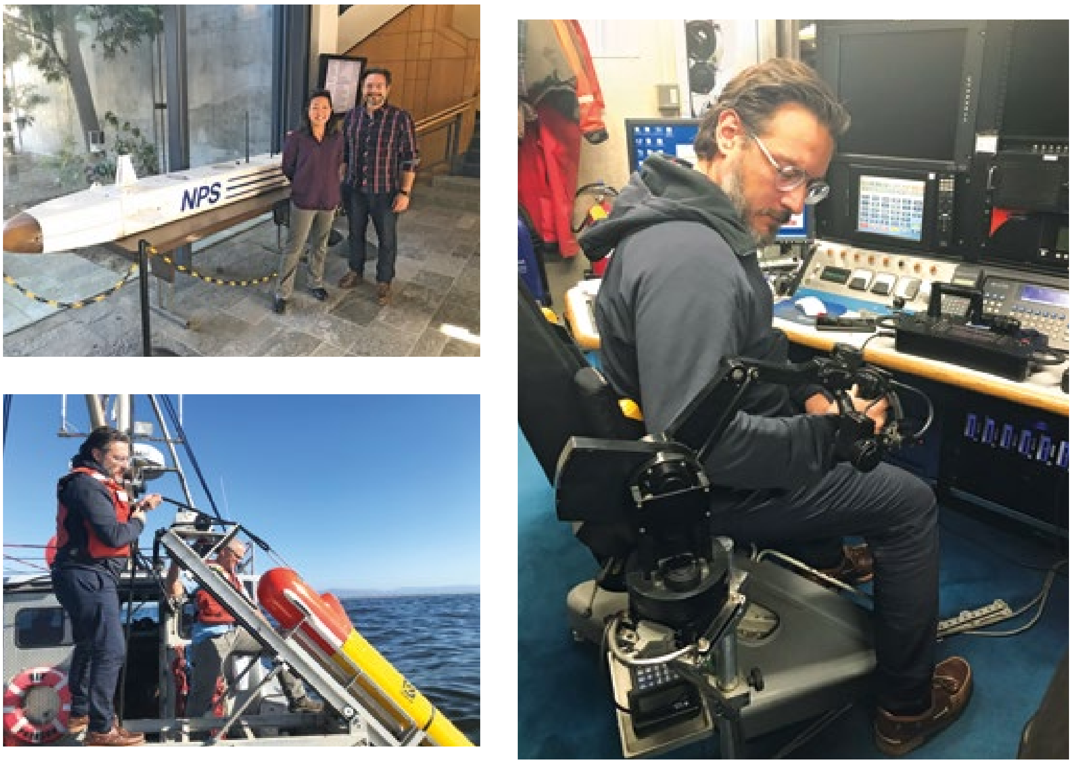


Fig. 1, Sami Haddadin visited multiple oceanographic research institutes with Leila Takayama, trying their teleoperation controls for ROVs, launching AUVs, and meeting ocean robotics scientists and engineers © Leila Takayama.

Our approach:

Using a multidisciplinary approach, we leveraged our expertise in robotics controls, cognitive psychology, and human-robot interaction to develop prototypes for our ocean science and engineering collaborators at the Monterey Bay Aquarium Research Institute (MBARI). We observed and interviewed ROV pilots and users of MBARI's telepresence systems, designed and built prototypes of robot teleoperation interfaces for remotely operating robots, and conducted empirical studies of our prototype as well as other robot operation interfaces to evaluate their performance and identify fruitful directions for future research. ▸

[1] Crosby, A., et al. (2024).

1. Understanding ocean robot piloting

Sami Haddadin visited MBARI and the US Naval Postgraduate School with Leila Takayama to get a hands-on feel for how they operate their ocean robots (Fig. 1). Subsequently, our Focus Group observed ROV piloting sessions and interviewed users of MBARI's research vessel telepresence systems (2019–2022), including ocean scientists, ship's crew, and ROV pilots [1]. We learned that ROV piloting is incredibly challenging, especially with the current interfaces that occupy the ROV control rooms. To effectively fly ROVs, it is critical for robot operators to have sufficient situation awareness, e.g., deciding how hard to push the sampler on the sea floor, figuring out how far forward to reach to capture the jellyfish, or managing the tension on the tether that connects the ROV to the ship.

2. Exploring force feedback for ocean robot operators

While the gold standard for robot teleoperation uses high-precision force-feedback input devices, we took a low-cost approach to en-

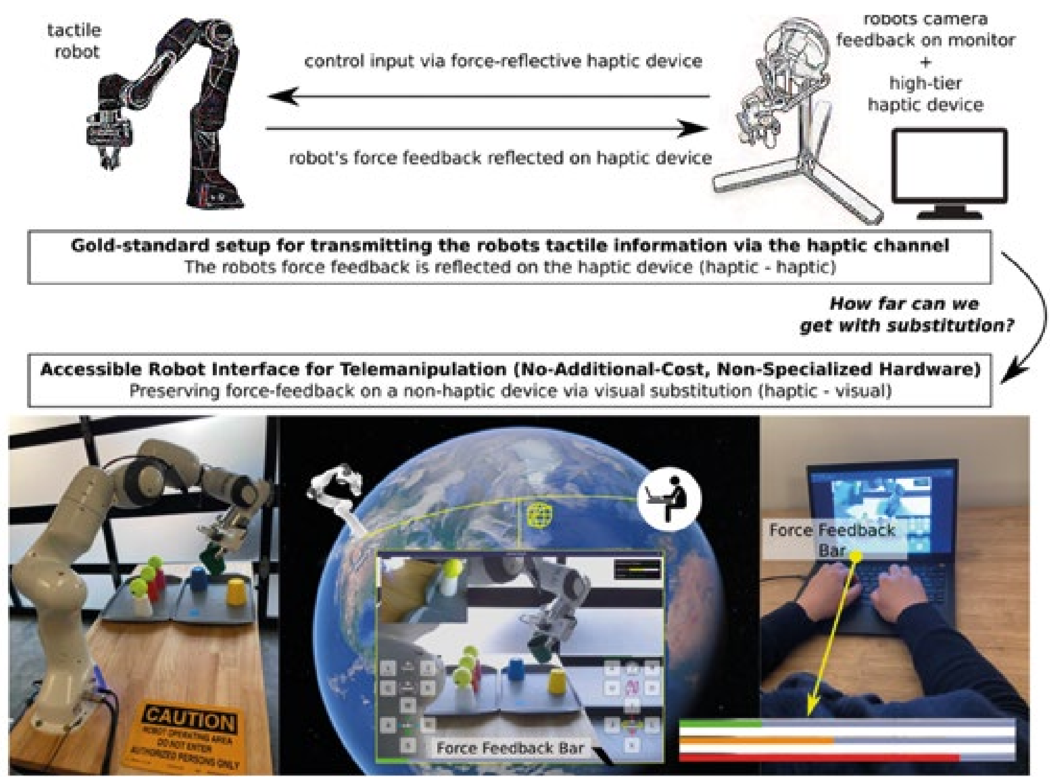


Fig. 2, Our Accessible Robot Interface for Telemanipulation (A-RIFT) offers visual, auditory, and force-feedback information to remote people via low-cost personal computing hardware © TUM MIRMI (Moortgat-Pick, A., So, P., Sack, M.J., Cunningham, E.G., Hughes, B.P., Adamczyk, A., Sarabakha, A., Takayama, L., Haddadin, S. A-RIFT: visual substitution of force feedback for a zero-cost interface in telemanipulation. *2022 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, 3926-3933 (2022).)

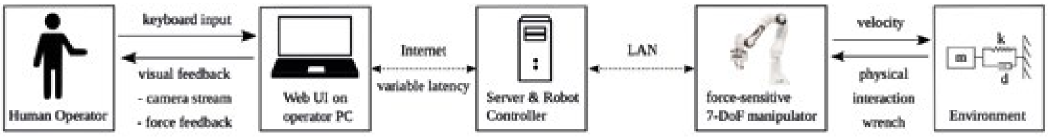


Fig. 3, A-RIFT hardware, software, and network configuration © TUM MIRMI (Moortgat-Pick, A., So, P., Sack, M.J., Cunningham, E.G., Hughes, B.P., Adamczyk, A., Sarabakha, A., Takayama, L., Haddadin, S. A-RIFT: visual substitution of force feedback for a zero-cost interface in telemanipulation. *2022 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, 3926-3933 (2022).)

hance the potential for increasing access to these types of jobs, using widely available personal computer hardware and software [2] (Figs. 2 and 3). Because people cannot feel force feedback with their home computing devices, we experimented with communicating force information through other modalities (e.g., visual and auditory). For our user study, we decided to use a visual bar at the bottom of their video display in the web browser, which became longer and redder when the robot arm experienced higher forces. In our user study, participants in Munich operated a robot arm on the TUM campus (slightly remote) and also operated a robot arm in Santa Cruz, California (very remote), flipping plastic cups and placing balls into those cups on a table. As expected, people performed better (i.e., placed more balls into cups) when operating the nearby robot than the very remote robot. When operating the very remote robot, people made fewer errors when they saw force feedback in the visual bar than when they were not presented with the visual bar. From this user study, we learned that visually rendered force-feedback information could improve very remote teleoperation of robot manipulators. This inspired us to explore other modes of sensory remapping (e.g., force information communicated via sounds, and depth information communicated via stereoscopic images [3]). ▸

[2] Moortgat-Pick, A. et al. (2022).

[3] Elor, A. et al. (2021).

Fig. 4, Alex Moortgat-Pick and Sami Hadaddin demonstrating A-RIFT to Bavarian Minister-President Markus Söder and Bavarian Science Minister Markus Blume, who remotely operated the Franka Panda robot in Santa Cruz, California, from Munich (2022) © TUM MIRMI.

[4] Lakshminarayanan, S. et al. (2024).

3. Enabling ocean robots to estimate forces

While our initial work was conducted on land, our follow-up studies were conducted underwater. Detecting forces experienced by ocean robots is especially challenging because there are many sources of strong forces to consider, including ocean currents and the robot's tether. We investigated whether we could use current machine learning techniques to estimate forces on these ocean robots, using inertial measurement units (IMUs) on a relatively low-cost BlueROV in a TUM laboratory test tank [4]. Our model-based approach outperformed other methods (e.g., support vector regression, bidirectional encoder representations from transformer) for estimating the forces being experienced by the ROV. This groundwork can be used to enable more autonomous behaviors such as collision avoidance, even when there is high latency in the connections between remote operators and the ROVs. It can also be used as a sensory information channel for robot pilots.

Future work:
Thanks to the support of the TUM-IAS Fellowship, our Focus Group has built collaborative relationships across continents and institutions, enabling us to expand the capabilities of ocean exploration teams. The results of our initial studies have demonstrated that we can improve situation awareness for robot operators by leveraging different perceptual channels. Furthermore, we might be able to estimate the forces being experienced by these ocean robots so that we can convey that information to robot operators as well as use that information for enabling more autonomous on-board capabilities. Whenever possible, we used low cost, widely available sensors and input devices (e.g., personal computers, gaming VR headsets, IMUs) so that the results of our work can be more readily accessed, used, and built upon by our broader research communities.

In close collaboration with Emma G. Cunningham (UW Madison), Michael J. Sack (Cornell University), and Benjamin P. Hughes, Kevin Weatherwax, Alison Crosby (all University of California, Santa Cruz) and Peter So, Alexander Moortgat-Pick, Anna Adamczyk, Dr. Daniel-Andre Dücker (all TUM), and Prof. Andriy Sarabakha (Aarhus University).

Video of Leila Takayama's
Munich i_presentation:
www.youtube.com/watch?v=eldm-IrowYY ■

Selected publications

Lakshminarayanan S., Duecker, D., Sarabakha, A., Ganguly, A., Takayama, L. & Haddadin, S. Estimation of external force acting on underwater robots. *2024 IEEE 20th International Conference on Automation Science and Engineering (CASE)*, 3125-3131 (2024)

Moortgat-Pick, A., So, P., Sack, M.J., Cunningham, E.G., Hughes, B.P., Adamczyk, A., Sarabakha, A., Takayama, L. & Haddadin, S. A-RIFT: visual substitution of force feedback for a zero-cost interface in telemanipulation. *2022 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, 3926-3933 (2022).

Crosby, A., Takayama, L., Martin, E.J., Matsumoto, G.I., Kakani, K. & Caress, D.W. Beyond bunkspace: telepresence for deep sea exploration. *2024 IEEE Conference on Telepresence*, 16-23 (2024).

Elor, A., et al. Catching jellies in immersive virtual reality: a comparative teleoperation study of ROVs in underwater capture tasks. Proceedings of the *27th ACM Symposium on Virtual Reality Software and Technology*, 1-10 (2021).

For a full list of publications, please visit
www.ias.tum.de/ias/takayama-leila

Focus Group: Visual Computing

Prof. Luisa Verdoliva (University Federico II of Naples), Hans Fischer Senior Fellow | **Artem Sevastopolsky (TUM),** Doctoral Candidate
Host: **Prof. Matthias Nießner (TUM)**

Prof. Luisa Verdoliva

Toward more general deepfake detection through anomaly-based analysis

This project aims to develop new methods for the creation and detection of synthetic media, also known as deepfakes, with the goal of improving the ability to generalize against novel AI-generative models. The approach focuses on detecting fakes by understanding the characteristics of authentic content and identifying manipulations as anomalies deviating from the real class.

[1] Cozzolino, D., Rössler A., Thies, J., Nießner M. & Verdoliva, L. ID-Reveal: Identity-aware DeepFake Video Detection. *IEEE/CVF International Conference on Computer Vision (ICCV)*, 15108-15117 (2021).

[2] Cozzolino, D., Pianese, A., Nießner, M. & Verdoliva, L. Audio-Visual Person-of-Interest DeepFake Detection. *IEEE Conference on Computer Vision and Pattern Recognition (CVPR) Workshops*, 943-952 (2023).

Thanks to the rapid progress in AI-generated media, creating false images and videos with a high level of realism has become very easy. Coupled with ubiquitous social networks, this allows for the viral dissemination of fake news and raises serious concerns about the trustworthiness of digital content in our society. Traditional methods for verifying data authenticity are typically supervised and require very large training datasets that include both real and fake samples. A main issue is that new methods for generating synthetic data are proposed by the day, and such approaches cannot generalize to new generative models not included in the training set.

The goal of this project is to fill this gap and propose an approach that ensures generalization. Instead of relying on labeled real and fake data, we use only pristine samples, treating manipulations as anomalies relative to a learned model that captures the natural statistics of real-world imagery. Our collaborative efforts have focused on the following areas: detecting facial manipulations in videos, including face generation and recognition, as well as identifying AI-generated content in images.

To advance research in this field, we have been organizing a Workshop on Media Forensics at CVPR since 2021. The workshop has been a successful event and gave us the possibility to bring together researchers, foster collaboration, and benchmark progress in deepfake detection.

Identity-based deepfake video detection

Our key insight is that each person has specific characteristics that a synthetic generator likely cannot reproduce. Hence, the approach focuses on learning an individual's biometrics, particularly their unique facial motion patterns, to detect potential inconsistencies. This represents a paradigm shift from traditional supervised methods. Instead of addressing the problem "Is this video real or fake?" our goal is to answer the question "Is this the person they claim to be?" – thus emphasizing person-specific verification. Being trained only on real videos, our method, called ID-Reveal [1] (Fig. 1), is independent of the specific type of manipulation. This work has been extended to deal with both audio and video [2], where we leverage a contrastive learning paradigm to learn the moving-face and audio segment embeddings that are most discriminative for each identity (see Fig. 2). Thanks to our multimodal approach, we can detect manipulations in both video-only and speech-only data, as happened when investigating realistic cases involving known individuals [3].

AI-generated image detection

To identify fully and locally AI-manipulated content in generic images, we rely on low-level traces, which are invisible forensic artifacts embedded in the image. We extract a learned noise-sensitive fingerprint (Noiseprint++) that bears traces of in-camera processing steps [4]. When images are manipulated, these telltale traces may be corrupted, an event that, if detected, allows one to carry out powerful forensic analyses. This is trained in a self-supervised manner using only pristine images taken from more than 1,000 different camera models. The scientific and practical impact of this work is evident from the fact that the technique has already been integrated into the Image Verification Assistant tool [5], which is used by journalists for fact-checking. ►

[3] www.restofworld.org/2023/indian-politician-leaked-audio-ai-deepfake

[4] Guillaro, F., Cozzolino, D., Sud, A., Dufour, N. & Verdoliva, L. (2023).

[5] https://mever.iti.gr/forensics

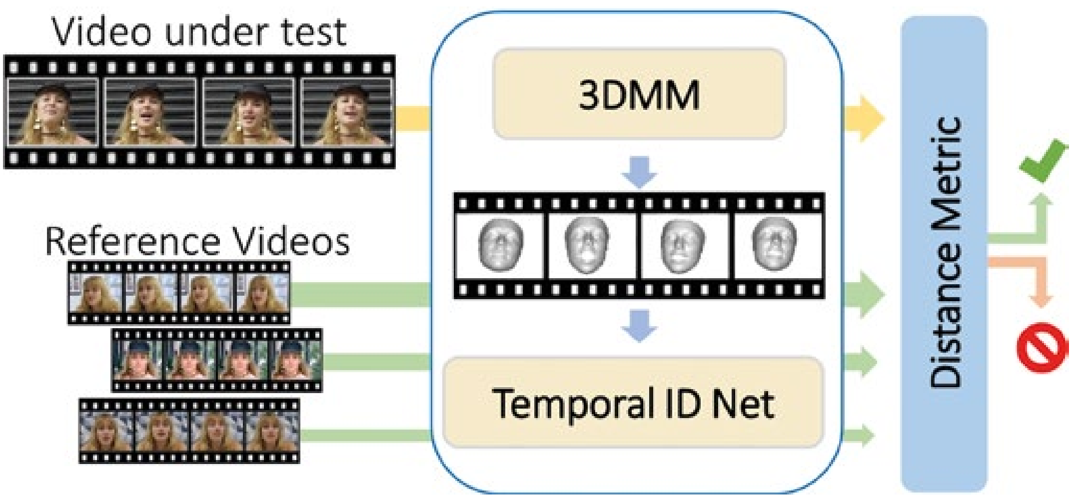


Fig. 1, ID-Reveal is an identity-aware deepfake video detection. From each frame it extracts a 3-D Morphable Model (3DMM) and estimates a temporal embedding, which is used as a distance metric to detect fake videos based on only a few reference videos of the person under test.

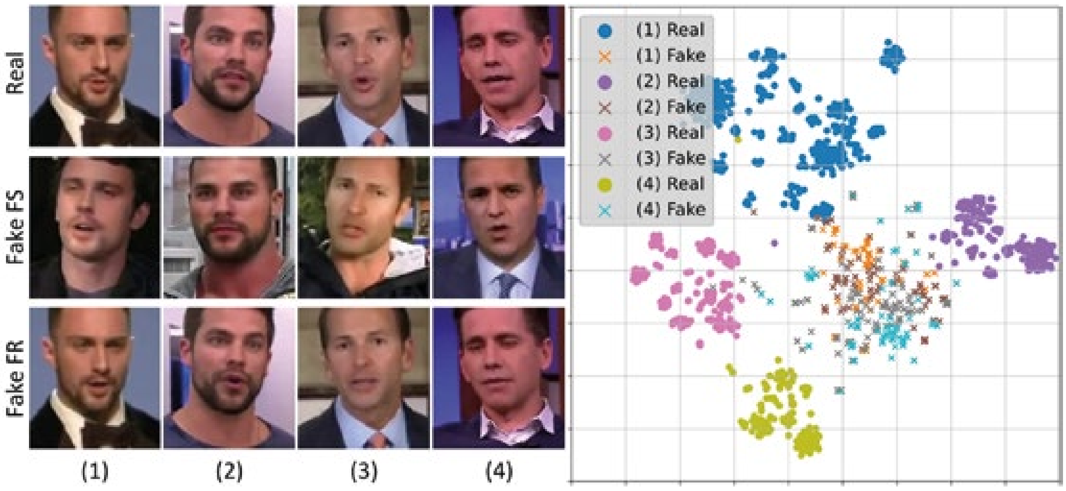


Fig. 2, We present a scatter plot of 2-D projections obtained via t-SNE for selected embedded vectors (audio-video feature concatenations) from real (circles) and fake (crosses) videos of four identities shown on the left. The vectors form distinct clusters for each individual, with manipulated counterparts generally distant from their real counterparts.

We have proposed an alternative strategy for fully generated image detection that is again based on an accurate statistical model of the real class [6]. Our key idea is to use a lossless coder to learn a reliable statistical model of real images. Lossless coding is a mature field of research based on sound information-theoretic concepts. Most image lossless coders work by predicting the value of each pixel based on a suitable known context and then encoding the prediction error. If the image is real, it follows the intrinsic statistical model of real images, and its pixels are not too surprising for the encoder. On the contrary, the pixels of synthetic images happen to exhibit unexpected values, thereby causing a coding cost larger than expected.

TUM-IAS doctoral candidate research

The TUM-IAS supported the doctoral candidate Artem Sevastopolsky in this project. The research initially focused on enhancing facial recognition, while also releasing two training datasets for unsupervised pretraining and a large-scale protocol for bias estimation [7]. Additionally, we developed a generative model for 3-D human heads that combines flexible animation with high detail preservation [8]. The collaboration has resulted in a paper accepted at ICCV 2023 and another scheduled for presentation at 3DV 2025.

Future research

There is still much room for research in this field, and there are many aspects that deserve deeper investigation. Below, we highlight a few key directions for future investigation.

Intent characterization: The boundary between real and fake is blurring as AI becomes commonplace for tasks such as compression and enhancement. In the near future, when generative AI will be everywhere, should we still call these images fake? Instead, the focus should shift to characterize the intent behind media, whether real or AI-generated.

Explainability: Similarly, understanding the meaning of AI-generated images in relation to their context will allow us to make sound decisions about their harmful potential. More generally, being able to provide an interpretation of the score provided by the detector would help to make more convincing decisions.

[6] Cozzolino, D., Poggi, G., Nießner, M. & Verdoliva, L. (2024).

[7] Sevastopolsky, A., Malkov, Y., Durasov, N., Verdoliva, L. & Nießner, M. (2023).

[8] Sevastopolsky, A. et al. (2025).

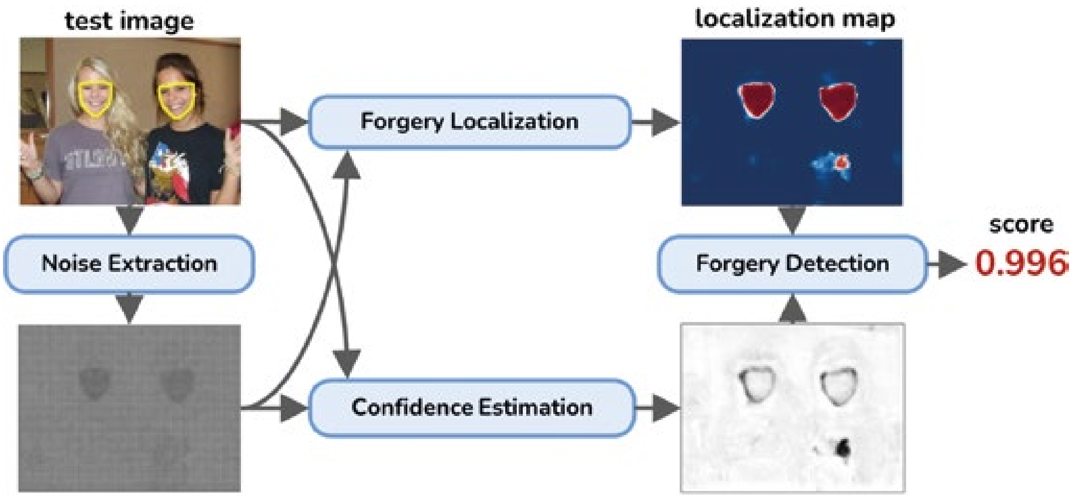


Fig. 3, Our method detects and localizes image forgeries (in yellow) by extracting Noiseprint++ and combining it with the RGB image to generate an anomaly localization map. Noiseprint++ also helps compute a confidence map, highlighting less reliable regions (black areas, e.g., false positives). The confidence and anomaly maps are used together to produce a global integrity score.

Robustness to adversarial attacks: Although there are research studies that analyze the performance of detectors in the presence of adversarial attacks, only a few detectors are designed with the aim of withstanding such attacks.

Active methods: In recent years, research has focused mainly on passive methods, but modern active approaches offer valuable tools to enhance forensic capabilities. Some embed invisible watermarks to certify authenticity, while others insert imperceptible signals to disrupt editing tools and prevent malicious use. ■

Selected publications

Cozzolino, D., Rössler A., Thies, J., Nießner M. & Verdoliva, L. ID-Reveal: Identity-aware DeepFake Video Detection. *IEEE/CVF International Conference on Computer Vision (ICCV)*, 15108–15117 (2021).

Sevastopolsky, A., Malkov, Y., Durasov, N., Verdoliva, L. & Nießner, M. How to boost face recognition with StyleGAN? *IEEE/CVF International Conference on Computer Vision (ICCV)*. 20924–20934 (2023).

Guillaro, F., Cozzolino, D., Sud, A., Dufour, N. & Verdoliva, L. TruFor: Leveraging all-round clues for trustworthy image forgery detection and localization. *IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, 20606–20615 (2023).

Cozzolino, D., Poggi, G., Nießner, M. & Verdoliva, L. Zero-Shot Detection of AI-Generated Images. *European Conference on Computer Vision (ECCV)*, 54–72 (2024).

Sevastopolsky, A. et al. HeadCraft: Modeling High-Detail Shape Variations for Animated 3DMMs. *International Conference on 3D Vision (3DV)* (2025).

For a full list of publications, please visit
www.ias.tum.de/ias/verdoliva-luisa

Where do the TUM-IAS Fellows come from?

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Dr. Zhenchang Xing
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Prof. Andreea Molnar
Swinburne University of Technology

Austria

Prof. Karin Nachbagauer
University of Applied Sciences Upper Austria

Belgium

Prof. Michel Géradin
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Prof. Jihyun Lee
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Chile

Prof. René Botnar
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Shandong University

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Chinese Acadamy of Sciences

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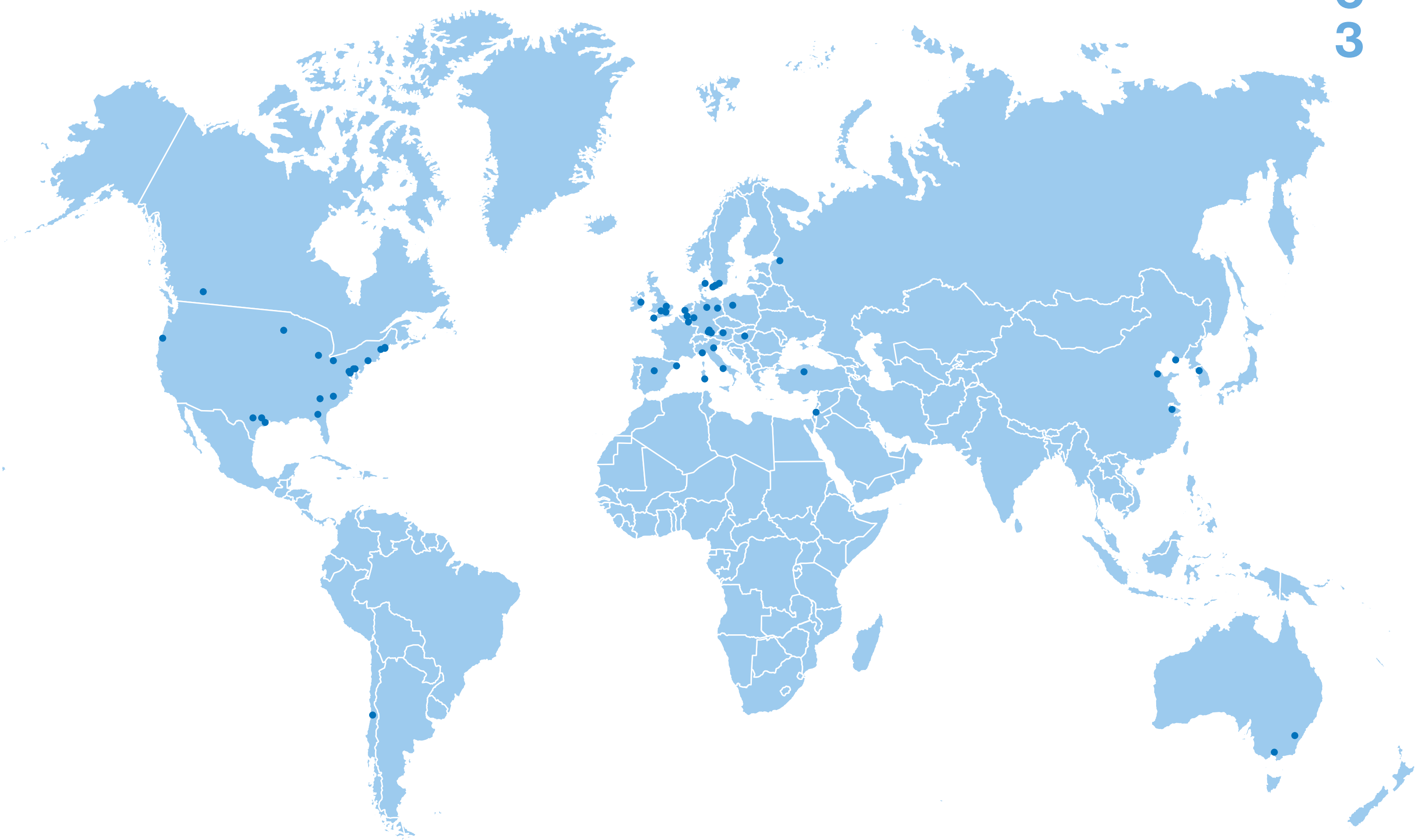

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Facts and Figures

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Excellence Strategy, Clusters of Excellence, and TUM Budget

After having played a central part in the first two rounds of the Excellence Initiative (2006–2012 and 2012–2019), the TUM-IAS became a permanent institution of TUM, financed out of the general TUM budget.

In addition, the IAS receives funding from the current Excellence Strategy, thanks to its Anna Boyksen and Albrecht Struppler Clinician Scientist Fellowships and Philosopher in Residence program. In addition, the TUM-IAS is collaborating with the Cluster of Excellence e-conversion, which finances several TUM-IAS@e-conversion Hans Fischer Senior Fellowships. This program currently funds a total of three fellowships.

Third-party funding

TÜV SÜD Foundation

In 2023 and 2024, three Philosophers in Residence were appointed – the TÜV SÜD Foundation and the Excellence Strategy fund this new one-year Fellowship. One more Philosopher in Residence can be appointed in 2025.

The TUM-IAS has a long collaboration history with the TÜV SÜD Foundation. After funding short-term Visiting Professorships for several years, the foundation funded two Hans Fischer (Senior) Fellows in 2016 and 2019 respectively. With its support for these Fellowships, the foundation aimed to promote energy efficiency and climate protection research, test procedures, product and plant safety, and compliance management.

Siemens AG

Since 2018, Siemens AG has provided TUM-IAS with a total of EUR 4.6 million over two funding periods, enabling the appointment of two additional Hans Fischer (Senior) Fellowships annually. After the first six Siemens-funded fellowships concentrated on Simulation and Digital Twin and Future of Autonomous Systems/Robotics, the focus is now on the Industrial Metaverse. So far, 10 Fellowships funded by Siemens AG have been appointed at TUM-IAS.

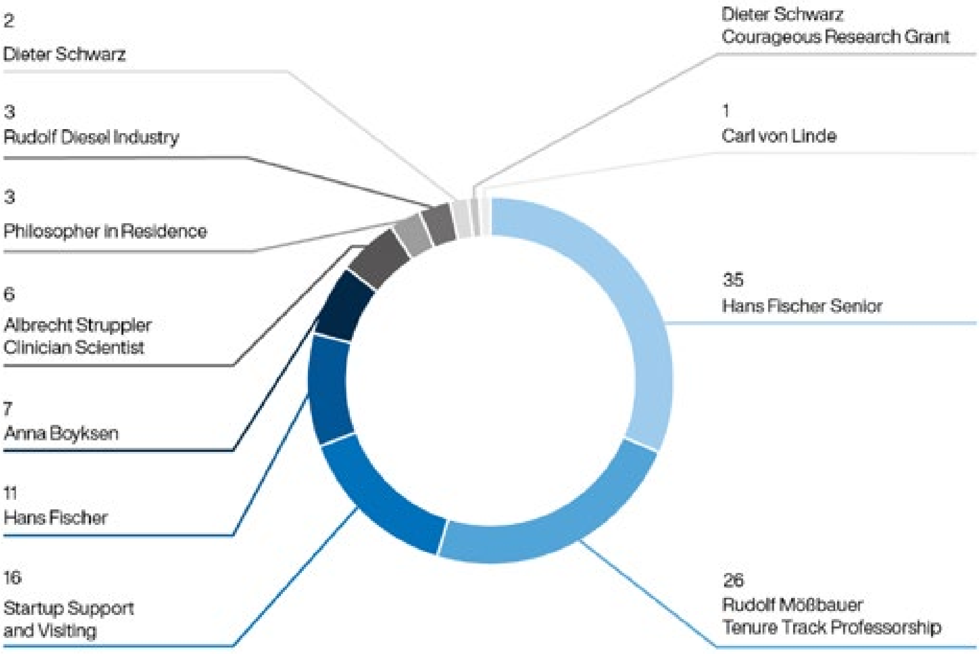
TUM Georg Nemetschek Institute Artificial Intelligence for the Built World

Since 2022, the TUM Georg Nemetschek Institute has funded one Hans Fischer (Senior) Fellowship per year, focusing on Artificial Intelligence for the Built World. A third Fellowship was awarded in 2024 (see Welcoming Our New Fellows).

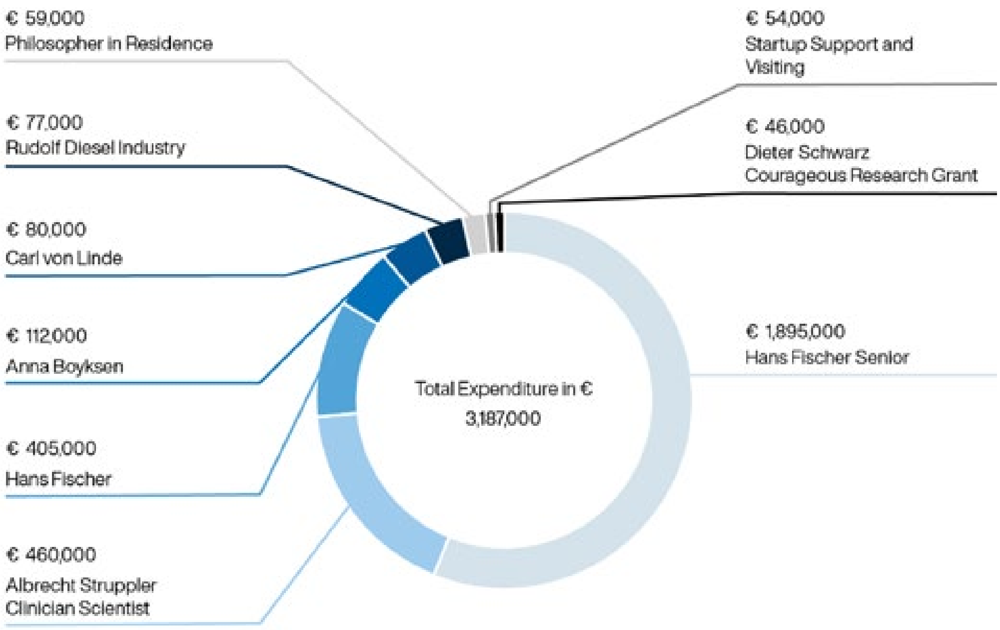
Dieter Schwarz Foundation

Since 2024, the Dieter Schwarz Foundation has funded two new Fellowships at TUM-IAS each year. The Dieter Schwarz Fellowship aligns with the existing Hans Fischer (Senior) Fellowships, attracting renowned international scientists from outside TUM who intend to explore innovative, high-risk topics in the key areas researched at the TUM Campus Heilbronn. Additionally, the Dieter Schwarz Courageous Research Grant, endowed with one million euros, has been awarded annually since 2024. It supports outstanding international scientists from outside TUM who intend to use groundbreaking technology to propose a radical solution to a major challenge in the area of "Digitization and Sustainability."

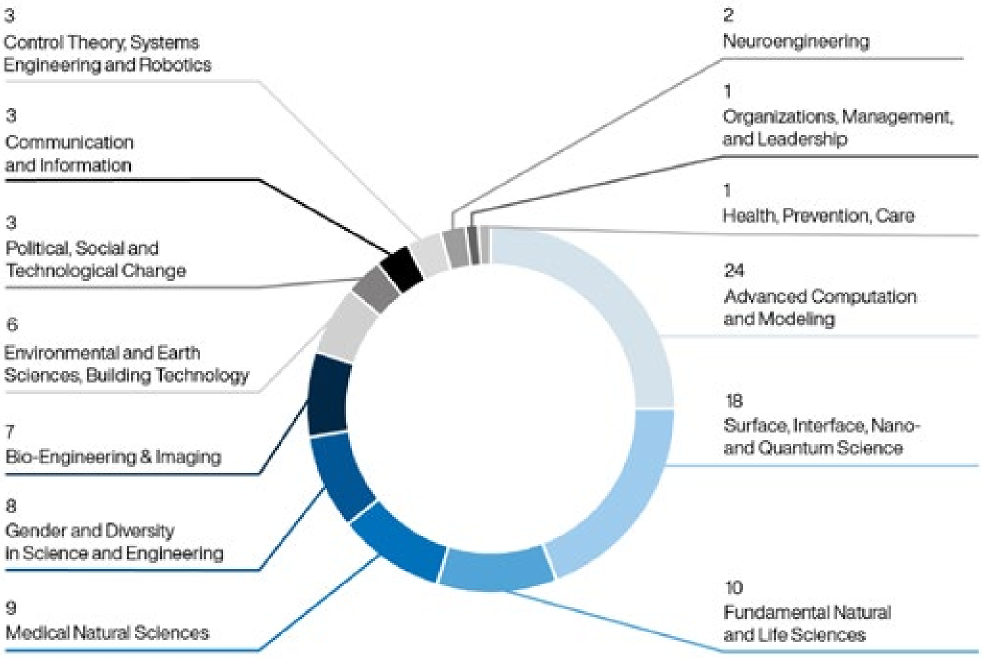
Fellow Distribution by Fellowship Category in 2024



Expenditure per Fellowship Category in 2024

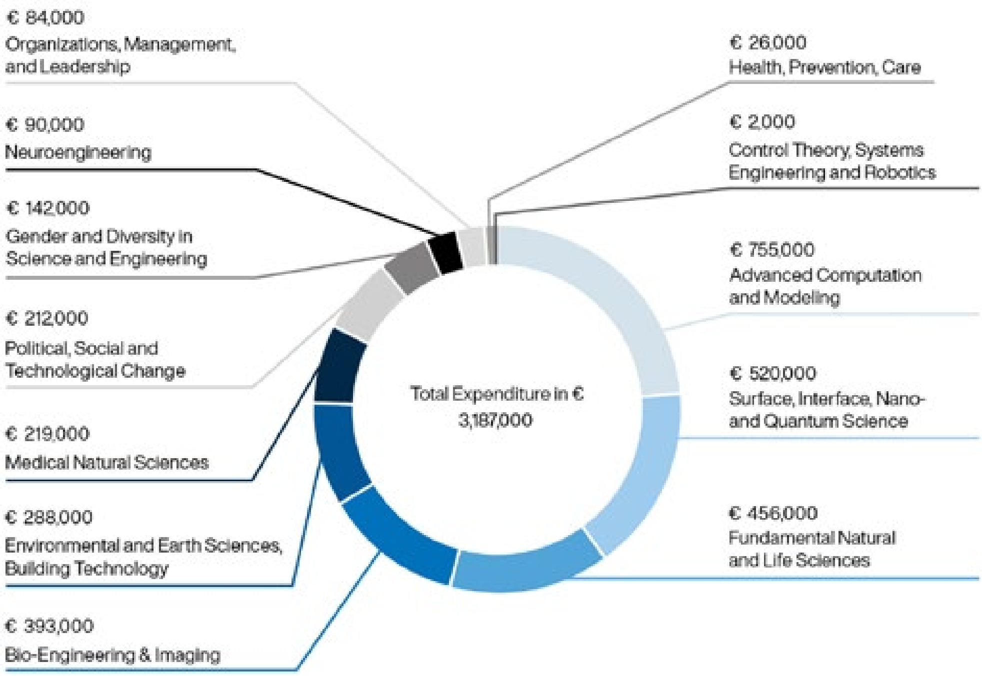


Fellow Distribution by TUM-IAS Research Area in 2024*

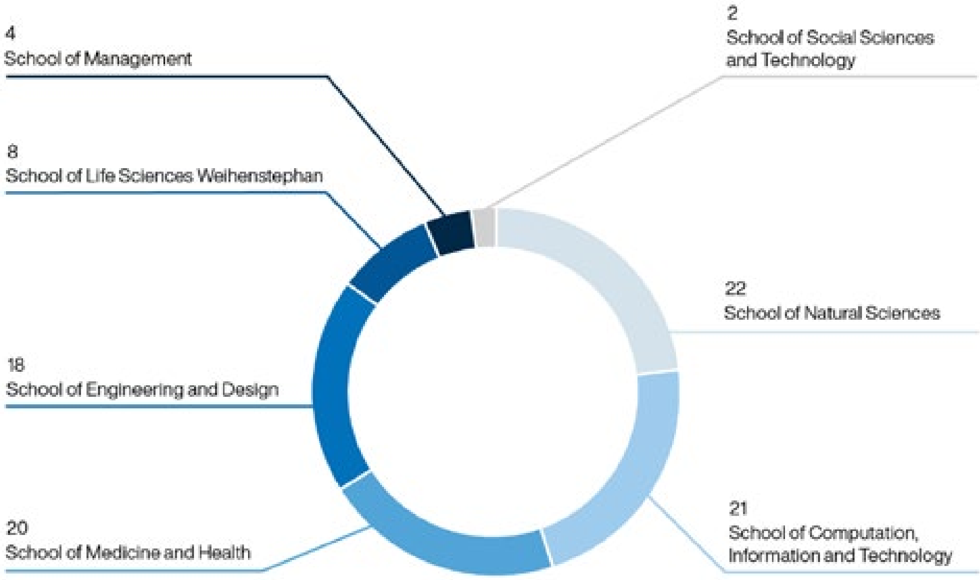


*Startup Support and Visiting Fellowship not taken into account here.

Expenditure per TUM-IAS Research Area in 2024

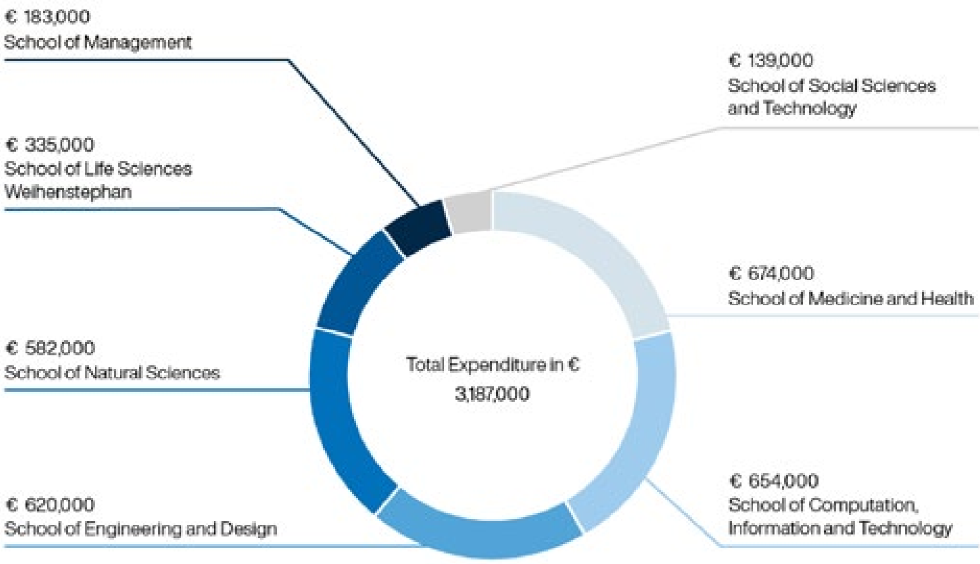


Fellow Distribution by TUM School in 2024*



*Startup Support and Visiting Fellowship not taken into account here.

Expenditure per TUM School in 2024



Board of Trustees

(status: January 2025)

The Board of Trustees is formed by a group of international advisors from academia, research support organizations, and industry. It advises the TUM-IAS director on general scientific, organizational, and technical issues. The Board also defines the general strategy and standards of the TUM-IAS.

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Advisory Council

(status: March 2025)

The TUM-IAS Advisory Council is composed mainly of TUM faculty, representing the different research areas of the university and the TUM-IAS. One of its prime functions is advising on the suitability and ranking of Fellow nominations the TUM-IAS receives for its various Fellowship programs. In addition, the Council advises on the scientific and technological course of the TUM-IAS, on the basis of an assessment of the potential and needs of the university. The Advisory Council usually meets three times a year.

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Prof. Dr.-Ing. André Borrmann, Computational Modeling and Simulation; Director TUM Georg Nemetschek Institute

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Prof. Cathleen Zeymer, Protein Chemistry

TUM-IAS Management Office

(status: January 2025)

Meet the TUM-IAS Management Team, which is responsible for our Fellowship Programs, liaison with our Fellows, workshops and conferences, our guesthouse, and all other TUM-IAS services. (7.4 full-time equivalents)

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