

2021



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# 04 TUM President's Foreword

**We are always reinventing ourselves – top universities are constantly evolving, otherwise they fall behind in the competition. TUM is currently undergoing a fundamental transformation process. Fifteen faculties will become seven schools.**

Four new schools have already been founded and have begun their work in the new constellation, with three more to follow by the end of 2023. The purpose of this realignment is to more efficiently transform the development potential in research and teaching into innovations, to accelerate technology spin-offs, and to make TUM as a whole more adaptable to future tasks and new framework conditions.

Important elements of the reorganization are the Integrative Research Centers as transdisciplinary cross-sectional institutions. They link the new schools with each other in order to create further innovation spaces.

The TUM Institute for Advanced Study has a special role to play here. With more than 60 collaborative projects by international Fellows and TUM Hosts based there, it is committed to cutting-edge research, internationality, and interdisciplinarity like no other TUM institution. The TUM-IAS is ideally interwoven with the schools and, with unconventional thinking across disciplinary boundaries, provides new insights that in many cases stand for social responsibility.

## **Sustainability**

And that is exactly what will matter. Climate change and sustainable action are among the greatest challenges we will face in the coming years and decades. More than ever, society needs the full creative power of our university community, our entrepreneurial courage to change, and a new sense of responsibility.

Sustainability is already a firm cornerstone of our TUM strategy today. We align our research, our teaching, our continuing education program, and also the campus management at our five main locations with it. To

name just a few examples: M Cube stands for our sustainable mobility project, which will receive 45 million euros in funding from the German government over the next nine years. The Green Hydrogen Future Lab will be funded by the German Federal Ministry of Education and Research for the next three years. Likewise, our students were successful in the Carbon Removal Student Competition and were able to implement the significantly more efficient use of methane from biogas plants. The entire Straubing campus, with 21 professorships, is dedicated to the topics of bioeconomy and sustainability. These projects show how important this task is to us and how deeply and diversely it is already anchored in research and teaching today.

In recent years, the TUM-IAS has placed a major focus on energy research in a wide range of disciplines – from catalysis research to optimized semiconductors and novel materials for photovoltaic cells. Sustainability needs such ambitious research for more efficient energy use.

## **Quantum sciences and technologies**

Since its founding in 2005, the TUM-IAS has been working with many projects close to the focal points of TUM. Quantum science and quantum technologies have been among them for years. In 2018, TUM was successful with its partners Ludwig-Maximilians-Universität, the Max Planck Institute of Quantum Optics, and the Walther Meissner Institute for Low Temperature Research and won support for the Cluster of Excellence Munich Center for Quantum Science and Technology. In 2021, we jointly launched the Munich Quantum Valley, which will be supported by the Free State of Bavaria with 300 million euros over the next few years. Quantum computing, quantum cryptology,





transfer to industry, education and training – these are some of the goals of the new Quantum Valley. In addition, TUM is investing in new professorships in these fields. BMW AG is funding an endowed chair on quantum algorithms and applications.

#### Transfer to market – from labs to ventures

The industrial technology leaders in Europe have been conducting cutting-edge research at the highest level for decades. Since 2005, the Rudolf Diesel Industry Fellowships of our TUM-IAS have succeeded in bringing together top-class researchers from industry and university on a longer-term basis.

We are placing the transfer to society on an even broader basis. Whether it is knowledge and skills, technologies, or education and training – the path from invention to innovation is multifaceted. That's why we're setting up the new Venture Labs. In specially equipped laboratories, workshops, and IT centers, spin-offs at the interfaces of engineering, natural and life sciences, artificial intelligence/information technology, and medicine in particular will be given a unique boost. This joint initiative of TUM and UnternehmerTUM, our partner for innovation and start-ups for over 20 years, offers founders a comprehensive ecosystem with the necessary

development environments. Our offerings range from technical and social infrastructure to entrepreneurship education and support through a network consisting of high-profile entrepreneurs, mentors, industry partners, academic/domain experts, and investors. Here, too, we have been able to attract top-class partners such as the BMW Group, BayWa AG, Nemetschek Group, and the entrepreneurs Andreas and Thomas Strüngmann, who together are providing around 30 million euros for this purpose.

In this reorganization of the Technical University of Munich, with its focus on research, transfer, sustainability, and internationality, the TUM-IAS plays a central role with cutting-edge research, interdisciplinarity, and internationality, to which you all contribute as Fellows, Members, and Friends. I look forward to meeting you at the General Assembly 2022 at the TUM-IAS. ■

Prof. Thomas F. Hofmann  
President

# TUM-IAS Director's Message

**Crises such as the pandemic or the war in Ukraine act like a burning glass and force us to rethink. In the spring of 2022, many failures are visible, and the consequences weigh heavily on us. In Europe, too, 30 years after the war in Yugoslavia, we are once again a long way from stable peace and from realizing the goals that global societies set themselves with a view toward sustainability.**



All the more, however, the challenge to the sciences in their entire breadth and to research remains to keep the flame of creativity burning. Under COVID-19, we have learned new, efficient ways of working together, and in future meta-worlds, virtual and physical meeting spaces will intermingle even more strongly worldwide to generate progress through the exchange of ideas.

The transformation to greater sustainability is one of the greatest challenges facing science, business, and society, also in terms of peacekeeping. This basically comes as no surprise. Exactly 60 years ago, in 1962, Rachel Carson published her most important work, *Silent Spring*, which urgently described the drastic consequences of the use of pesticides and herbicides for fauna, flora, and humans. In 1972, the Club of Rome presented its first major study, *The Limits to Growth*. It has lost none of its relevance 50 years later. It is more urgent than ever, not only for us researchers, but for all of us: to think and act sustainably – together, across borders, worldwide. TUM and the TUM-IAS take this up and are guided by this principle in their scientific work and teaching. For us, sustainability is one of our strategic pillars today. This is reflected in the projects of our Fellows with their TUM Hosts and PhD candidates (Focus Groups) and also in the activities of our partner, the International Expert Network on Earth System Preservation (IESP).

The research of the international TUM-IAS Fellows in Focus Groups, located at the various departments and Schools of TUM, is highly specialized and oriented toward fundamentals, often only comprehensible in detail to experts in the field. However, a closer look at the results often reveals concrete application references, e.g., energy-saving chemical processes, new and more efficient semiconductor materials, digital twins for simulations in the various engineering sciences, computational models for securing water supplies, or more precise and earlier diagnostic possibilities in medicine, as well as in earth observation.

Therefore: Even if the pandemic leads to severe restrictions and the war causes deep cuts and the need for far-reaching changes, the creativity and willingness to take risks shown by excellent, committed scientists of all ages in the working environment of our TUM inspire hope. Essential for the development and promotion of creative achievements are encounter and exchange, combination and recombination of knowledge and experience, and finally the often quoted “one percent inspiration, ninety-nine percent perspiration” (Thomas A. Edison).

The TUM Institute for Advanced Study offers its Fellows, Members, and friends exactly that: an “exchange place of knowledge,” as TUM President Thomas Hofmann calls it. That is why our Fellowship Program is so important, and I am very pleased to have seen and met many Fellows at the TUM-IAS in recent months, despite travel restrictions.

To mitigate the impact of the pandemic on our projects, we have extended the terms of Fellowships that have already begun, as well as doctoral funding. New programs that we announced last year, such as the Innovation Networks and the Albrecht Struppler Clinician Scientist Fellowships, have started successfully. This year, we are awarding the first Fellowships of the Georg Nemetschek Institute Artificial Intelligence for the Built World, based at TUM. More about this on the following pages.

We transformed our weekly “Wednesday Coffee Talks,” where Fellows and TUM scientists reported on their

work, into an online format, reaching more people, including more students, than before – not only at our five TUM locations, but worldwide! This event unites our Fellow community, which is recruited from all continents.

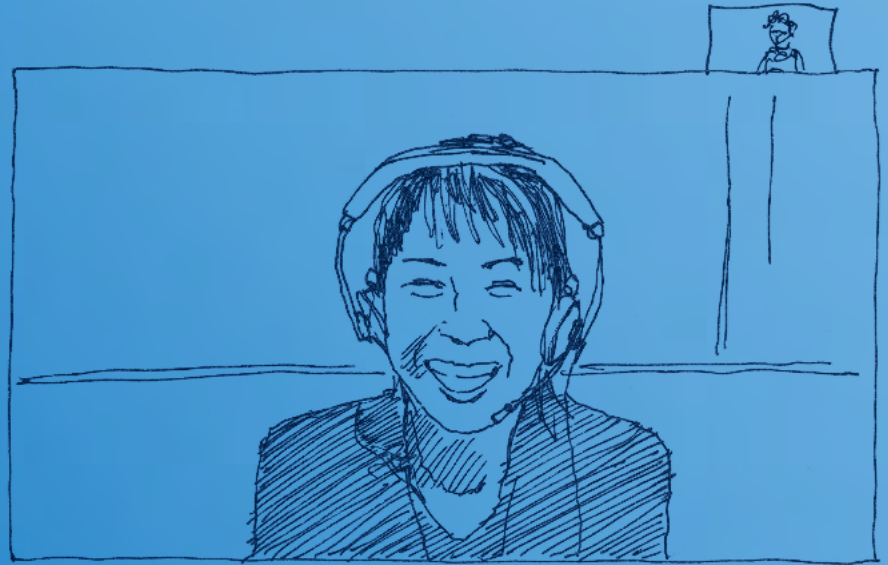
From the many positive developments that you can read about on the following pages, I would like to single one out here as particularly gratifying: Some of our Fellows are among the world’s most cited scientists in their fields. It fills me with pride that we were able to win them as TUM-IAS Fellows. If you look at the publications of all Fellows since the founding of the TUM-IAS, they are cited more often than average. They also report their research results in the top five percent of the relevant journals with above-average frequency. This means that the Fellows of the TUM-IAS with their Focus Groups at the Schools and departments of TUM are globally judged to be particularly relevant in terms of generating scientific and technical progress.

This outstanding scientific output is made possible by the generous support that the TUM-IAS receives from various sources. Here I would like to thank in particular Siemens AG and the TÜV Süd Foundation, which have provided us with considerable support in recent years. In 2021, we were able to award three Anna Boyksen Fellowships, the funding for which comes from the Excellence Strategy of the German federal and state governments – they also deserve thanks. Finally, my thanks go to the Free State of Bavaria, which finances our university, and thus also the TUM-IAS, from tax revenues. ■



Prof. Michael Molls  
Director





# Actions, Awards, Events

During 2021 we turned ideas into actions,  
distant communication into a new asset.  
And again, our Fellows and Members  
were honored with numerous awards.





# Actions

## Extension of Fellowships due to the pandemic

The COVID-19 pandemic, with long and diverse travel restrictions worldwide, brought personal international exchange largely to a standstill, and workshops and conferences were cancelled. Many projects of our TUM-IAS Fellows, e.g., those based on joint laboratory work, had to be postponed, as well as study trips. Also, PhD candidates funded under the Fellowships were mostly unable to visit their supervisors at their home institutions abroad. To mitigate these challenges, we have extended the terms of Fellowships that have already started as well as PhD funding.

## Cooperation with the Alexander von Humboldt Foundation

Since the founding of the TUM-IAS in 2005, award winners of the Alexander von Humboldt Foundation (AvH) are also Members of our Institute. In order to better link the funding programs of both institutions, to strengthen cooperation, and to create synergies in the support of international scientists, the TUM-IAS will in the future assume the central interface function between TUM and AvH. It will be the university-wide contact for various Humboldt Foundation programs, advise and support professors in nominating suitable candidates, and network Humboldt award recipients more intensively with each other, with TUM-IAS Fellows, and with TUM scientists.

## Another round of TUM Innovation Networks

In 2021, TUM published for the second time the call for proposals for Innovation Networks dedicated to fostering cross-disciplinary research in cutting-edge topics with a “high risk/high gain” approach. On a long-term perspective, they are meant to build the foundations for large-scale consortia and potential funded collaborative research projects.

The TUM-IAS supports this strategic initiative of TUM Agenda 2030 through the orga-

nization of Exploratory Workshops. These events aim at elaborating the most promising selected ideas submitted in the first phase of the call. In total, TUM researchers submitted 13 ideas for this call. After a first evaluation by the Innovation Networks Board and TUM experts, seven ideas were shortlisted. Subsequently, four Exploratory Workshops took place from December 1 to 10, 2021. Following the workshops, each group submitted a final concept paper for a TUM Innovation Network. These concept papers were evaluated by external reviewers. Finally, the Innovation Network Board made a funding suggestion to the TUM Board of Management, which selected, out of the four proposals, two Innovation Networks for a four-year period of funding in February 2022:

Exoskeleton and wearables enhanced prevention and treatment (eXprt), **Prof. Gordon Cheng** (TUM Department of Electrical and Computer Engineering) and **Prof. Joachim Hermsdörfer** (TUM Department of Sport and Health Sciences) and Next generation drug design (NextGenDrugs), **Prof. Matthias Feige** (TUM Department of Chemistry, TUM-IAS Rudolf Mößbauer Tenure Track Assistant Professor).

These two Innovation Networks will be launched in spring of 2022 and are in addition to the first three – ARTEMIS, RISE, and Neurotech – that successfully started in 2021 and are now running with more than 30 junior scientists involved.

## New Albrecht Struppler Clinician Scientist Fellowship launched

This Fellowship, launched in 2021, is designed for physicians working at the TUM University Hospital Klinikum rechts der Isar who intend to further develop an independent research profile while at the same time continuing their clinical qualification. The Fellowship is aimed at outstanding, high-potential early-career scientists who have already received or will shortly receive their certification as medical

specialist (Facharzt/ärztin) and who have already successfully secured third-party funding. The Fellowship offers a relief of 50 percent from clinical duties, which gives Fellows time to carry out a transdisciplinary research project in collaboration with scientists from a department/school different from the TUM School of Medicine.

The Fellowship is named after Albrecht Struppler (1919–2009), the first chair of neurology at TUM and a pioneer in building a bridge from the neurosciences to engineering. With this program, the TUM-IAS would like to encourage out-of-the-box ideas and cross-disciplinary exchanges that may otherwise get lost in the busy everyday clinical routine, and reinforce health and medical sciences with perspectives and expertise from non-medical disciplines.

The Fellowship lasts three years, during which the Fellow will continue his/her duties at the University Hospital to a reduced extent (relief of 50 percent). Since it is the aim of this Fellowship to bridge medicine with other scientific fields represented at TUM, a cooperation partner/group from a TUM department/school other than the TUM School of Medicine is compulsory. During the Fellowship, the Fellow is welcome to make use of the office space at the TUM-IAS building. The Fellow also actively contributes to interdisciplinary TUM-IAS events.

### TUM-IAS Fellowship Calls

We were able to welcome 15 new Fellows in 2021 in the categories Hans Fischer (Senior) Fellowship, Anna Boyksen Fellowship, and Albrecht Struppler Clinician Scientist Fellowship. Their home countries are as far away from each other as possible, ranging from Spain, the Netherlands, Denmark, and Hungary to Russia, Australia, and the USA. They are visiting seven departments as well as the TUM University Hospital Klinikum rechts der Isar. Two Fellowships for scientists specialized in the fields of Simulation and Digital Twin and Future of Autonomous Systems and

Robotics are funded by Siemens AG. Two of the Hans Fischer Senior Fellows are working in the Cluster of Excellence e-conversion.

For ten years now, TUM has been appointing promising talents as Tenure Track Assistant Professors (W2), after a thorough selection process organized by the TUM-IAS. The TUM Faculty Tenure Track is the performance-oriented career model for young scientists with international experience and offers the realistic prospect of advancing to a tenured W3 professorship from the very beginning. The Fellowship is named after TUM professor Rudolf Mößbauer (1929–2011), who was awarded the Nobel Prize in Physics in 1961 for his 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 start possible in their careers, they are equally affiliated with the TUM-IAS as Fellows. In 2021, Rudolf Mößbauer Tenure Track Assistant Professors have been appointed in the research areas of Learning Sciences and Educational Design Theories (**Prof. Anna Keune**) and Behavioral Science for Disease Prevention and Health Care (**Prof. Nikkil Sudharsanan**).

➔ For details on our new Fellows, please see Chapter “Welcoming Our New Fellows” beginning on page 18.

TUM-IAS Fellows among Highly Cited Researchers

The frequency of citations of a study is a good indicator of research quality. To determine the Highly Cited Researchers, the US company Clarivate each year evaluates the Web of Science database it operates, which records scientific publications from a broad range of subjects.

The new edition of the evaluation shows the scientists who were cited most frequently in their respective fields between 2010 and 2020. Researchers who are cited particularly often in different fields are listed in the Cross-Field category. In total, the list comprises around 6,600 people in no particular order, including the following TUM-IAS Fellows:

- **Prof. Ib Chorkendorff** (Chemistry), DTU Copenhagen
- **Prof. Naomi Halas** (Materials Science), Rice University
- **Prof. Laura Herz** (Cross-Field), University of Oxford
- **Prof. Bernhard Küster** (Cross-Field), TUM
- **Prof. Peter Nordlander** (Materials Science), Rice University
- **Prof. Ingrid Kögel-Knabner** (Agricultural Science), TUM
- **Prof. Shuit-Tong Lee** (Cross-Field), Suzhou University
- **Prof. Johannes Lehmann** (Environment and Ecology and Agricultural Sciences), Cornell University
- **Prof. Takao Someya** (Cross-Field), University of Tokyo and RIKEN

Research output

University rankings (i.e., Shanghai Ranking, Times Higher Education, QS World University Ranking) assess the research quality of universities by different indicators such as the numbers of publications, and the research influence of universities is evaluated by indicators such as the number of citations. In both national and international rankings, TUM is among the top-rated German universities.

Since 2007, TUM-IAS Fellows have contributed 3,303 publications to the TUM total num-

ber of publications (based on Scopus database). These publications have been cited almost 130,000 times (status: March 31, 2022). Citation analysis reveals that publications produced by TUM-IAS Fellows mostly in cooperation with their respective TUM Hosts have a considerably higher average citation impact than all publications by TUM in the same period of time (2007 to present): 39.3 vs. 25.0 average number of citations per publication (see Tab. 1). These data demonstrate that the research performance of the TUM-IAS has a positive effect on the ranking indicators of TUM.

Entity	Publications	Citations	Ø Number of Citations per Publication
TUM-IAS	3,303	129,818	39.3
TUM incl. IAS	111,471	2,791,689	25.0
Mean: 2007–2022		Data Source: Scopus © 2022 Elsevier	

Table 1

The presence of publications in the most influential journals in the world is shown by the “number of publications in top journal percentiles.” Bibliometric analysis reveals that the percentage of publications in the 5 percent most-cited journals (defined by the journal metrics SCImago Journal Rank SJR, see Tab. 2) is much higher for publications from TUM-IAS Fellows in comparison to the overall publications by TUM. These data indicate that the research output generated by TUM-IAS Fellows contributes significantly toward TUM’s national and international reputation as one of Germany’s top universities.

Entity	Publications in Top 5% Journal Percentiles (using SciVal/SJR metrics)	
	in %	absolute
TUM-IAS	39.2	1,205
TUM incl. IAS	23.7	23,536
Mean: 2007–2022		Data Source: Scopus © 2022 Elsevier

Table 2



# Awards

We are delighted and proud that our Fellows and partners have again received top-class awards in 2021:

**Prof. Luisa Verdoliva** became IEEE Fellow in January 2021 for her contributions to multimedia forensics. **Prof. Job Boekhoven** received the Lecturer Award of Verband der Chemischen Industrie for 2021.

**Dr. Barbara Solenthaler** was given the Günther Enderle Best Paper Award of the Eurographics conference 2021.

TUM-IAS Alumnus Fellow **Prof. Andrzej J. Buras** received the Max Planck Medal of the German Physical Society (DPG), honoring his outstanding contributions to applied quantum field theory of fundamental interactions, especially in the field of flavor physics and quantum chromodynamics. The Max Planck Medal is the DPG's highest honor for outstanding achievements in the field of theoretical physics.

TUM-IAS Alumna Fellow **Prof. Jia Chen** received the Arnold Sommerfeld Prize 2021 of the Bavarian Academy of Sciences and Humanities for fundamental contributions to research on climate change and urban pollution. She was also named as Member of Global Young Academy (GYA).

TUM-IAS Fellow **Prof. Mathias Senge** received the Irish Laboratory Award for 2021. His group, which is a leader in the field tetrapyrroles and has published widely on Hans Fischer's pigments of life, the porphyrins, is Chemical Laboratory of the Year.

The Euler medal of the European Community on Computational Methods in Applied Sciences (ECCOMAS) was awarded to TUM-IAS Alumnus Hans Fischer Fellow **Prof. Alessandro Reali**. The Euler medal recognizes outstanding and sustained contributions to the area of computational solid and structural mechanics.

**Prof. Reinhard Heckel** received the Young Scientist Honor from the Werner-von-Siemens-Ring foundation 2021.

**Prof. Gustavo Goldman** was chosen as the 2021 Moselio Schaechter awardee of the American Society for Microbiology (ASM), for being a role model in leadership and commitment in the field of microbiology.

## ERC Grants

TUM-IAS Fellow **Prof. Hendrik Dietz** and Host **Prof. Wolfgang A. Wall** were awarded the prestigious ERC Advanced Grants.

## TUM Distinguished Affiliated Professors and new TUM-IAS Members

The TUM-IAS welcomes the TUM Distinguished Affiliated Professors as Honorary Fellows and members of the TUM-IAS community.

The former President of the Nanyang Technological University and biochemist **Prof. Bertil Andersson** received the TUM Distinguished Affiliated Professorship award on October 7, 2021. Since the appointment has been made jointly with the TUM School of Life Sciences, he became honorary professor both at the TUM Department of Chemistry and at the TUM School of Life Sciences in Weihenstephan.

**Prof. Rainer Blatt**, experimental physicist and Scientific Director of the Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, joined as a new TUM Distinguished Affiliated Professor on November 11, 2021. With his pioneering experimental demonstrations of basic building blocks and algorithms of quantum processors, he has paved the way toward useful quantum computing systems and new research directions in quantum technology. Rainer Blatt received the Stern Gerlach Medal in 2012 and the John Stewart Bell Prize in 2015. He has been coordinator of the Munich Quantum Valley since 2021.



European Research Council  
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# Events

2021 saw the resumption of the face-to-face meetings as well as the larger conferences, but these are now held online.

## TUM-IAS General Assembly

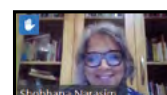
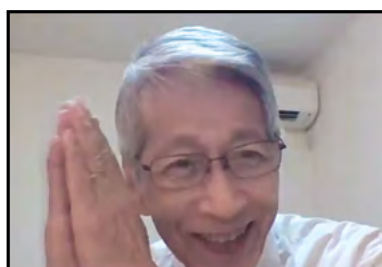
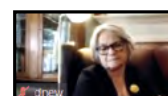
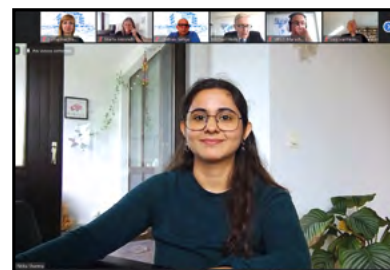
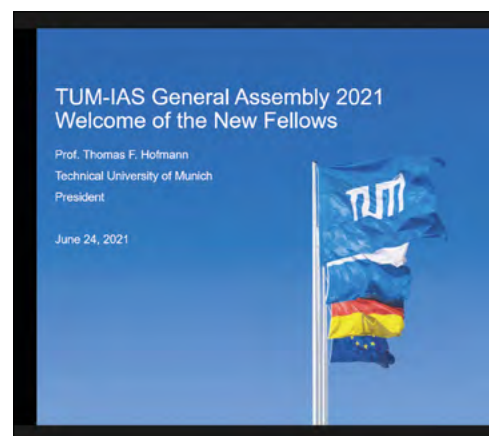
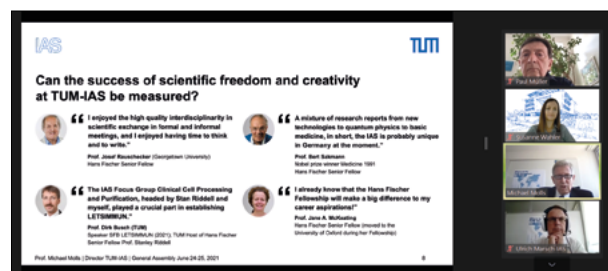


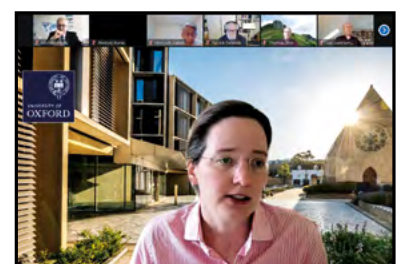
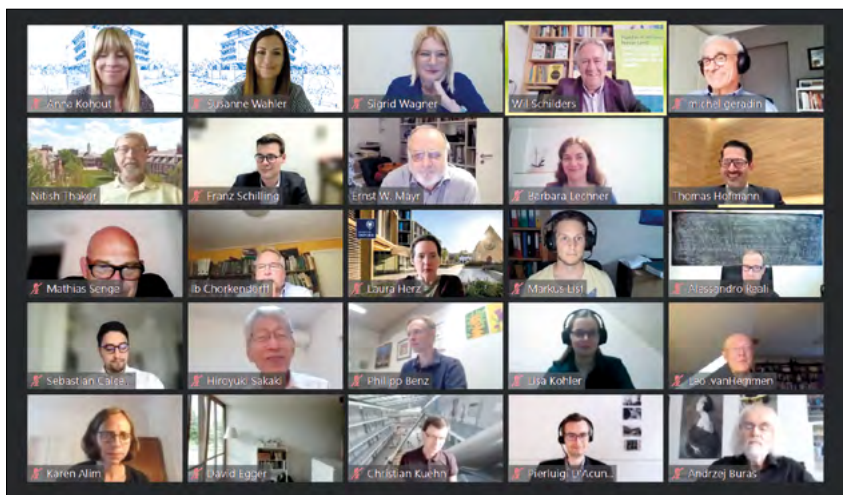
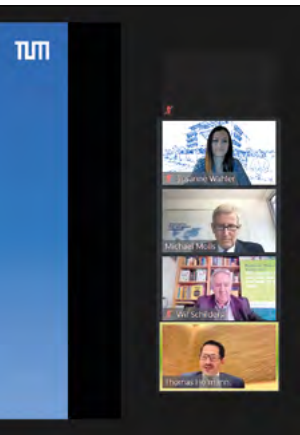
Prof. Michael Bordt

More than 120 Fellows, Hosts, alumni and friends met online on June 24 and 25 for our General Assembly. Over two days, Fellows presented a wide variety of topics from the projects at the TUM-IAS in 30 talks and sessions.

For the first time, the Linde Lecture opened our General Assembly. It commemorates Carl von Linde, one of the first professors at the young Technical University of Munich founded in 1868 and a pioneer in cooling technology. The new Linde Lecture is intended to set an example of how critical reflection, theory-driven research, and practical implementation can push the boundaries of our knowledge and enable humanity to set out for new shores.

Predestined as a speaker was therefore Prof. Michael Bordt SJ, who is a member of the Jesuit Order and teaches at the Munich School of Philosophy. He is a board member of the Institute for Philosophy and Leadership and offers consulting, guidance, and workshops for executives in top positions of large medium-sized companies and corporations. In his Linde Lecture, Prof. Bordt explored what we can learn from crises – including the Covid-19 crisis – and which positive aspects we can transfer into the future.





### Thermoacoustics in Combustion

The Symposium on Thermoacoustics in Combustion in September was jointly organized by **Prof. Thomas Sattelmayer**, Chair of Thermodynamics, **Prof. Mirko Bothien**, TUM-IAS Rudolf Diesel Industry Fellow, and **Dr. Luca Magri**, TUM-IAS Hans Fischer Fellow. More than 64 papers from 12 countries on combustion instabilities made this the largest congress worldwide in this field.

### IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)

**Prof. Leonidas Guibas** (TUM-IAS Hans Fischer Senior Fellow) and **Prof. Matthias Niessner** (Visual Computing & Artificial Intelligence), held the first Workshop on Language for 3D Scenes in June. This was the first workshop on natural language and 3D-oriented object understanding of real-world scenes. Their primary goal was to spark research interest in this emerging area and to benchmark progress in connecting language to 3D to identify and localize 3D objects with natural language.

### China in the Global Economy

In October, an international workshop focused on China's role in the global economy and its governance. It was organized by **Prof. Eugénia da Conceição-Heldt**, Chair of European and Global Governance, and **Prof. Susan Park**, TUM-IAS Hans Fischer Senior Fellow.

### Workshop on Network Dynamics

Power grid networks or synchronously firing neural oscillators in the brain – these are examples of networks of dynamical nodes. The collective dynamics – and therefore the functionality – of such network dynamical systems are determined by the individual dynamics of each node as well as the interaction between nodes. A workshop, organized by the TUM-IAS Focus Group Network Dynamics, brought together experts on networks, dynamics, and data working on pure and applied topics in network dynamics with a particular focus on adaptive networks. TUM-IAS Hans Fischer (Senior) Fellows **Dr. Christian Bick** and **Prof. Dr. Krasimira Tsaneva-Atanasova** organized this virtual workshop.

### Future of Scientific Evaluation

In a virtual fireplace evening, **Prof. Kai Müller**, TUM-IAS Fellow and Rudolf Mößbauer Tenure Track Assistant Professor, discussed alternatives to classical peer review.

### Dr. Markus Söder, Prime Minister of Bavaria, visited Prof. Jia Chen

**Dr. Markus Söder**, the minister-president of Bavaria, recently visited a research station for greenhouse gases in the urban environment called MUCCnet (Munich Urban Carbon Column network), operated by **Prof. Jia Chen**, TUM-IAS Alumna and TUM professor. “We can only reduce emissions efficiently if we understand them,” Dr. Söder said. The minister-president was on the roof of a TUM building learning about a sensor network for measuring greenhouse gases that is unique worldwide.



### Wednesday Coffee Talks

Our “Wednesday Coffee Talks – Scientists meet Scientists” series gives insights into



The second workshop in October in Bad Wörishofen, also attended by almost 30 participants, was dedicated to the motto “Stronger Commitment and Responsible Dynamics Are Needed! Approaches in Science, Technology and Education.” The focus was on the Sustainable Development Goals (SDGs) of the UN and their hesitant and slow implementation, as well as future activities.

→ A detailed report of the IESP starts on p. 62.

TUM research to a larger public. In 2021, we had more 25 online talks throughout the year. The new online format brought us a much larger audience from different regions around the world. We covered research from “Making Artificial Intelligence Trustworthy” to “Hyperactive Signals driving Cancer.”

### IESP Workshops

The International Expert Network on Earth System Preservation (IESP) held an online workshop in February on “Water and Agricultural Management” with 30 participants. It focused on the future of water supply in southern Germany and Bavaria.







# Welcoming Our New Fellows

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

# Fellowship Program



## **Anna Boyksen Fellowship**

for outstanding top-level female professors who intend to explore gender- and diversity-relevant themes in the context of the TUM subject portfolio



## **Rudolf Mößbauer Tenure Track Assistant Professorship**

for outstanding, high-potential early-career scientists



## **Rudolf Diesel Industry Fellowship**

for highly qualified researchers from industry



## **Albrecht Struppler Clinician Scientist Fellowship**

for excellent senior physicians working at the TUM University Hospital Klinikum rechts der Isar



## **Hans Fischer Fellowship**

for outstanding early-career scientists from outside TUM

## **Hans Fischer Senior Fellowship**

for renowned international scientists from outside TUM



## **Carl von Linde Fellowship**

for excellent TUM faculty members



## Prof. René Botnar

King's College London



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Marcus R. Makowski (TUM School of Medicine) | **TUM-IAS Focus Group:** CardioMRI | **TUM-IAS Research Area:** Bio-Engineering & Imaging

Coronary artery disease (CAD) remains one of the leading causes of mortality worldwide. The early detection of CAD enables targeted risk stratification and prophylactic treatment of patients most at risk of having a heart attack. While invasive X-ray coronary angiography and non-invasive computed tomography coronary angiography (CCTA) are the gold standard imaging modalities for the assessment of CAD, both are limited by long-term risk from ionizing radiation and short-term risk of contrast agent-mediated kidney damage. Cardiovascular magnetic resonance (CMR) could be a safe, non-invasive, ionizing radiation- and iodinated contrast-free alternative for the imaging of coronary artery stenosis. However, widespread clinical implementation of CMRA is currently limited due to long and unpredictable scan times, lower spatial resolution (usually 1–2 mm anisotropic), and image quality degradation related to cardiac and respiratory motion. To address these limitations, the CardioMRI Focus Group will develop high-resolution free-breathing 3D coronary MR angiography (for patients unable to hold their breath) employing deep learning-based super-resolution reconstruction and motion estimation methods.

## Dr. Elena del Valle

Universidad Autónoma de Madrid



**Fellowship:** Hans Fischer Fellowship | **Hosts:** Prof. Gerhard Kramer, Prof. Kai Müller (TUM Department of Electrical and Computer Engineering) | **TUM-IAS Focus Group:** Novel Quantum Light Sources | **TUM-IAS Research Area:** Surface, Interface, Nano- and Quantum Science

Since the invention of the laser, classical photonics has developed into one of our most reliable, efficient, and powerful technologies. Consequently, photonics is expected to play a leading role in quantum technologies as well. Currently, the bulk of the effort in quantum photonic science and technology focuses on quantum communication and is based on the development of ideal single-photon sources as the key components. Here, sources based on semiconductor nanostructures, such as semiconductor quantum dots, offer the most desirable properties: on-demand operation, high brightness, high purity, and high generation rates. However, most real-world applications will need multiphoton states of light, for example to provide redundancy against photon loss. Moreover, having efficient, controlled, and pure multiphoton sources will open new perspectives beyond quantum communication, for example in photonic quantum computation, quantum sensing, and metrology. The major technological goal of this Focus Group is to develop the multiphoton sources of tomorrow.

## Prof. Naomi J. Halas

Rice University



**Fellowship:** Hans Fischer Senior Fellowship | **Hosts:** Prof. Jonathan Finley, Prof. Ian D. Sharp (TUM Department of Physics), Prof. Emiliano Cortés (Department of Physics, LMU) | **TUM-IAS Focus Group:** Sustainable photocatalysis using plasmons and 2D materials (SusPhuP2M) | **TUM-IAS Research Area:** Surface, Interface, Nano- and Quantum Science

This TUM-IAS Focus Group is pursuing the development of novel photocatalytic nano-reactors built from novel two-dimensional materials and their heterostructures decorated with novel plasmonic light-harvesting structures. It brings together TUM groups led by Jonathan Finley and Ian D. Sharp at the Walter Schottky Institute and the Hybrid Nanophotonics and Plasmonic Chemistry chair at LMU and is led by Hans Fischer Senior Fellow Naomi J. Halas. The group explores chemically reactive sites in 2D materials and their heterostructures and combines them with nanoscale plasmonic reactors to enhance light-matter coupling and provide local catalytic activity. Goals aim at (1) the exploration of ultrafast carrier photokinetics and photochemistry at the surface of tailored 2D heterostructures, (2) understanding of carrier generation and relaxation pathways as well as the role of hot-electron and photo-thermal effects, (3) tailoring of the design of plasmonic noncatalytic antennas and colloids decorating the 2D materials, and (4) testing and optimizing the use of such hybrid systems for field-induced photocatalysis.

## Prof. Maja Horst

DTU – Technical University of Denmark



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Ruth Müller (TUM Department of Science, Technology and Society) | **TUM-IAS Focus Group:** Responsible Innovation Communication | **TUM-IAS Research Area:** Political, Social and Technological Change

We aim to develop research and teaching in the area of public communication of emerging technology using artificial intelligence (AI) as an exemplary case. In particular, we will focus on the representation of scientists in public discourse as well as the role scientists play in producing public narratives. As a strategic priority, AI is expected to have disruptive and transformative effects in many industries and in the public sphere as well. Simultaneously, some voices in the public sphere also consider AI a threat to social values and practices. We focus on the effects of such a highly charged public and policy communication environment on the conditions for responsible research and innovation within AI. Radical expectations about the potential of future technology are important for the generation of resources, but they can also have adverse effects, for instance on the political decision-making to allow, postpone, or deny experimental use of big data or AI in public services. Communication and responsiveness are therefore not add-ons to AI development, but essential constituents of responsible technology development.

## Prof. Anna Keune

TUM School of Social Sciences and Technology



**Fellowship:** Rudolf Mößbauer Tenure Track Assistant Professorship | **TUM-IAS Focus Group:** Learning Sciences and Educational Design Technologies | **TUM-IAS Research Area:** Gender and Diversity in Science and Engineering

Education in STEM and digital skills continues to face lopsided gender representation. Leveraging socio-material historicities for learning promises to foster sustainable and equitable STEM education. The Focus Group is positioned at the intersection of learning sciences and design scholarship and focuses on advancing the understanding of how materials can foster STEM domain understanding for all students, transform what counts as STEM participation, and widen who participates. Guided by constructionist and post-humanist theoretical commitments as well as participatory approaches to design, the Focus Group investigates creative design technologies and computational crafts in school and out-of-school settings to advance understanding of a) the materiality of STEM learning, b) gender equity in STEM, and c) design technologies for inclusive STEM learning by leveraging creative tools and materials.

## Prof. Frank Keutsch

Harvard University



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Jia Chen (TUM Department of Electrical and Computer Engineering) | **TUM-IAS Focus Group:** Air Pollution and Climate | **TUM-IAS Research Area:** Environmental and Earth Sciences, Building Technology

Human activities are directly related to the rise and environmental impacts of the Anthropocene, which have resulted in fundamental changes in the composition of Earth's atmosphere. These changes include increased concentrations of both long-lived greenhouse gases, such as carbon dioxide, and short-lived pollutants such as tropospheric ozone and particulate matter. The resulting impacts on humans and the environment span large spatial and temporal scales, from local urban air pollution to global climate. In this Focus Group, we investigate drivers of urban air pollution using novel sensors and modeling approaches in order to improve the understanding of the most effective mitigation strategies for tropospheric pollution such as ozone and particulate matter within the context of human health and climate. In addition, we develop novel measurements and modeling methods to detect greenhouse gas sources and sinks as well as solutions for mitigating climate change. We also investigate approaches such as solar geoengineering, which is not a solution but potentially could reduce impacts of climate change, albeit with currently highly uncertain risks. The ultimate objective of the work is to enable policy makers to evaluate different approaches for improving air quality and combating climate change.

## Prof. Antonia Larese

Università degli Studi di Padova



**Fellowship:** Hans Fischer Fellowship | **Host:** Prof. Kai-Uwe Bletzinger (TUM Department of Civil, Geo and Environmental Engineering) | **TUM-IAS Focus Group:** Digital Twins of Civil Structures and Protection Systems in a Climate Change Perspective (REACT) | **TUM-IAS Research Area:** Advanced Computation and Modeling

As a consequence of the increasing frequency of extreme events, existing civil infrastructures are often exposed to stresses that may significantly exceed those assumed in their design, leading to a high possibility of loss of effectiveness and integrity. The ultimate goal of our Focus Group is to improve our knowledge on the behavior of infrastructures under extreme hydrological events such as floods and landslides. To this end, we will develop and validate advanced computational high-fidelity coupled models able to simulate the interactions between fluid, soil, and structures, optimized for large-scale computations. Moreover, we will address the huge complexity of such models, studying proper reduced-order models (ROMs) to get real-time accurate results and to overcome their intrinsic deterministic nature. With this aim, uncertainty quantification techniques and novel machine learning approaches are needed to handle the huge amount of monitoring and simulated data, to obtain the correct model parameters and control the errors.

## Dr. Jihyun Lee

University of Calgary



**Fellowship:** Anna Boyksen Fellowship | **Host:** Prof. Michael Zäh (TUM Department of Mechanical Engineering) | **TUM-IAS Focus Group:** Inclusion and Diversity in the Manufacturing Sector in Industry 4.0 | **TUM-IAS Research Area:** Gender and Diversity in Science and Engineering

The Focus Group on Inclusion and Diversity in the Manufacturing Sector in Industry 4.0 involves Anna Boyksen Fellow Dr. Lee (University of Calgary) and her Host Prof. Zäh (TUM). It aims to build new strategies to promote women's participation in manufacturing through digital skills training and enhancing linkages between academia and industry. Insights gained from the analysis will be applied to training female students in the area of advanced manufacturing. The anticipated outcome of this proposal will be strategic guidelines for universities to minimize the gender gap in current and future manufacturing sectors. This outcome will bring socio-economic benefits to Germany, Canada, and other countries.

The long-term objectives are to create a better working environment in manufacturing with gender equality and work-life balance and to overcome labor shortages by training skilled female talent in the manufacturing sector. Skilled female talent will benefit not only manufacturing companies but also society. The deliverables from the project's long-term objectives will be adjusted for the platform of each country and will be used to implement female talent training programs in manufacturing.

## Prof. Örs Legeza

Wigner Research Centre for Physics



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Gero Friesecke (TUM Department of Mathematics) | **TUM-IAS Focus Group:** Novel Tensor Network Methods for Strongly Correlated Quantum Systems | **TUM-IAS Research Area:** Advanced Computation and Modeling

The main research interests focus on the development of novel tensor network state (TNS) methods and their application to strongly correlated quantum many-body systems to simulate and study magnetic properties in solid states, exotic quantum phases, complex molecular clusters, ultracold atomic systems, or nuclear structures. For the method development we combine established methods for simple networks (MPS, MERA, tensor trees) with concepts from quantum information theory and computational mathematics to push the current frontier of moderate system size to much larger and more complex systems.

## Dr. Anastassia Makarieva

Petersburg Nuclear Physics Institute



**Fellowship:** Anna Boyksen Fellowship | **Host:** Prof. Anja Rammig (TUM School of Life Sciences) | **TUM-IAS Focus Group:** Drought Mitigation through Ecosystem Restoration: Challenges and Opportunities | **TUM-IAS Research Area:** Fundamental Natural and Life Sciences

Plant transpiration profoundly influences atmospheric processes. Natural forest ecosystems have evolved a number of mechanisms to stabilize the terrestrial water cycle. While our understanding of them remains incomplete, direct anthropogenic destruction and climate change are disrupting these stabilizing feedbacks. Conversely, preservation and restoration of natural ecosystems bear the promise of enhancing the water cycle resilience, including protection from extremes such as droughts, floods, and violent winds, as well as avoidance of tipping points toward aridity. The Focus Group will explore theoretical problems of how forest-mediated processes affect atmospheric dynamics, including scaling up individual plant processes to synoptically relevant scales. The research will combine TUM's technical and scientific excellence with the knowledge of climate-regulating functions of least disturbed forest landscapes, most of which in Eurasia are located within Russian borders. The goal is to present quantitative evidence about the importance of natural forests for water-related aspects of regional and global climate stability. The research will highlight the results obtained by female scientists on the post-Soviet space, whose contributions so far remain underrepresented in the international literature.

## 2 6

### Dr. Andreea Molnar

Swinburne University of Technology



**Fellowship:** Anna Boyksen Fellowship | **Host:** Prof. Anne Brüggemann-Klein (TUM Department of Informatics) | **TUM-IAS Focus Group:** Diversity in Information Technology | **TUM-IAS Research Area:** Gender and Diversity in Science and Engineering

Despite increasing awareness and efforts made to attract women in computing, they are still poorly represented in information technology (IT). This Focus Group aims to identify and characterize initiatives that promote information technology among women and groups that are not usually represented in computer science. It will consider personal factors of influence, such as values, identity, and life mission. It also aims to determine how IT departments should act during the application process to increase the likelihood that interested students will take the crucial step and enroll once they have been accepted.

### Prof. Peter Nordlander

Rice University



**Fellowship:** Hans Fischer Senior Fellowship | **Hosts:** Prof. Jonathan Finley (TUM Department of Physics), Prof. Stefan Maier (Department of Physics, LMU) | **TUM-IAS Focus Group:** Sustainable Photocatalysis using Plasmons and 2D Materials (SusPhuP2M) | **TUM-IAS Research Area:** Surface, Interface, Nano- and Quantum Science

The synthesis of chemicals is crucial for society but requires an enormous amount of energy. Recent research at Rice University has introduced a new paradigm for the efficient capture and conversion of light to chemical energy, via the antenna-reactor concept. In this project we will explore the full parameter space in terms of materials for antenna-reactor complexes, from plasmonic and dielectric materials as antennas to nanostructured 2D materials as reactors. The latter have great potential for energy conversion due to their high surface-to-volume ratio, the possibility of incorporation of defects, their molecular capture capabilities, and the potential for optoelectronic tuning. Our goal is to determine the optimum combinations of materials for efficient light capture and energy conversion for selected chemical reactions via a comprehensive work program involving theoretical and numerical modeling of light capture, charge generation and transfer, and reaction kinetics, nanofabrication of hybrid antenna-reactor complexes, and fundamental studies of their response using single particle ultrafast spectroscopy and super-resolution microscopy.



## Prof. Daniela Pfeiffer

TUM University Hospital rechts der Isar



**Fellowship:** Albrecht Struppler Clinician Scientist Fellowship | **TUM-IAS Focus Group:** X-Ray and Computed Tomography Research | **TUM-IAS Research Area:** Bio-Engineering & Imaging

The aim of the Focus Group is to improve detection, precise diagnosis, and therapeutic follow-up of lung diseases such as COPD, lung cancer, and infectious diseases (including COVID-19). From a technical perspective, the Focus Group is mainly interested in novel methods for medical X-ray and computed tomography (CT) imaging, with a main focus on photon-counting CT technology, spectral CT applications, dark-field and phase contrast imaging, and machine learning in clinical applications.

## Prof. W. H. A. (Wil) Schilders

Eindhoven University of Technology



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Hans-Joachim Bungartz (TUM Department of Informatics) | **TUM-IAS Focus Group:** Scientific Machine Learning | **TUM-IAS Research Area:** Advanced Computation and Modeling

Computational scientific discovery is at an interesting juncture. While traditionally we have models of lots of different scientific phenomena, our computational capabilities appear unable to keep up. Solving such problems requires tedious work on suitable algorithms as well as getting code to run on GPUs and supercomputers. The next step forward is a combination of scientific computing and machine learning, combining mathematical models with data-based reasoning, presented as a unified set of abstractions and a high-performance implementation. This new area of research is referred to as scientific machine learning.

Mathematics will be essential in addressing the challenges that we encounter in the rapidly evolving field of scientific machine learning. The objective of the Focus Group is to develop new mathematical and computational methods combining physics-based and data-based models, especially also model order reduction methods suitable for application to such hybrid models. Important will be the incorporation of underlying properties, implying the development of mimetic numerical methods.

## Prof. Nikkil Sudharsanan

TUM Department of Sport and Health Sciences



**Fellowship:** Rudolf Mößbauer Tenure Track Assistant Professorship | **TUM-IAS Focus Group:** Behavioral Science for Disease Prevention and Health Care | **TUM-IAS Research Area:** Communication and Information

We study ways to improve the effectiveness of health systems by infusing insights about human behavior into the design and delivery of care and health messaging. We aim to create health systems that engender trust and encourage individuals to seek essential care as well as to engage in preventive health behaviors.

We focus on three major research areas:

1. Prevention of cardiovascular diseases in South and Southeast Asia
2. Improving the effectiveness of health insurance for vulnerable populations in India
3. Communicating health advice and information to the public in an age of misinformation and low trust in science

Our work draws heavily from behavioral science and economic theory. Using randomized experiments and evaluations, we investigate behavior change approaches that are low-cost and scalable. These include interventions delivered through mobile phones and digital platforms, design changes to the health care environment, and approaches that affect behavior through the framing and communication of information to the public.

## Prof. Nitish Thakor

Johns Hopkins University



**Fellowship:** Hans Fischer Senior Fellowship | **Host:** Prof. Gordon Cheng (TUM Department of Electrical and Computer Engineering) | **TUM-IAS Focus Group:** Human-centered Neuroengineering | **TUM-IAS Research Area:** Neuroengineering

Our vision is to take inspiration from the most complex and complete “robot,” the human. More specifically, we want to take inspiration from the human brain to provide intelligence to robots and prostheses. While this is our ambitious vision, our more specific goals pertain to using the bio/neuro-inspired approach we call neuroengineering to implement and transfer some key principles of human sensation, perception, and cognition to robotic mechanisms. Our model robot is the dexterous upper-limb prosthetic hand, a marvel of mechatronics that we have implemented in a dexterous multi-fingered prosthetic hand.

Prof. Cheng (TUM) and Prof. Thakor (JHU) share the interest and expertise in the field of neuroengineering, setting their goal as learning from the human sensory and motor systems, as well as from the brain and its cognitive network (expertise of Prof. Thakor), to create next-generation humanoid robots (expertise of Prof. Cheng). This Focus Group is pursuing the creation of an experimental platform for the examination of sensorimotor embodiment, whereby for example an amputee can learn to restore his or her sense of touch and the ability to act in the world.



## Dr. Benedikt Zott

TUM University Hospital rechts der Isar



**Fellowship:** Albrecht Struppler Clinician Scientist Fellowship | **TUM-IAS Focus Group:** Neuroglial circuits in health and disease | **TUM-IAS Research Area:** Fundamental Natural and Life Sciences

Neuropsychiatric diseases such as Alzheimer's disease are characterized by the dysfunction of neurons, which, due to the high connectivity of the brain, leads to the impairment of neuronal and glial circuits and even hemodynamic dysregulation. Our main goal is to better understand these complex circuits under physiological conditions and their breakdown in the diseased brain. We use two-photon imaging of calcium or glutamate and electrophysiology to detect neuronal and/or glial activity in the living brain of model organisms in real time. By performing behavioral experiments, we can monitor how disturbed circuit functions translate to clinical deficits. Furthermore, we can modulate circuit activity by pharmacology and opto- or chemogenetics. Finally, we test strategies to restore normal activity patterns in the brains of diseased individuals, which might facilitate the identification of drug candidates against Alzheimer's disease and other related pathologies.

**In Focus**

# Machine learning

In the brain's natural intelligence and in DNA, evolution has produced systems for processing, communicating, and storing information that remain unrivaled by technology – and never cease to inspire scientific exploration and creative innovation. TUM-IAS Fellow Reinhard Heckel and his collaborators combine artificial intelligence and information theory to improve existing technologies and devise new ones, such as data storage in synthetic DNA.



**Machine learning is a broad and expanding field of artificial intelligence with diverse, multifaceted branches. The Machine Learning Focus Group of the TUM Institute for Advanced Study centers on the research interests of Reinhard Heckel, who joined the Technical University of Munich in 2019 as an assistant professor in the Department of Computer and Electrical Engineering.**

A Rudolf Mößbauer Tenure Track Fellow of the TUM-IAS, Heckel leads research that explores the fundamentals of so-called deep learning, enables systems to learn from few and noisy examples, and applies deep learning to solving inverse problems in science, engineering, and medicine. In addition, he is a pioneer in encoding and decoding information for storage in the biological molecule DNA.

On behalf of the TUM-IAS, science journalist Patrick Regan spoke with Reinhard Heckel via videoconference in January 2022. Their conversation has been edited for clarity and length.

**Q: Artificial intelligence in general, and deep networks and deep learning in particular, are not just hot topics but have scored some achievements – in the study of protein folding, for instance – that may have real-world consequences. What are the areas you see as most interesting and promising? Are there any areas where you think proponents might risk claiming too much, or expecting too much?**

There are some areas where machine learning works particularly well, and it's well known that it works well. Those are computer vision and natural language processing. I would say most people who work on deep learning work on applications in one of those two areas. Computer vision is very broad. It includes vision for self-driving cars, building apps that can detect how you do an exercise, and it ranges from things like that to surveillance applications and more. Similarly, natural language processing ranges from applications like summarizing news to translating languages or helping as assistants, like chatbots, or also more sophisticated things like supporting other computer scientists in

writing code faster. There are a lot of applications, and it works really well. I personally work in the area of using deep learning for signal and image reconstruction problems.

**Q: Speaking of imaging, you've worked on both radar and MRI. How do you approach these different technologies, and how do these relate to each other?**

Radar and MRI are both imaging technologies. They have in common that a device collects measurements of an object through a physical process. In MRI, the object may be a person's brain. The measurement device is a magnetic coil that takes the measurement. In radar a device sends a signal and receives a response, which is the measurement. In both examples, and really any imaging system, there's a physical process that describes a relationship between the image and the measurement.

Traditionally algorithms that reconstruct an image from measurements were designed without machine learning. Experts, physi-





Patrick Regan (left) and Prof. Reinhard Heckel (right) in conversation via video conference.

cists or engineers, were handcrafting sophisticated algorithms and designing sophisticated models for images and other signals. Most current imaging technologies still work with those traditional algorithms.

But scientists and engineers have realized in the past five years that for all those imaging problems, deep networks work extremely well, and yield significantly better image quality.

**Q: With radar, you have little or no control over the space in which you're making the measurement, whereas with MRI you can engineer a lot of the constraints. So is learning applicable in different ways to those two situations?**

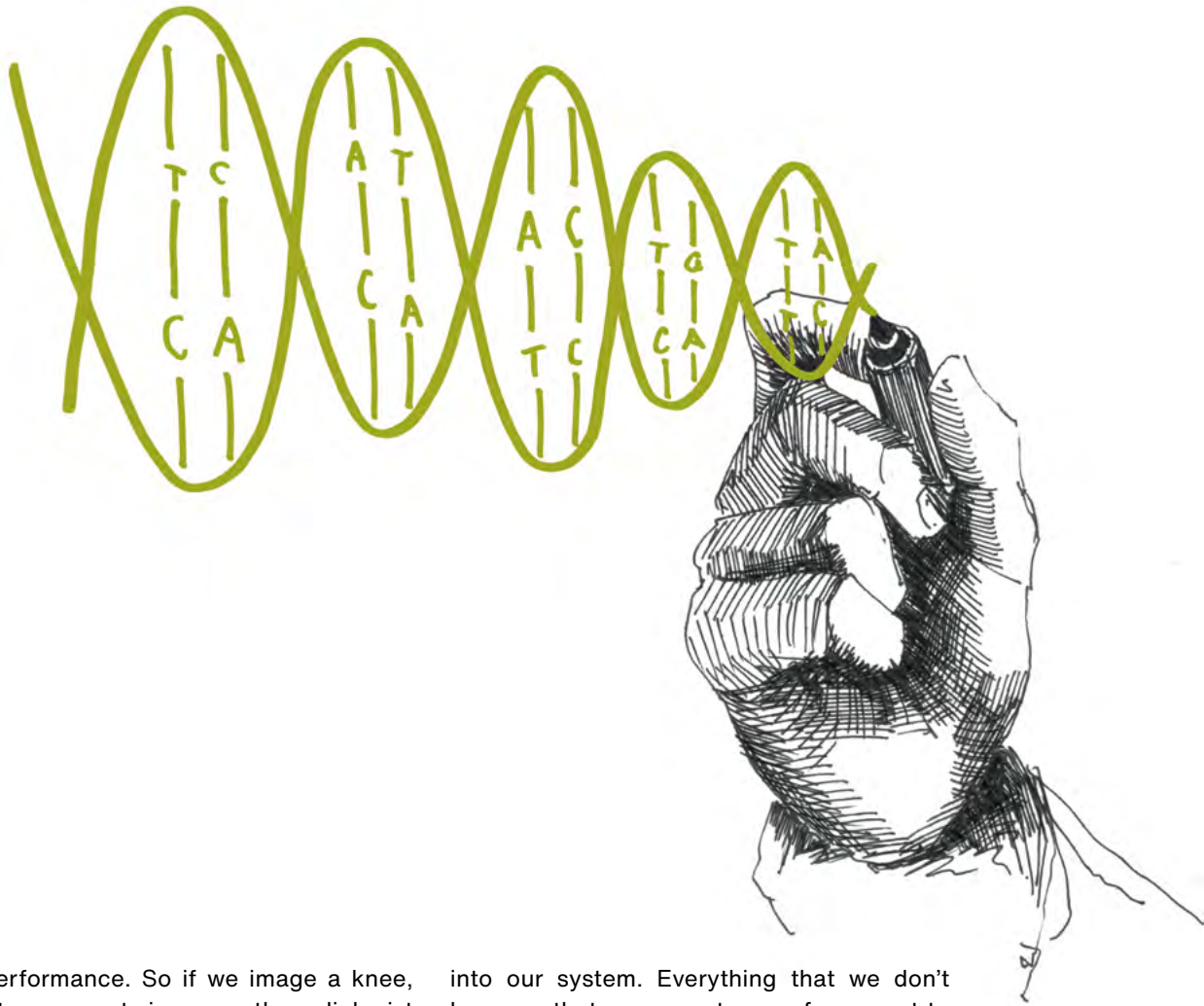
Those technologies are actually quite similar in a way. For an MRI scanner, you can design the sequences that you are running, and thus decide how to take measurements. And similarly in radar you can decide on the signal that you're sending. The reason deep networks perform well in both domains is that both radar and MRI images are difficult

to model accurately using mathematics, and deep networks can learn very good models from data.

For example, it's difficult to mathematically model how a brain looks. But if I show you a few images of a brain, then it's easy for you to tell me what is or is not a brain. Or if I show you a brain and then I draw something, it is easy for you to see that this is not an image of the brain. But it's very difficult to formulate such intuition in computer code. And that's why, in these kinds of problems, machine learning helps a lot. Because it's very helpful for the algorithm to have such knowledge built in. If you're imaging a brain, it's very helpful for the algorithm to know what a brain looks like.

**Q: Do you continue to be active in this area? What does the research focus on?**

In our research, we're interested in developing algorithms that are "learned" from data. We use learning to derive the algorithm itself from data. We are interested, of course, in ►



good performance. So if we image a knee, we want an accurate image so the radiologist can make a good diagnosis based on that.

We're also interested in understanding the inner workings of deep learning-based algorithms, and in providing guarantees about properties like robustness. Our concern is the following. Let's say the algorithm is trained on data from measurements with a particular MRI scanner and a particular patient population in Munich. Then someplace else, the algorithm is applied to data from a slightly different scanner, and another technician operates the scanner, and the patient population is different. I still need to be sure that my algorithm works well as intended. And that is very challenging. Ensuring robustness is what keeps us busy.

**Q: How do you improve the robustness?**

By measuring robustness, identifying robustness issues, and fixing them. We measure robustness by performing experiments on data collected by us, or we work with scientists who collect data. Then we construct algorithms where we build everything that we understand explicitly into the model, the physics for example. Everything that we know, we want to build

into our system. Everything that we don't know, or that we are not sure of, we want to leave open, so that we can learn it on the basis of data. This algorithm design approach works very well.

**Q: And then the process of improvement is writing new code, or asking the networks to do something?**

Sometimes it's not clear what can lead to an improvement. It could be that all you need to do to improve your system is to collect more data, or it could be that you need to improve your model, or it could be that if you have much more data you actually use a different model. If you have much more data, you have more to learn from, and if you have more to learn from, you need to hard-code less into your model. And if you hard-code less in your model, you also have fewer biases in the model that you hard-coded. So you use different models, for example, in a setup where you have a lot of data. We are always thinking about these models and performing experiments to validate whether they work well. We carefully test hypotheses to design a good algorithm. Sometimes we might have an idea about what should work, and that then becomes a hypothesis that we

test. After testing such a hypothesis on data, we go back and forth until we have a well performing and robust system.

**Q: So there's an iterative process of refining the models and algorithms.**

Yes.

**Q: Now, does this connect directly with the DNA storage, or is that a completely separate item?**

It's pretty separate. But I really hope that the idea from imaging that we can learn an algorithm is also applicable in DNA storage. We've started looking into that, because in DNA storage systems, there are situations where we don't have satisfying algorithmic solutions. Specifically, we have algorithms that work but take a lot of computational resources. We want to build algorithms that are significantly faster, and one idea about how to design such algorithms is to learn them from data using deep networks. So there is a connection, but it started out completely separate. Now I am trying to use similar ideas.

**Q: Let's talk about DNA-based information storage. As I understand it: With DNA, you're translating binary code into A-T and G-C bonds? So you use a conventional computer to translate digital information into a sequence of these four amino acids, and then you chemically synthesize strands of DNA with that exact sequence? Then the physical DNA is somehow applied to a surface that can provide you later with samples that can be sequenced, and the recovered sequence can be translated to the original digital data? OK so far?**

Yes, everything is correct.

**Q: So this might, like quantum computing, be practical as long as there are applications that justify the extra effort. For DNA information storage, what would such applications be?**

DNA data storage is already practical today for some specific applications. Of course, there are some storage applications like active working memory in a computer where DNA doesn't make sense. But then there are storage applications where DNA makes a lot of sense. Those are applications where we want to store data with a very high information density. The information density that we already achieve on DNA today is by orders of magnitude higher than what we achieve on tape or on a hard disk.

**Q: So, information per unit of area or volume.**

Exactly. A lot of information in a very small space. And the second reason we are interested in DNA storage is longevity. Data on DNA lasts very long.

**Q: It's counter-intuitive, isn't it. We and all other living things are, in the grand scheme of things, fleeting phenomena. But this molecule outlasts us somehow.**

Yes, there are some good examples demonstrating DNA's longevity. DNA has been found, preserved, in the bones of horses that lived 400,000 years ago. And researchers have been able to extract DNA from the bones of a mammoth more than a million years old. Sometimes insects are found in amber, and from those you can also extract the DNA. If DNA is preserved in a dry form, then it can last very long. ►

***“The information density that we already achieve on DNA today is by orders of magnitude higher than what we achieve on tape or on a hard disk.”***

PROF. REINHARD HECKEL

TGTAGTTGAAGCCAGCCATATCAGGTAACC  
 AGTCTACTAGCCAAAGGBCCTGCAAAACCCB  
 TTCTGCGTAACTGAGCGGATGTATTCC  
 GATAAGTACTCTGTAATTGTGTTGATCGAT  
 GGAGCAGATCATCGAACCGATTGATATA  
 TCTATCTACTTCTAACTGATTATCGTC  
 TCGTTGGGAATGGTTTCCGCTCTCAAC  
 TTTAAGCGCGTTACGATCTGTCTACTTGT  
 GCGCATTTGTGTCTTTATCGAATAGAAC  
 AATATAATTCTGTTATATACATCTCTTC  
 ACGTGAAGTCTTTCTTATAGGTAGAACAT  
 TATAGGANGGTGTACGCGTCTGCTTTTC  
 CCGAGAGACCTAGTCAACCTCTTATTGG  
 CATTCGCGATGAGTCTGATCTTGTGGACG  
 TTGTCACTTTAGTCAGCCACAGTGAGCAC  
 GGGTAAGTCTGTTGTTAGGACTCGAGGG  
 CCACTTCTGCGCTATAGGATCACTGCGG  
 TGACC TGCGCATGCGATTACACGAAAT  
 ACGAGACGGGCACTACAGGATGTATAT  
 TCTGCTCGAGGCTGGATGAGTATAGCTC  
 CTAGGAGGCGACCGAGACTACTTAGAT  
 ATTAGGATTTCTATTCCTGCTGCGGAGT  
 GTGATCGAGACTGCGACACAAAGAAATGT  
 TATCAACTCTGCGCTTAAAGACTAAGAC  
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 TGTCTAGATTAATTTTGTAGCTCCGA  
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 GCGACAGCTCAATGAATGATACAAAGGCT  
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 GAGATGAGGAAATGATGATGGTGGCCCG  
 GTTGTGTGTTAGGCGCTAAACATGT  
 TACGCACTCAACACTCTAAGGCGCTTGG  
 TACTGCACTGCTTATGCTATCGTCC  
 GAGCTGCTGATCTCAACGCAACACCACT  
 CATCTAGTTAAGACTGTGCTGCTATCA  
 AGCTTGGTAGGAGCTAGGCTCTTAAAC  
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 AGTCTACTAGCAGAGGCTCGAAGCCCG  
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 GCGCATGTGTCTTATGAGACTGAGAC  
 AATATATCTGTTATATACATCTCTTC  
 ACCTGAAGTCTTCTTATAGGTAGAACAT  
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 CCGAGAGCAGCTAGTCAACCTCTATTTC  
 CATTTGCTGATGATGATAGGTTTGGACCG  
 TTTTCACTTTAGTCAACACAGTGAGCAC  
 GGGTAAGTCTGTTTATAGGACTGAGG  
 CCACTTCTGCTATAGGATCACTGCG  
 TGACTGCGCATGATTAACGCGAAGT  
 ACAGGACAGGCGAGTACAGGATGTATAT  
 TCTGCTGAGGCTGATCACTCAAGCTC  
 CTAGGAGGCGACCGAGACTACTTAAGAT  
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 GGTCCAACTCAACTGATCAGGAGTCACT  
 TTCTAAGGCAACAAATCACGATCGCTGA  
 GCGGTTCCTCGCGGTGATCGGTGAT  
 GAGATGAGGAAATGATGATGGTGGCCCG  
 GTTGTGTGTTAGGCGCTAAGCAATGT  
 TACGCACTCAACACTCTAAGGCGCTTGG  
 TACTGCACTGCTGCTTATGAGTATCGTGC  
 GAGCTGCTGATCTCAAGCAACACCACT

A list of short DNA sequences (one per line) on which data is stored.

**Q: I'm still grappling with how you package it so that a person in the future will recognize what it is and know what to do with it. That question seems comparable to labeling nuclear waste as hazardous in a way that future generations should understand, something people are working on right now. The potential longevity of data stored in DNA makes me think of the Voyager space probes, which are carrying information about us and our world into the universe beyond the solar system. As unlikely as it may be that the golden disks will ever be retrieved and understood, if that does happen, the information they contain might have outlived human civilization. Potentially, what you're working on may not be so different.**

That's a good point. It's also a separate problem in a way, an important problem. If you want to store something for a long time, you still have to remember how you stored it and what you even mean with all that information. Even if we write sentences in English, we have to understand the language, and on a lower level there are additional ways we write data and encode it, and we have to remember "in what technical language" we wrote that information. This meta information has to be preserved as well, potentially close to the storage medium. The Voyager golden records are a good example. They were included aboard the Voyager spacecrafts and are a sort of time capsule. Those records carry information on how to read the information on the disks.

**Q: Right, there are instructions on how to play it. So there are a bunch of important steps involved. Where are you placing most of your emphasis?**

For the DNA project, I put all my energy into the encoding and the decoding. My chemist collaborator, Prof. Robert Grass, does all things chemistry. I essentially tell them, here is what we need to write, and then they write it on DNA, carry out an experiment, and return the read DNA back to me. Everything in between encoding and decoding is really the job of a chemist.

**Q: Your main collaborators are still in Zurich?**

Yes, at ETH Zurich. That's a collaboration that's been going for ten years now.

**Q: Do you foresee any application that would correspond to short-term working memory in a computer or communication system?**

No, not really. There are different things that you want from memory. In some indifferent applications you want to store a lot of data. There are applications where the data should be very dense. There are applications where the data should last very long. And there are applications where the data should be accessible very quickly. Depending on what you're interested in, one storage medium is better than the other. DNA will never be extremely fast to access. It will never be as fast to read and write as the working memory in your computer. Some chips have memory access times of 10 nanoseconds and less. But then there are some things you can only do with DNA right now. For example, we had one project where we stored the music of a rock band in DNA. We put it in spray paint, and the band made a graffiti painting with it.

**Q: So the painting could be sampled, the sample could be sequenced, and the resulting digital file could then be played?**

Yes. If you scratch off just a tiny piece of the painting and take it to the chemist, Prof. Grass, he can extract the DNA, and then you give the data to me to decode it, and you get all the music back.

**Q: So in the graffiti painting, there would be millions of copies of this sequence.**

Millions.

**Q: And each one is like a hologram of the original file?**

Right. You have millions and millions of tiny copies everywhere, and if you take just a little bit, you can get all your data back. I don't see how you could do that with anything else right now. And you can even embed it in plastic and things like that. So there are applications for which DNA is already interesting now.



**Q: To what extent is this approach to encoding and decoding tied to classic information theory? At the time information theory was first being developed at Bell Labs, other researchers there were creating some of the essential components for digital computing and communications. Information theory and transistor-based electronics seem to be made for each other. This makes me wonder: Is there something else that might be “made for” DNA? DNA may suggest potentials that a binary operation, or even superposition scenarios, could not do or would not even suggest. Are you tempted to rethink information theory?**

That’s a good question. We used a lot of the coding theory that was developed at that time, and we build on the information theory that was developed at that time. When there a new storage medium, like DNA, arises you need to develop new or update current information theory for the particular problem. So what is particular about DNA, why it is necessary to develop new codes, is the following. Typically when you store information or you send a signal, you just have a relatively long string of data. In a hard disk, it’s just written on your disk. And you know where you wrote it. It’s just physically there. That’s what’s different about DNA. In our bodies, DNA is very long, it’s a very long sequence, about three billion nucleotides. But we cannot write long pieces of DNA. It’s not possible now, and it doesn’t look as if it’s going to be possible any time soon. What we can do is write very short pieces of DNA. Those pieces are typically a hundred nucleotides long.

**Q: Analogous to packets in data communications? Or so-called shotgun sequencing in DNA analysis?**

It’s related to shotgun sequencing. We do shotgun sequencing because it’s difficult to read long pieces of DNA. If we could just read the entire DNA of a person, we wouldn’t need shotgun sequencing. We can only write and read short pieces of DNA, so we have to split long pieces of DNA into smaller ones to read it, and that’s why scientists do shotgun sequencing.

**Q: So part of the encoding process is splitting it up?**

Exactly. However, even if you split things up into blocks, you typically know where these blocks are. But in DNA, you have the following situation: We can write short pieces of DNA, and we can write as many as we want. But then the writing is imperfect. We make a lot of errors when we write.

**Q: So you had to invent error correction for DNA as well?**

We didn’t have to invent it. We could build our codes on the work of Shannon, Hamming, Reed and Solomon, and others. But we had to make specific information theory for the DNA data storage channel. A channel model distorts the information at its input. For DNA, we have a very different channel model, and when you have a different channel model, then you have to study that, and you have to study the capacity again, which Shannon defined. Then you have to develop codes for that. Essentially you use the language of information theory.

**Q: Even though you’re dealing with this chemically synthesized material.**

Exactly. It’s really nice that you brought this up, because that’s really what I’m doing. That’s why the encoding and decoding is interesting. If you could write a long piece of DNA, then we could use established techniques. I would think: All these information theory problems are solved already, so I’m just going to use existing codes. There wouldn’t be much to do from a research perspective. That would also be fine, right? Then I would have worked on something else. But one other thing that’s specific to DNA is that you also have deletions and insertions. That makes it difficult too, because we don’t have good codes for deletions and insertions, and we actually don’t understand fundamental questions on the capacity of deletion and insertion channels. ►

**Q: But I'm guessing you're not looking for a biomimetic approach to coding.**

No. We are not trying to mimic biology in any way. You mentioned that transistors and information theory are kind of made for each other. The one thing you can do very easily with DNA is to copy it. That's very cheap. But other than that, we are not trying to use biological approaches. I don't think it makes that much sense. There are also some error correction mechanisms in biology, but it's very inefficient because of the computational limitations that biology has. So I don't think there's anything there to mimic, unfortunately.

**Q: Last question on DNA. What do you imagine a DNA-based archive or library would look like at some point in the future? How do you picture people interacting with this information source, putting things in and taking things out?**

I think eventually it's going to look more or less like a USB stick. There is already a device only slightly larger than a USB stick that can read DNA. I imagine if it's ever going to really become a thing like that, it will probably be a device that can read and write the DNA, so you can put information in and out.

**Q: Something using microfluidics integrated with electronics?**

I think that's the vision. But who knows what will happen? It can also be that DNA storage will just not take off for long-term storage of information, but then it'll likely have another application area. For example, for marking products or embedding information in them, you might use DNA storage as an industrial tool. That's the first thing that will happen, I think. Because it's much easier. You don't have to store so much information. You can make use of the fact that you need to copy it.

**Q: So, for example, the information could be in the ink on the label?**

Yes, the information can be in the ink. DNA can be embedded in many objects. It can be in olive oil, to mark where the olive oil is coming from. The first successful applica-

tions of DNA storage are going to be things like that.

**Q: So it could have applications in control and logistics.**

That's right.

**Q: Your last position was in the Computer and Electrical Engineering Department at Rice University, and clearly that's a good place to be. How did TUM lure you away?**

Rice is actually a fantastic research environment. It's a small department but functions very well. The people are very nice and supportive, and it's very good for young scientists. TUM was interesting, first, because within Germany it is the best university, so it attracts good students. And it's a big university, with lots of students. If you have a lot of students, then there are also many especially good students. That makes it easier to find good PhD candidates at TUM, and good PhD candidates are super important. That was one of the main reasons I came here.

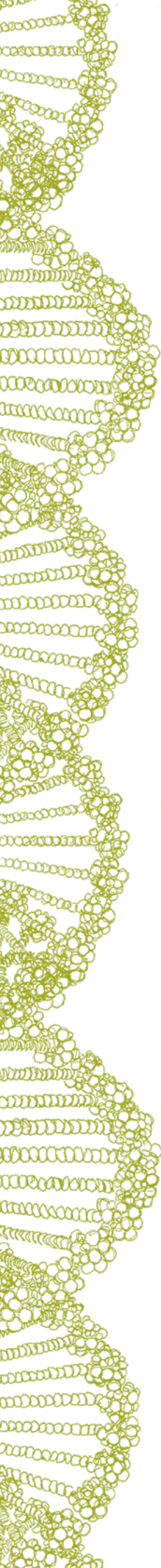
**Q: Did the Mößbauer Tenure Track program and the connection to the TUM-IAS offer any special advantages that played a role in your decision?**

That did make it more interesting. The TUM-IAS provided funding to start with and to build a lab. That was very helpful. That gave me extra freedom at the beginning. The money is not tied to one or the other thing. That's very important at the beginning. I traveled quite a bit, and I bought some equipment like computers that you can't easily purchase with public grants. So the freedom of having the funding and being able to use it for anything I want was very important. I think that is very important in general. Ideally, money in research should come with very few strings attached. Then it's going to be used most efficiently.

**Q: What kinds of topics are your current PhD candidates working on?**

In imaging we have seen that image reconstruction problems can be solved by tradi-





***“In imaging we have seen that image reconstruction problems can be solved by traditional algorithms without any learning, but we can do much better when we learn the algorithms from data, that is, if we take a data-driven approach to imaging.”***

PROF. REINHARD HECKEL

tional algorithms without any learning, but we can do much better when we learn the algorithms from data, that is, if we take a data-driven approach to imaging. The reason is that machine learning algorithms can learn very effective prior assumptions about the data. So they learn structure about the data. In imaging, the algorithms learn what natural images look like.

I think this idea is much more broadly applicable. For example, we are interested in other types of data, such as proteins. In medicine and chemistry it is very important to know what a given protein looks like, for drug discovery and other applications like that. To image and use a protein in a computer system, we want to view the protein as protein, not as an image of a crystal. Because it moves and occurs in different configurations. You don't want to view it as a 3D object. You want to see and model it for what it is, and for this neural networks and machine learning can be very effective.

One concrete project we are working on is how to learn prior assumptions about such objects. Of course we can work with imag-

es of such objects, but then we're not really interested in the image per se, we're interested in a representation of that object. The same thing goes for other types of data. For example, in communications, potentially, you have a channel, and it's not an image, but it also has some representation. And what I'm interested in, and also what a lot of my PhD candidates are working on, is how we can take the idea of learning in algorithms to other fields and other types of data.

**Q: Are any of them working on the DNA side yet?**

I just found an excellent young student. She started in April 2022 to work on DNA data storage, and I'm very excited about what she'll do. It's been a bit more difficult to find such an excellent student for DNA storage than for machine learning. A student in that area needs to have similar skills, but many of today's students want to work on machine learning, because it is hot right now. There was a time when all the smart students wanted to work in information theory. Now a lot of the best students want to do machine learning. ■







# Scientific Reports

When their research projects come to an end, we ask our Fellows to contribute a Final Scientific Report with 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 Supramolecular Chemistry

**Prof. Job Boekhoven (TUM)**, Alumnus Ruldbf Mfbbauer Tenure Track Assistant Professor | **Dr. Marta Tena-Solsona (TUM)**, Postdoctoral Researcher



**Prof. Job  
Boekhoven**

# Assembling molecules using chemical reactions

**The Supramolecular Chemistry Focus Group develops molecular self-assembly regulated through chemical reaction cycles. We use this method of creating molecular assemblies to synthesize materials with life-like properties; this approach might ultimately be used to synthesize life.**

**[1]** van Rossum et al. (2017); RieB et al. (2020).

**[2]** Tena-Solsona et al. (2017).

We design molecules to bond with each other through reversible, non-covalent interactions. As a result, these molecules stack on top of each other to form larger structures, a process called self-assembly. Life could not exist without such molecular assemblies; a cell's membrane, cytoskeletal network, and nucleus are exemplary structures. Besides biology, we also find assemblies of molecules in everyday materials such as gels, soaps, foams, and liquid crystals. The question we ask ourselves is, could we design molecules that assemble and form structures as intricate, complex, and beautiful as living ones? Could we synthesize life?

One of the reasons we cannot, yet, is because life operates out of thermodynamic equilibrium, whereas most of our knowledge in supramolecular chemistry applies to assemblies in equilibrium. Living systems, including the cell, are not thermodynamically stable but require a constant influx of energy (a cell will require nutrients to survive). As a result, most biological assemblies are controlled by energy consumption and dissipation kinetics [1]. Part of our group has concentrated on advancing the fundamental understanding of

molecular self-assembly out of equilibrium. We designed molecules to self-assemble when driven by chemical reactions, which is very similar to how biology self-assembles its molecules. With that approach, we aimed to understand better why and how biology regulates structures and their function with chemical reactions. We also aimed to create materials with more life-like properties, such as materials that make autonomous decisions, for example to adapt to changes in their environment. Finally, we envision that such knowledge can help us understand better the fundamental principles of life, which could shed light on our own origins and potentially enable steps toward the synthesis of life.

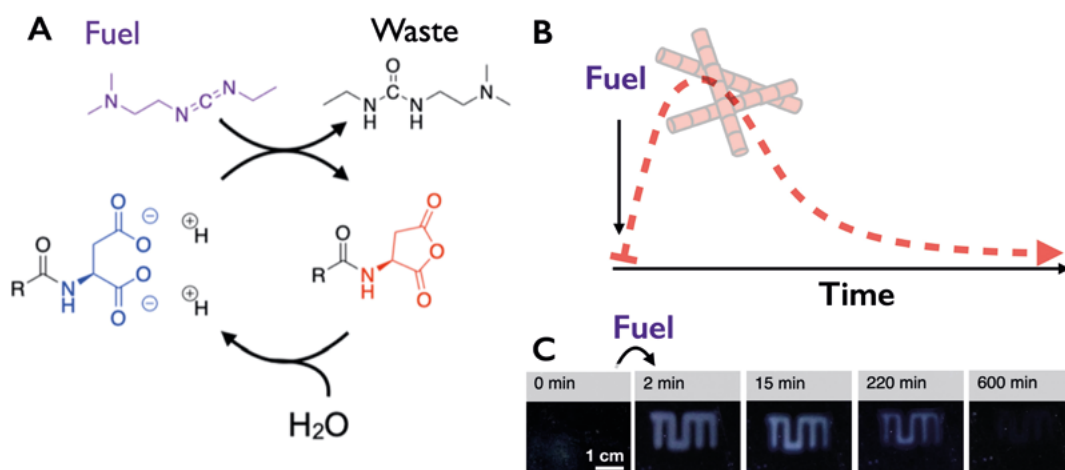
We first designed a chemical reaction cycle that can act as the engine for our molecular assemblies (Figure 1A) [2]. That reaction cycle "burns" up a chemical fuel to operate. While doing this, it activates and deactivates molecules for self-assembly. In this manner, molecules can only self-assemble after being chemically activated by an energy-consuming reaction. Simultaneously, they are spontaneously deactivated by a deactivation reaction. Thus, this type of self-assembly is a



non-equilibrium process (it constantly requires energy to sustain), which is fundamentally much closer to the way biology organizes its supramolecular structures.

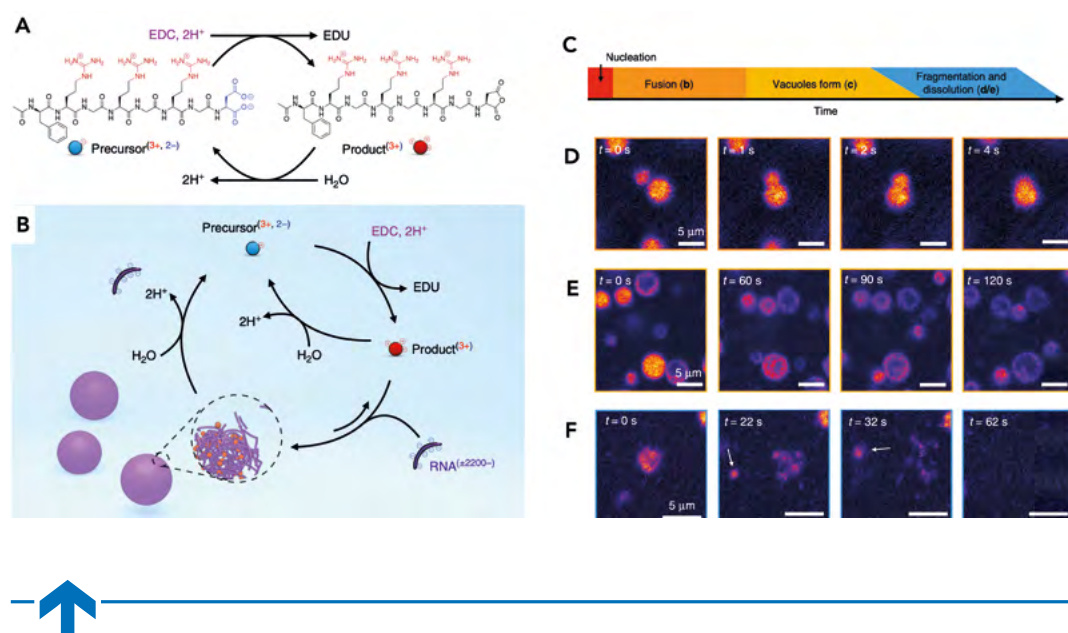
We introduced a chemical reaction cycle that fulfills the above requirements. It uses carboxylic acid derivatives as precursors and carbodiimide-based condensing agents as fuel. The carboxylic acids are converted into metastable anhydrides (activation) when fuel is added. These anhydrides rapidly hydrolyze back to carboxylic acids (deactivation). We designed the molecules such that they would assemble into supramolecular architectures or phase-separate into droplets in the activated state. Under these condi-

tions, the self-assembly process is kinetically controlled; that is, if a lot of fuel is present, activation outcompetes deactivation and the assemblies grow. If the system is starved of fuel, the assemblies collapse. A molecular assembly is only temporarily present if a finite amount of fuel is added. We demonstrated that this could be used as a self-erasing ink or a hydrogel that self-abolishes. In more recent work, we have shown that the assemblies can also be used to deliver drugs with tunable release profiles; we can set how rapidly and for how long a specific drug is released from its carrier. Thus we have used our approach of non-equilibrium self-assembly to control the decay profile of materials. ►



**Figure 1.** Chemically fueled self-assembly. **A)** Scheme of the chemical reaction cycle for the fuel-driven formation of a transient product. The dicarboxylate precursor (blue) is converted into an anhydride product (red) by consumption of a carbodiimide (fuel). The aqueous anhydride is unstable and rapidly hydrolysis back to the original precursor. Because of the loss of charges when anhydride is formed, the product self-assembles upon certain concentration. **B)** The result of the chemical reaction cycle is that the product and its associated properties are only temporarily present after fuel addition. **C)** Using a chemical fuel as an ink, the TUM logo can be written by supramolecular assemblies. As these assemblies are fuel-dependent, the message disappears as the message runs out of fuel.





**Figure 2.** Chemically fueled coacervate-based droplets. **A)** Molecular design of the peptide that switches affinity for RNA. **B)** Schematic representation of the chemical reactions playing a role in the formation of droplets. **C)** The lifetime of a chemically fueled droplet. After application of fuel, the droplets emerge. In the first minutes of their life, they rapidly fuse with other droplets. After 10 minutes, the first observation of their decay is evident, i.e., vacuoles start to form. As the system runs low on fuel, droplets start to dissolve. In some cases, dissolution results in asymmetric self-division. **D–F)** Confocal microscopy time lapses of the above-mentioned events.

[3] Donau et al. (2020); Späth et al. (2021).

As we learned how to use our new chemical reaction cycle to drive self-assembly, we focused on bigger research questions: Can we use the transduction of chemical energy to sustain synthetic life? For that, we created a synthetic compartment that would serve as our synthetic life form. The compartments we developed are vesicles (like the cell wall), oil droplets, and complex coacervates. Each of these compartments was sustained by our chemical reaction cycle; thus each of these compartments emerged in response to energy, was sustained for some time, and then decayed when energy was depleted. Emergence, death, and compartmentalization are all hallmarks of life.

We wish to highlight one of these chemically fueled assemblies, the complex coacervate-based droplets [3]. In this work, we designed a peptide coupled to the above-mentioned chemical reaction cycle (Figure 2A and B). In its precursor state, this peptide does not interact with RNA. In contrast, in its product (activated) state, the peptide can form a complex coacervate with RNA (it can glue together the RNA). The result is that RNA-containing coacervate-based droplets emerge in response to fuel (Figure 2C). Initially, the droplets are small, but they rapidly grow due to fusion and by taking up more droplet materials (Figure 2C). When fuel is running low but not fully depleted, the drop-

lets show signs of their evolution toward death. Large holes appear within them, so-called vacuoles (Figure 2E). In the final stage of their “life,” which coincides with the time when all fuel is depleted, these droplets lose their integrity and fall apart, though not before one final spectacle: The droplets fall apart into hundreds of tiny droplets that eventually dissolve (Figure 2F).

We believe these droplets have great potential in our design of synthetic life. First, they show some living systems traits, including emergence, death, and self-division. Moreover, these droplets have an aqueous inner compartment and can up-concentrate water-soluble molecules from their environment.

Their ability to harvest nutrients from their environments opens the door to Darwinian evolution. In the next steps in our search for synthetic life, we would combine these droplets with autocatalytic reaction cycles, such that the droplets can synthesize the building blocks for their existence.

In summary, our Focus Group has made significant strides toward supramolecular chemistry out of equilibrium by introducing a simple, versatile chemical reaction cycle. The reaction cycle is now being used by other chemists worldwide. We used the cycle to demonstrate a new concept in materials science and to enable advances toward the synthesis of life. ■

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**For a full list of publications please see** <https://www.ias.tum.de/ias/active-fellows/boekhoven-job/>

## Focus Group Environmental Sensing and Modeling

**Prof. Jia Chen (TUM)**, Alumna Rudolf Mößbauer Tenure Track Assistant Professor | **Dr. Shrutilipi Bhattacharjee (TUM)**, Postdoctoral Researcher | **Florian Dietrich, Xinxu Zhao (TUM)**, Doctoral Candidates



**Prof. Jia Chen**

# Urban greenhouse gas and air quality monitoring

[1] Dietrich et al. (2021).

[2] Chen et al. (2016).

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[4] Chen et al. (2020); Toja-Silva, F., Chen, J., Hachinger, S., Hase, F. CFD simulation of CO<sub>2</sub> dispersion from urban thermal power plant: Analysis of turbulent Schmidt number and comparison with Gaussian plume model and measurements. *Journal of Wind Engineering and Industrial Aerodynamics* 169, 177–193 (2017). <https://doi.org/10.1016/j.jweia.2017.07.015>.

**Our research tackles two of today's most urgent challenges: climate change and air pollution. My group and I have not only developed new types of sensors, but also carried out research on interdisciplinary issues, including the development of novel mathematical methods and atmospheric models. We have initiated two pilot projects, unique in the world, to quantify urban greenhouse gas emissions and air quality.**



**Figure 1,** Illustration of the Sensornetwork MUCCnet including satellite measurements, air quality sensor network, and emission inventory.

### Worldwide unique greenhouse gas network

In 2019, my group established a fully automated long-term sensor network in Munich to measure CO<sub>2</sub>, CH<sub>4</sub>, and CO [1], which is based on the differential column measurement (DCM) principle that I developed [2]. The network consists of five solar-tracking Fourier transform infrared (FTIR) spectrometers integrated into our patented automated enclosure systems [3]. The configuration of the network is depicted in Figure 1. Four stations are located on the outskirts of the city to capture the inflow/outflow column concentrations in arbitrary wind conditions. One inner-city station serves as a permanent downwind site for half of the city.

The fully autonomous DCM sensor network in Munich is the first of its kind and unique worldwide. With this network, my group monitors the long-term greenhouse gas trends in Munich and traces unknown emission sources with unprecedented accuracy [4]. We are currently developing an extension to the sensor system that will measure NO<sub>2</sub> and O<sub>3</sub> in the future. Our automated enclosure systems are deployed not only in Munich, but also in places at extreme latitudes, and with difficult access and demanding climatic conditions, e.g., in Finland, north of the polar circle, and in Uganda at the equator [5]. The system in Uganda provides the first ground-based observations of greenhouse gas columns over East Africa, thus enabling the study of wetland emissions, which account for a third of global methane growth. The modeling approaches we developed have also been used to assess emissions in other cities in the world [6].

### A new concept for assessing urban air quality

To assess the human exposure to air pollutants and define the best mitigation strategies for NO<sub>x</sub> and PM, we need to gain a better understanding of their spatial distributions at the neighborhood level. The very limited spatial coverage of the present governmental stations, however, prevents us from achieving this goal. Further, the governmental stations do not necessarily capture the street level pollutant exposure, as their inlets are positioned 4 m above the ground. Our in situ mobile measurements reveal a discrepancy of 48% between the governmental stations and the spatially averaged street-level data in their vicinity [7]. My group is currently setting up an autonomous NO<sub>x</sub>, PM, CO and O<sub>3</sub> network in Munich, consisting of 50 stand-alone sensor systems. My group developed these systems, which are characterized by very low power consumption, an IoT (Internet of Things) communication interface, and a compact and lightweight design. The sensor network will provide air quality measurement data with a high spatial (every 200 m) and temporal (1 min) resolution. To ensure data quality, these sensors will be automatically calibrated twice a week, using high-precision mobile reference sensors. The calibration process will be supported by machine learning algorithms to compensate for cross-sensitivity, drift, and aging effects. ►

[5] Dietrich et al. (2021).

[6] Jones, T. S., Franklin, J. E., Chen, J., Dietrich, F., Hajny, K. D., Paetzold, J. C., Wenzel, A., Gately, C., Gottlieb, E., Parker, H., Dubey, M., Hase, F., Shepson, P. B., Mielke, L. H. & Wofsy, S. C. Assessing urban methane emissions using column-observing portable Fourier transform infrared (FTIR) spectrometers and a novel Bayesian inversion framework. *Atmos. Chem. Phys.* 21, 13131–13147 (2021), <https://doi.org/10.5194/acp-21-13131-2021>; Zhao, X., Marshall, J., Hachinger, S., Gerbig, C., Frey, M., Hase, F. & Chen, J. Analysis of total column CO<sub>2</sub> and CH<sub>4</sub> measurements in Berlin with WRF-GHG. *Atmos. Chem. Phys.* 19, 11279–11302 (2019), <https://doi.org/10.5194/acp-19-11279-2019>.

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**[9]** Shekar, A. et al. (2020b); Castro, A. O., Chen, J., Zang, C. S., Shekhar, A., Jimenez, J. C., Bhattacharjee, S., Kindu, M., Morales, V. H., Rammig, A. OCO-2 Solar-Induced Chlorophyll Fluorescence Variability across Ecoregions of the Amazon Basin and the Extreme Drought Effects of El Niño (2015–2016). *Remote Sensing* 12, 1202 (2020), <https://doi.org/10.3390/rs12071202>.

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**[11]** Bhattacharjee, S. & Chen, J. (2020).

### Application of satellite data

I am a member of the NASA OCO satellite science team and use this one-of-a-kind dataset of global CO<sub>2</sub> concentration and SIF (solar induced fluorescence) to study important questions relating to CO<sub>2</sub> emissions. For example, we were able to reveal that CO<sub>2</sub> emissions from the Nile Delta are about 1% of the global anthropogenic emissions, which is significantly more than previously assumed [8].

Apart from identifying greenhouse gas sources worldwide, we are also interested in how

climate change affects the behavior of carbon sinks [9]. We also employ the data of the European Sentinel-2 satellite in our studies: With the help of a neural network, this data was used to quantify the distribution of the invasive eucalyptus population in Portugal [10].

Moreover, we pursue innovative approaches to data fusion, which are of vital importance in analyzing satellite data. My group developed the Semantic Kriging method, which creates new possibilities for spatial interpolation of measurement data [11]. ■

### Selected publications

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**For a full list of publications please see** <https://www.ias.tum.de/ias/chen-jia/>



**Figure 2,** South station of MUCCnet in Taufkirchen.

## Focus Group Modeling Spatial Mobility

**Prof. Rolf Moeckel (TUM)**, Alumnus Rudolf Mößbauer Tenure Track Assistant Professor | **Prof. Kelly Clifton (Portland University)**, Alumna Hans Fischer Senior Fellow | **Dr. Ana Tsui Moreno Chou (TUM)**, Postdoctoral Researcher | **Qin Zhang (TUM)**, Doctoral Candidate



Prof. Rolf Moeckel

# Agent-based model of people and travel behavior

**This team develops agent-based models for the simulation of travel behavior, demographic transitions, housing markets, and traffic flows. The microscopic integration of these models allows for a consistent analysis at the agent level. Implications for health, well-being, and the environment are of particular interest.**

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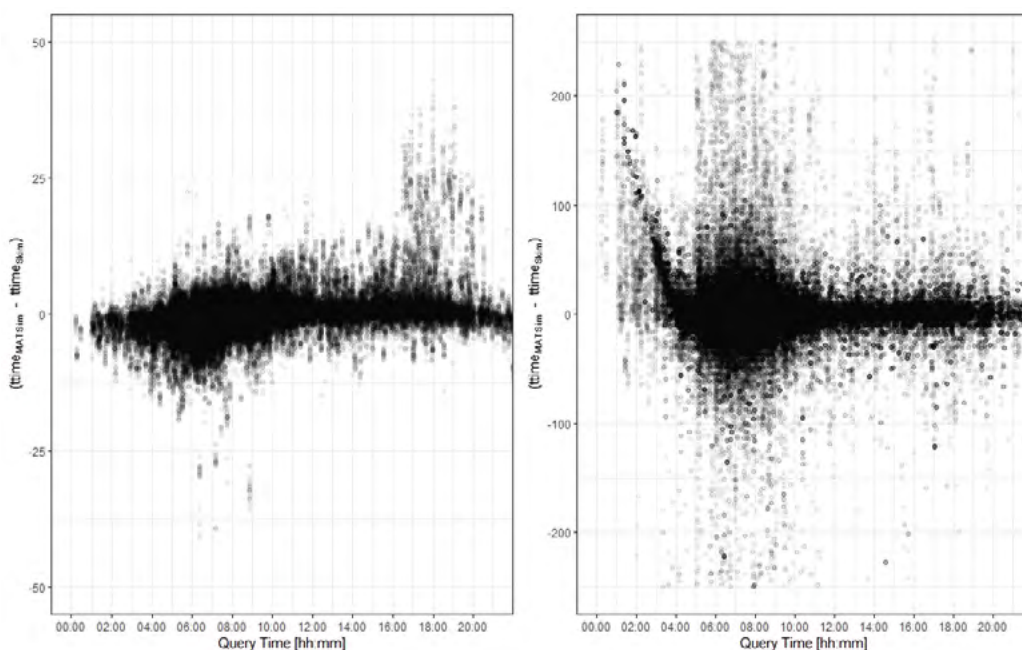
The Focus Group Modeling Spatial Mobility (MSM) was established in 2015 and focuses on integrated land use/transport modeling and travel behavior research. After Prof. Moeckel was granted tenure in 2021, it was renamed Travel Behavior (TB) to better account for the larger scope of research. Currently, the team works on model development of land use, transport, and related models, such as environmental impact models and health models. This also includes the spatial analysis of travel behavior and location choice of households and firms. The interaction between land use and transport is of particular interest.

An integrated land use/transport modeling suite was implemented for the Munich Metropolitan Area. The base year is 2011, and the model simulates land use and travel behavior through 2050. The study area consists of 444 municipalities with a population of 4.5 million, subdivided into 4,924 automatically generated zones [1]. The study area has been delineated on the basis of commuter flows. The modeling suite consists of the land use model SILO [2], the travel demand model

MITO [3], and the assignment model MATSim. The former two were developed from scratch by this research group, and the latter was developed at ETH Zurich and TU Berlin. All three models are built as agent-based models that simulate individual households and persons.

In cooperation with Hans Fischer Senior Fellow Dr. Kelly Clifton from Portland State University, the existing modeling suite was extended by the pedestrian model MoPeD [4]. MoPeD coefficients were reestimated with Munich data and integrated with the above-described SILO/MITO/MATSim modeling suite. All models developed by this research group are open source under the GNU license and provided at <https://github.com/msmobility> free of charge. Interested users are welcome to download, use, and further develop these models. As far as legally possible, data to run these models are shared as well.

Complementing this work is the exploration of walking behaviors and the links to health outcomes using novel data sources. The emergence of longitudinal, location-based data offers the potential to understand the



**Figure 1,** Difference between agent-based travel times (ttimeMATSim) and morning-peak skim-based travel times (ttimeSkim) for auto (left) and transit (right) in minutes.

variability of individual activity and travel patterns. We have used Google Location History data to better understand travel behavior over a longer time period and to explore the impact of life events on travel behavior. In cooperation with Dr. James Woodcock from the University of Cambridge, we are adding a health model to our models to explore the impact of active mobility on the individual health status.

A novel aspect of the work conducted at TUM is the agent-based integration of land use and transport models. Traditionally, so-called

skim matrices are calculated that provide travel times from zone to zone at a given time of day. In our microscopic integration, highly aggregate skim tables are not required anymore, but rather individual queries of travel time are calculated between two x/y coordinates at a specific time of day [5]. Figure 1 shows the resulting difference. Differences in transit (right figure) are substantially larger than for auto (left figure), as the true schedule at a given time (agent-based integration) is more accurate than the skim-based travel time (traditional integration) queried during the morning peak. ►

[5] Kuehnel, N. et al. (2020b).



- [6] Kuehnel, N. & Moeckel, R. (2020a).
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Special attention was given to the simulation of traffic noise. Traffic noise has severe health impacts. Traffic noise can lead to sleep disturbances, tinnitus, and cardiovascular diseases, and it increases the risk of heart attack by 20% for every sixth person in Germany. Figure 2 shows the simulated traffic noise volumes in Munich, accounting for shielding and first-order reflections. While major arterials create high noise levels, inner courtyards are often very quiet despite central locations.

The impact of traffic noise volumes on housing costs were analyzed econometrically. It was found that moderate noise levels between 55 and 65 dB(A) lead to a price reduction of six percent while high noise levels above 65 dB(A) reduce housing cost by ten percent [6]. This has severe equity implica-

tions. Residents with higher income (who tend to have higher auto-ownership rates and tend to generate more traffic noise) often are able to buy out of traffic noise, while people with lower income may not be able to afford a quiet place to live [7].

The agent-based (but trip-based) travel demand model MITO is currently replaced with an activity-based travel demand model. Such models do not simulate trips for the sake of traveling, but rather simulate activities at different locations, and travel results as a necessity to conduct these activities. The model covers an entire week to allow for adjustments (such as postponing grocery shopping by a day) and to better represent leisure travel, which is more common on weekend days. ■

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**For a full list of publications please see** <https://www.ias.tum.de/ias/moeckel-rolf/>



**Figure 2,** Simulated traffic noise LDEN (day-evening-night noise level) in dB(A) in Munich

## Focus Group Population Epigenetics and Epigenomics

Prof. Robert Schmitz (University of Georgia), Alumnus Hans Fischer Fellow | Yadollah Shahryary (TUM), Doctoral Candidate | Host: Prof. Frank Johannes (TUM)



Prof. Robert Schmitz

# Investigating spontaneous epigenetic variation

**Genetic variation is a major driver of trait variation. Missing from previous efforts is an understanding of how epigenetic variation contributes to this process. We focus on innovating methods, studying experimental and natural plant populations, and developing mathematical models to better understand the role of epigenetic variation in trait variation.**

We study how chemical modification to the DNA sequence (DNA methylation) varies naturally in plants. It is well known that some of these changes lead to turning off the gene, whereas others currently have no known function. Much of the effort in this area is focused on how development or the environment affects these chemical modifications. Our group is unique in that we specifically focus on spontaneous changes to DNA methylation that accumulate naturally. Our work has demonstrated that spontaneous changes to DNA methylation accumulate over cell division and generational time, yet the origins of these changes remain unknown. Additionally, we study if there are any functional consequences associated with these spontaneous epigenetic changes. Finally, our discoveries that spontaneous epigenetic variation accumulates with time and at a rate much higher than the spontaneous DNA mutation rate provides a unique opportunity use spontaneous epigenetic variation as a molecular clock.

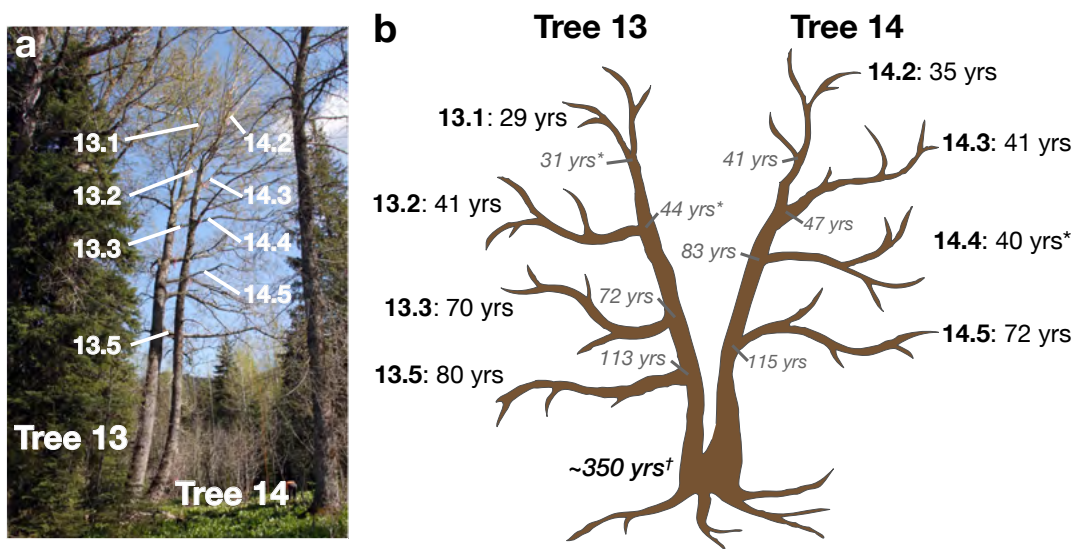
To better understand the role of spontaneous epigenetic variation, we use both natural

and experimental plant populations ranging from plants that have short annual life styles to those that are long-lived perennials. The natural life history of each plant species provides an opportunity to evaluate how it influences the rate and spectrum of spontaneous epigenetic variation. Our studies can be classified into two distinct classes: 1) studies of natural epigenetic variation and 2) studies of experimentally induced epigenetic variation.

1) Natural epigenetic variation: We initiated a survey of natural spontaneous changes in DNA methylation in a collection of more than 750 wild isolates of *Arabidopsis thaliana*. Each of these isolates represents a different individual of a genetically distinct population. We characterized the DNA methylation status of genes into three categories: unmethylated, gene body DNA methylated, and genes that had transposon/repeat-like methylation patterns. We observed that the vast majority of genes were consistently in an unmethylated state, regardless of the geographical origin. A rare fraction of genes was present in transposon/repeat-like methylation state.

Approximately 15% of genes were classified as gene body DNA methylated, and this class exhibited the greatest amount of variation in genes between different wild isolates. We explored the basis for this variation and observed a unique pattern that suggests that the variation observed is associated with DNA methylation pathways that were primarily thought to function only in transposon/repeat regions of plant genomes. This research has opened a new path of research to better understand how these distinct regions of the genome interact to lead to spontaneous epigenetic variation.

2) Experimentally induced variation: The major breakthrough that we made prior to beginning this Fellowship was that spontaneous epigenetic variation accumulates over time. This conclusion was based on the use of *A. thaliana* mutation accumulation lines where experimental populations of single seed descent lineages were created from a single founder individual. This experimental setup allowed us to control the known relationship and time between parent and progeny individuals. ►



**Figure 1.** Photograph and schematic drawing the studied tree. This wild poplar, located in Mt. Hood, Oregon, experienced a decapitation event ~300 years ago. Tree 14 re-sprouted from the stump, and ~80–100 years later Tree 13 re-sprouted. **(a)** Leaf samples were collected from the labeled terminal branches. **(b)** Age was estimated for both the end of the branch (black font) and where it meets the main stem (gray italics). Ages with \* indicate age was estimated using diameter; all other estimates were from core samples.



One major hypothesis is that that spontaneous epigenetic variation forms as a by-product of reproduction when DNA is inherited from one generation to the next. To test this hypothesis, we isolated DNA from eight different branches of a long-lived perennial poplar tree that is approximately 350 years old. This experimental setup allows us to explore if spontaneous epigenetic variation accumulates with time independent of sexual reproduction. We were able to trace back the accumulation of changes to DNA methylation to a common ancestral cell and determine the extent of spontaneous DNA methylation variation. An important discovery was that these variations in DNA methylation exist even though none of the samples were collected from across generations. These results show that spontaneous changes to DNA methylation, which sometimes are linked to gene expression and trait variation, accumulate as a result of cells replicating their DNA within generations and not between generations.

In parallel, we have designed additional mutation accumulation populations whereby we have used founder plants that are mutant in key enzymes we hypothesize influence the rate and spectrum of spontaneous epigenetic variation. At the same time, have leveraged our expertise in plant epigenomics to better understand features that might underlie why certain regions of plant genomes are more susceptible than others to spontaneous epigenetic variation. Combining these two approaches has led to the discovery that a minor portion of plant genomes contributes a major source of epigenetic variation, and this allows us to measure divergence time between individuals where not enough DNA mutations have done so to make accurate predictions of relatedness.

A number of major discoveries have resulted from this unique collaboration.

1. The epimutation rate is a product of cell division time and is independent of major epigenetic reinforcement strategies that plants use during sexual reproduction.

2. Epimutation rates are stable and predictable enough that they can be used to estimate age of individuals, providing a new molecular clock. This is especially powerful for use in situations in which there has not been enough time for DNA mutations to accumulate to a point where they are useful in determining relatedness and divergence time between individuals.

3. We have discovered that DNA methylation pathways important for silencing transposons and repeats are important for creating the spontaneous epigenetic variation observed in genes.

4. We have determined the molecular epigenomic properties of regions of the genome that are most susceptible to accumulation of spontaneous epimutations.

These results have led to a major breakthrough: We are confident that epimutation rates can be used to age-date individuals in plant populations in cases where there is not enough DNA sequence variation to do so. This has major implications for studying speciation and invasiveness, for mapping of relationships between clonally propagated plants, and for age-dating plants.

Our future research will explore how the epimutation varies between species and determine how applicable these epimutation models can be when used to evaluate divergence time between individuals. In parallel, we will continue our studies aimed at understanding how epimutations originated. We firmly believe understanding this process will provide clues as to why their functions exist in plants, which is still a mystery. ■

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**For a full list of publications please see**  
<https://www.ias.tum.de/ias/active-fellows/schmitz-robert-j/>



**Prof. Antonia  
Wachter-Zeh**

## Focus Group Coding for Communications and Data Storage

**Prof. Antonia Wachter-Zeh (TUM)**, Alumna Rudolf Mößbauer Tenure Track Assistant Professor | **Prof. Camilla Hollanti (Aalto University)**, Alumna Hans Fischer Fellow | **Prof. Eitan Yaakobi (Technion – Israel Institute of Technology)**, Hans Fischer Fellow | **Dr. Rawad Bitar (TUM)**, Postdoctoral Researcher | **Dr. Lukas Holzbaur (TUM)**, Alumnus Doctoral Candidate

# Coding and cryptography for privacy, security, and storage

**Our research lies in coding theory and cryptography with applications to privacy, security, storage, and machine learning. In this collaboration, we have worked on code-based cryptography to make our data resilient against capable quantum computers; coding for DNA-based data storage, to enable long-term high-density data storage; distributed data storage and private information retrieval.**

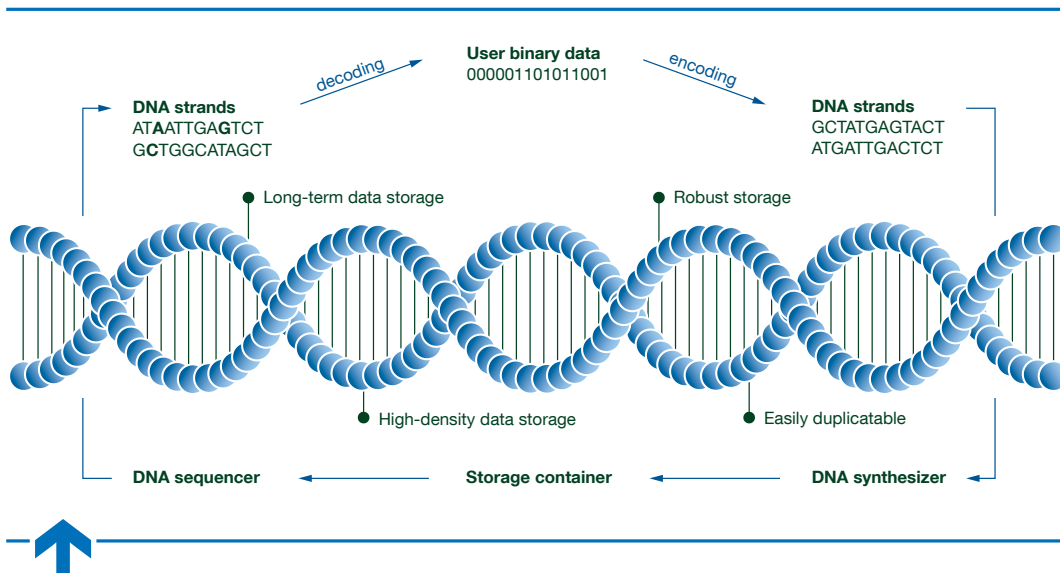
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### Post-quantum cryptography

Post-quantum cryptography, in particular code-based cryptography, promises to guarantee security even when capable quantum computers will break most classical public-key cryptosystems. In this collaboration, we have studied code-based cryptography in both Hamming and rank metrics.

We have derived a polynomial-time key recovery attack for a McEliece-type cryptosystem based on twisted Reed-Solomon codes, which proves that the proposed system is insecure. For the Hamming Quasi-Cyclic (HQC) proposal, which is a promising candidate in the third round of the NIST Post-Quantum cryptography standardization project, we have shown that, utilizing a power-side channel, we are able to mount an efficient key-recovery attack, which indicates that the proposed implementation of the system is not secure [1]. Further, we have investigated how so-called hints that stem from side-channel attacks reduce the work factor of general information set decoding algorithms [2].

Recently, we have focused on the rank metric, which allows the development of systems with smaller key and ciphertext sizes. Thereby, we have proposed and analyzed a new algorithm to solve the problem of decoding errors of rather large rank-weight with Gabidulin codes [3]. The complexity of this problem is of importance to assess the security of rank-metric code-based cryptosystems. Further, we have extended a cryptosystem based on Gabidulin codes where we modified the encryption and decryption algorithms of Loidreau's cryptosystem in order to achieve smaller key sizes. Besides Gabidulin codes, low-rank parity-check (LRPC) codes are very interesting for code-based cryptography due to their weak algebraic structure; therefore, we have defined and studied LRPC codes and their decoding over Galois rings [4]. The most important contribution here is that we have proposed a new a new code-based cryptosystem, called LIGA, based on the hardness of list decoding Gabidulin codes.



**Figure 1.** Storing data in strands of DNA involves converting the zeros and ones of digital data into the four bases of DNA: adenine (A), cytosine (C), guanine (G) and thymine (T). DNA storage has the potential to solve several problems such as life span and capacity of conventional storage media.

### Coding for DNA storage

DNA-based data storage, as shown in Figure 1, consists of DNA synthesis as the writing process, storage in a special storage medium, and DNA sequencing as the reading process. In contrast to conventional storage methods, due to the nature of DNA and the biological processes involved, special error patterns such as insertion, deletion, and substitution errors occur.

We have studied fundamental storage density limits of DNA storage systems [5]. These findings are among pioneering work that aims to provide guidelines on how to design error-correcting codes for the systems. Further, we provide code constructions that achieve high storage rates and allow for time-efficient decoding.

In terms of explicit error-correcting codes for DNA storage, we designed a code optimized to correct a combination of error types. As the combination of different error types is hard in general, we first focused in a first step on a code construction for a single de-

letion and a single substitution [6]. Furthermore, we have studied a new type of deletion error patterns: crisscross deletion patterns. Given an array where several rows and several columns are deleted or inserted, we aim to reconstruct the original array by introducing a certain underlying structure in the original arrays. Error-correcting codes for bursts of insertions and duplications, two types of errors frequently occurring in DNA storage systems, are presented in two more of our papers. We have also studied covering codes for insertion and deletion errors. The results are useful to design and analyze massively parallel clustering algorithms of synthetic DNA strands. We have further investigated codes that facilitate and speed up clustering algorithms by using “clustering-correcting codes” [7]. These codes further improve the accuracy of the clustered sequences.

Another focus was on codes over sets which lay the foundation for error-correcting codes in DNA storage systems as they protect unordered strands from vectors [8]. Our results allow on the one hand to understand ►

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- [10] Holzbaur, L. et al. (2020).
- [11] Holzbaur, L. et al. (2021).

the fundamental rate-limits of DNA storage systems and on the other hand provide efficient codes that allow for error correction of typical errors that arise in DNA storage.

One of the most costly bottlenecks of DNA-based data storage, in terms of cost and time, is the synthesis process. We have therefore shown how to add redundancy to DNA strands to allow for a faster and less costly synthesis [9]. In particular, for synthesis machines that synthesize a massive amount of DNA strands in parallel, we show how to save ~50% in time and synthesis material as compared to conventional methods.

### Coding for distributed data storage and private information retrieval

The huge amount of data that is constantly being processed has led to the construction of huge data centers spread over different locations. Each of these data centers consists of a network of storage disks or servers where the data is distributed among the servers. However, given the massive number of storage servers, server failures happen frequently. Therefore, it is necessary to store redundant data alongside the initial data via a storage code.

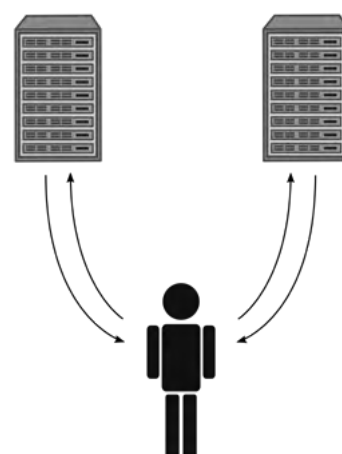
With the increase in usage of distributed services such as cloud storage and peer-to-peer networks, the importance of user privacy is constantly on the rise. Recently, private information retrieval (PIR) in the context of coded storage has gained a lot of interest. With PIR, a user is able to download a desired file from a database or distributed storage system (DSS) without revealing the identity of the file to the servers (see also Figure 2).

In this collaboration, we first have proven the capacity for DSS that are protected against server failures by erasure codes for the use

case where the user is only supposed to learn exactly what is desired, which is referred to as symmetric private information retrieval (SPIR).

In another work, the star product scheme has been adopted, with appropriate modifications, to the case of private (e.g., video) streaming [10]. It is assumed that the files to be streamed are stored in a distributed manner over several servers by an erasure code, and the download is carried out in a manner suitable for streaming applications.

Further, we have focused on how to optimally repair a certain number of failed servers by contacting the least number of other servers [11]. We have derived the trade-off between the redundancy and the failure tolerance of a storage system when the number of repair servers changes according to the number of failed servers. Moreover, this class achieves the best trade-off between redundancy and failure tolerance with this repair property. ■



**Figure 2,** Private information retrieval

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**For a full list of publications please see** <https://www.ias.tum.de/ias/wachter-zeh-antonia/>

# Functional Earth system services through resilient, diverse ecosystems

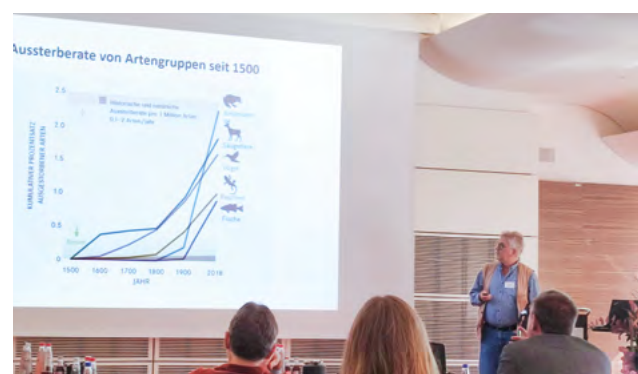
Since 2020, a series of global crisis has been exposing numerous shortcomings in the international society and the global economy. This visible systemic vulnerability underlined once more the human dependency on healthy planetary systems. IESP strongly believes that not to learn from a crisis is not to understand the crisis. At present, the experienced involuntary return to basic human needs shapes our perspectives towards the future. To maintain functional Earth systems and provide for healthy living spaces for human and non-human species, resilient ecosystems lie at the core. Their resilience grounds in diversity; ranging from cohabitating flora and fauna to landscape use and geo-engineering.

The SARS-CoV-1 pandemic, which can be viewed as a symptom of over-consumption and unsustainable economic activity [1] as well as biodiversity loss and declining natural habitats, offers us an opportunity to rethink and reset. How can we utilize the pandemic experiences to increase dynamics in realizing the 17 UN Sustainable Development Goals (SDGs), or better yet ensure that we achieve them?

In October 2021, IESP discussed these and related questions with a group of 26 experts from society, science, and politics in a three-day workshop. A jointly developed memorandum consists of six petitions we consider essential steps to leave posterity a world worth living in. The paper [2] highlights necessary transformations in agricultural land use, food trade, and institutional organization.

Among the discussants were the Russian physicists Dr. Anastassia Makarieva, a newly appointed Anna Boyksen Fellow at the TUM-IAS (Host: Prof. Anja Rammig), and her colleague Dr. Andrei Nefiodov, a visiting scholar invited by IESP to establish new trans-

national research connections. They are affiliated with the Russian Academy of Sciences, and their research focuses on water balance and moisture transport in boreal forest ecosystems. Weather extremes, water shortages, and consequential vulnerability to pests and diseases stress their natural health. Forested landscapes provide “sustainable biospheric processes” that are critical for human life on Earth.



Prof. Josef Settele (UFZ) elaborating on the accelerating extinction rate of species since the mid-20th-century.



Lifelong Learning: Plastic representation of the concept “sustainability” utilizing LEGO Serious Play®.

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- [3] Drewes, J. E. et al. LAND: schaf(f)t: WASSER. Bericht der Expertenkommission Wasserversorgung in Bayern (2021).

A functional landscape water regime is among the most important ecosystem services (ESS) humans depend on. For example, looking at the reach of hydrological and ecological problems in the main river basins in the western United States, which supply California and its agriculture, exposes the challenges for water supply in the Anthropocene. The current discussions on transforming the global agricultural and food systems neglect the importance of a healthy landscape water balance. Yet it is a prerequisite for vital conditions including biodiversity, plant health, and soil fertility. The impacts of climate change through unsustainable farming and building practices are also measurable in Bavaria, raising issues of distributional fairness and conflicts of use.

To raise more attention for the need to rewrite our water future, and to plant seeds for innovative ideas and collaborations, IESP hosted two digital workshops during the winter of 2020/2021. The first event served as a kick-off event for an expert commission on Bavaria’s future water supply. Its mission was to serve as an independent scientific body to assess the current state of the various water supply systems and to suggest measures to strengthen their resilience, given the increasing impacts of climate change. The second workshop discussed preliminary results and questions with different stakeholders. The commission’s report to the State Ministry for the Environment and Consumer Protection outlines measures that are crucial to improve and stabilize regional landscape water regimes while maintaining the local cultural landscape and mitigating conflicts of interest [3].

Such conflicts arise not only between nature and humans, but also at the intersections between interests such as the supply of drinking water, agriculture, and food production. Here, as in other sectors, COVID-19 exposed archaic work structures and was blamed, by parties deliberately diverting attention from existing structural deficits and missed opportunities, for long-standing crises. In the midst of this process, a German legal requirement for entrepreneurial care along global supply chains (LkSG) was passed and came into force. IESP’s 2022 summer workshop aims to illuminate the effects of this new law for agriculture and the agricultural sector’s transformation toward greater sustainability.

Sustainability is the core concept of IESP’s framework of thought on maintaining a healthy Earth system. Its variety of applications features in an edited volume following a joint workshop IESP organized with the TUM Emeriti of Excellence at the TUM Academy and Science Center in Raitenhaslach. Strategies for Sustainability of the Earth System, edited by Peter A. Wilderer, Michael Molls, Martin Grambow, and Konrad Oexle, is published with Springer Nature.

IESP’s current project “Landwirtschaft-Wasserwirtschaft-Klimawandel. Neue Perspektiven für Landwirtschaft und Umwelt” (2018–2023) is funded by the Bavarian State Ministry of the Environment and Consumer Protection. ■



# Where do the TUM-IAS Fellows come from?

## USA

**Prof. Leonidas Guibas**  
Stanford University

**Prof. Naomi Halas**  
**Prof. Peter Nordlander**  
Rice University

**Dr. Lothar Hennighausen**  
National Institute of Diabetes and  
Digestive and Kidney  
Diseases (NIH/NIDDK)

**Prof. Frank Keutsch**  
Harvard University

**Dr. Sani Nassif**  
Radyalis LLC

**Prof. Robert J. Schmitz**  
University of Georgia

**Prof. Henrik Selin**  
Boston University

**Prof. Noelle Eckley Selin**  
**Prof. Kathleen Thelen**  
Massachusetts Institute of  
Technology

**Prof. Natalia Shustova**  
University of South Carolina

**Prof. Thaddeus Stappenbeck**  
Cleveland Clinic

**Prof. Leila Takayama**  
University of California

**Prof. Nitish Thakor**  
Johns Hopkins University

## Canada

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Simon Fraser University

**Prof. Jihyun Lee**  
University of Calgary

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University of São Paulo

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Pontificia Universidad Católica  
de Chile

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Universidad de Buenos Aires

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University of Cambridge

**Prof. René Botnar**  
King's College London

**Prof. Laura Herz**  
University of Oxford

**Dr. Luca Magri**  
Imperial College London

**Prof. Krasimira Tsaneva-Atanasova**  
University of Exeter

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Free University of Amsterdam

**Prof. Ron Heeren**  
Maastricht University

**Prof. Wil Schilders**  
Eindhoven University of Technology

## Denmark

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Technical University of Denmark

**Prof. Maja Horst**  
DTU Technical University of Denmark

## Sweden

**Prof. Meike Schalk**  
KTH Royal Institute of Technology

## Belgium

**Prof. Michel Gérardin**  
Université de Liège

## Germany

**Prof. Daniel Cremers**  
**Prof. Bernhard Küster**  
Technical University of Munich

**Dr. Filippo Maglia**  
BMW Group

**Prof. Daniela Pfeiffer**  
**Dr. Benedikt Zott**  
TUM University Hospital  
rechts der Isar

### Rudolf Mößbauer Fellows at TUM

**Prof. Job Boekhoven**  
**Prof. Jia Chen**  
**Prof. Pierluigi D'Acunto**  
**Prof. David Egger**  
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**Prof. Ruben Portugues**  
**Prof. Franz Schilling**  
**Prof. Kathrin Schumann**  
**Prof. Nikkil Sudharsanan**  
**Prof. Antonia Wachter-Zeh**  
Technical University of Munich

## Ireland

**Prof. Mathias Senge**  
Trinity College Dublin

## Hungary

**Prof. Örs Legeza**  
Wigner Research Centre for Physics

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**Dr. Anastassia Makarieva**  
Petersburg Nuclear Physics  
Institute

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**Prof. Eitan Yaakobi**  
Technion

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Jawaharlal Nehru Centre  
for Advanced Scientific  
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Upper Austria

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**Prof. Eleni Chatzi**  
**Dr. Barbara Solenthaler**  
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**Dr. Elena del Valle**  
Universidad Autónoma de Madrid

## Italy

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University of Padua

**Dr. Sara Lucatello**  
INAF Osservatorio Astronomico di Padova

**Prof. Giuseppe Savaré**  
Bocconi University

**Prof. Luisa Verdoliva**  
University Federico II of Naples

## Australia

**Dr. Andreea Molnar**  
Swinburne University of  
Technology

**Prof. Susan Park**  
University of Sydney

# Facts and Figures

The TUM-IAS was established as a flagship of TUM's institutional strategy to promote top-level research in the Excellence Initiative of the German federal and state governments. After having played a central part in the first two rounds of the Excellence Initiative of the German federal and state governments (2006–2012 and 2012–2019), the TUM-IAS became established as a permanent institution of TUM, financed out of the general TUM budget.

With its Anna Boyksen and Albrecht Struppler Clinician Scientist Fellowships, the Institute contributed to the proposal of the current Excellence Strategy and is therefore receiving funding for its new initiatives. In addition, the TUM-IAS is collaborating with the Cluster of Excellence e-conversion, which is financing several TUM-IAS@e-conversion Hans Fischer Senior Fellowships. In 2021, a total of three Fellows had been appointed within this program.

Funded under the Excellence Strategy of the Federal Government and the Länder.

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## Third-party funding

### TÜV Süd Foundation

In 2015, the TÜV Süd Foundation and TUM agreed on introducing a "Hans Fischer Senior Fellowship awarded by the TÜV Süd Foundation." By funding this Fellowship, the TÜV Süd Foundation aims to support the exchange of internationally renowned scientists as well as sustainable projects in groundbreaking research fields: energy efficiency and climate protection, test procedures, product and plant safety, and compliance management. So far, two Fellows were appointed under this scheme.

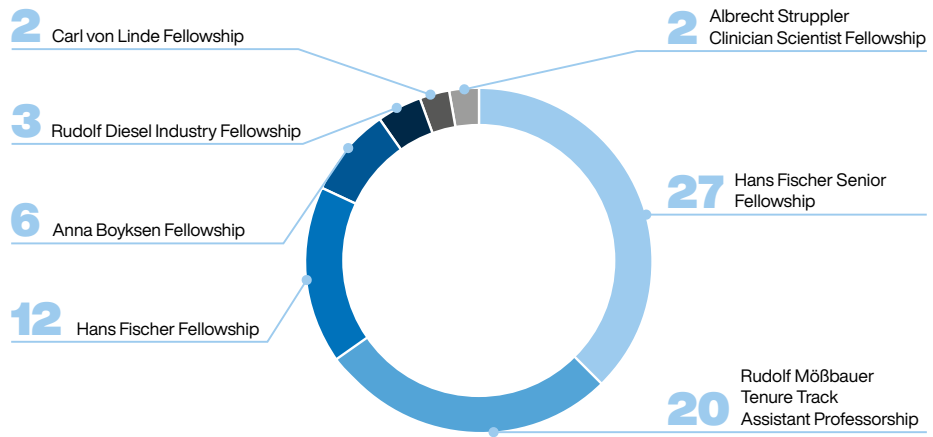
### Siemens AG

Siemens AG provides funding for six Hans Fischer (Senior) Fellowships with over two million euros. The research focus is on the fields of Simulation and Digital Twin and Future of Autonomous Systems/Robotics. The fifth and sixth Fellows were appointed in 2021.

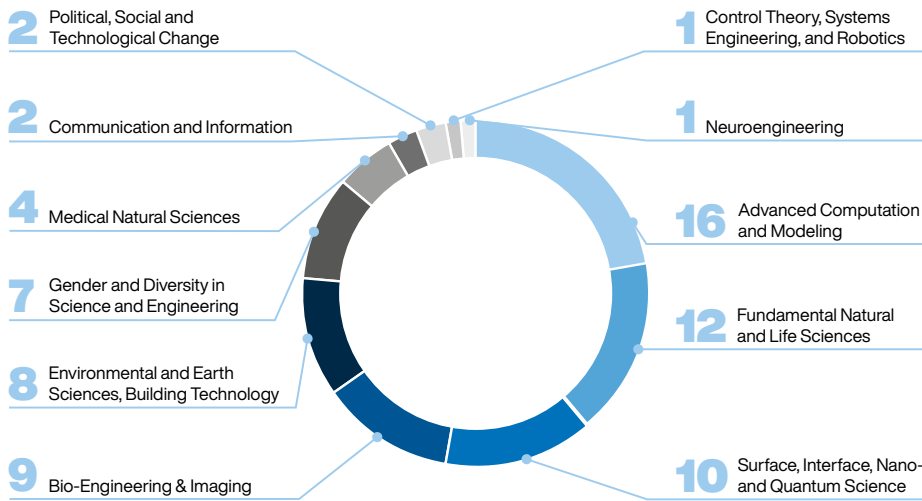
### Georg Nemetschek Institute Artificial Intelligence for the Built World

The Georg Nemetschek Institute provides funding for one Hans Fischer (Senior) Fellowship per year, focusing on the field of Artificial Intelligence for the Built World. A first Fellowship was included in the call published in December 2021.

**Fellow Distribution  
by Fellowship  
Category in 2021**

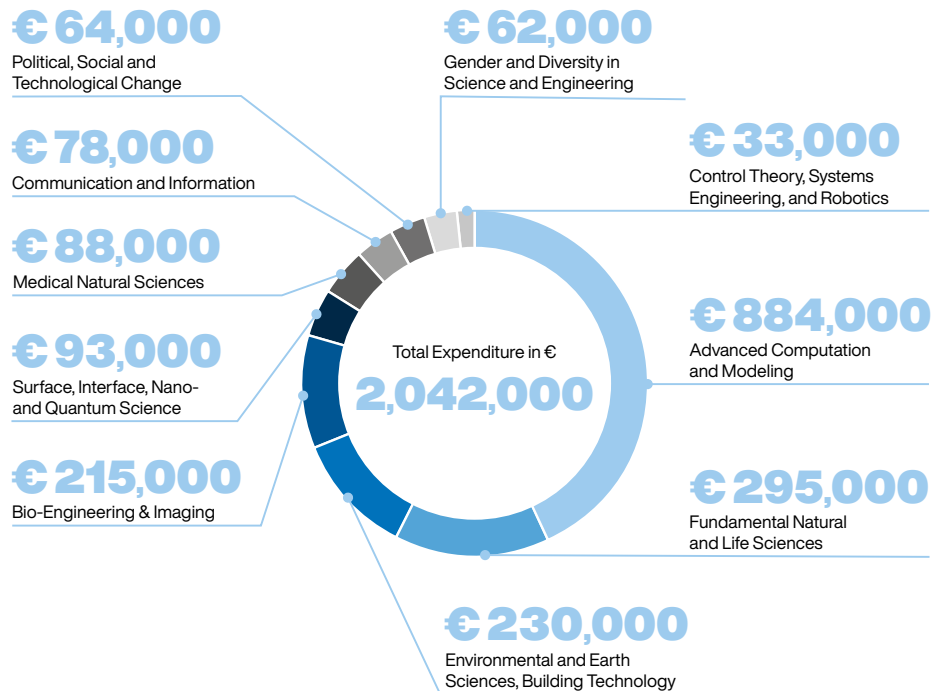


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**Fellow Distribution  
according to TUM-  
IAS Research Areas  
in 2021**

**Expenditure per  
TUM-IAS Research  
Area in 2021**





# Board of Trustees

(status: May 2022)

The Board of Trustees is formed by a group of international advisors from academia, research support organizations, and industry. It advises the director on general scientific, organizational, and technical issues. The Board also defines the general strategy and standards of the Institute.

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# Advisory Council

(status: May 2022)

The TUM-IAS Advisory Council is composed by TUM faculty, representing the different research areas of the university and this Institute. One of its prime functions is advising on the suitability and ranking of Fellow nominations the Institute receives for its various Fellowship programs. In addition, the Council advises on the scientific and technological course of the Institute, on the basis of an assessment of the potential and needs of the university. The Advisory Council meets usually three times a year.

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**Prof. Stephan A. Sieber**, Organic Chemistry II

**Prof. Ian F. C. Smith**, Georg Nemetschek Institute

**Prof. Simone Warzel**, Global Analysis

After nearly two terms of office, the membership of **Prof. Chris-Carolin Schön** has ended in 2022. We would like to express our sincerest thanks for being able to rely on her experience and insight during the evaluation of our Fellowship proposals and the selection of our new Fellows for so many years.

# TUM-IAS Management Office

(status: May 2022)

Meet the TUM-IAS Management Team, which is responsible for our Fellowship Program, liason with our Fellows, workshops and conferences, our guest house, and all other TUM-IAS services.  
(5.4 full-time equivalents)



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## IESP-Project Team

The IESP-Project Team within the TUM-IAS organizes research programs, conferences, and events as well as publications of the International Expert Network on Earth Systems Preservation.  
(1.5 full-time equivalents)



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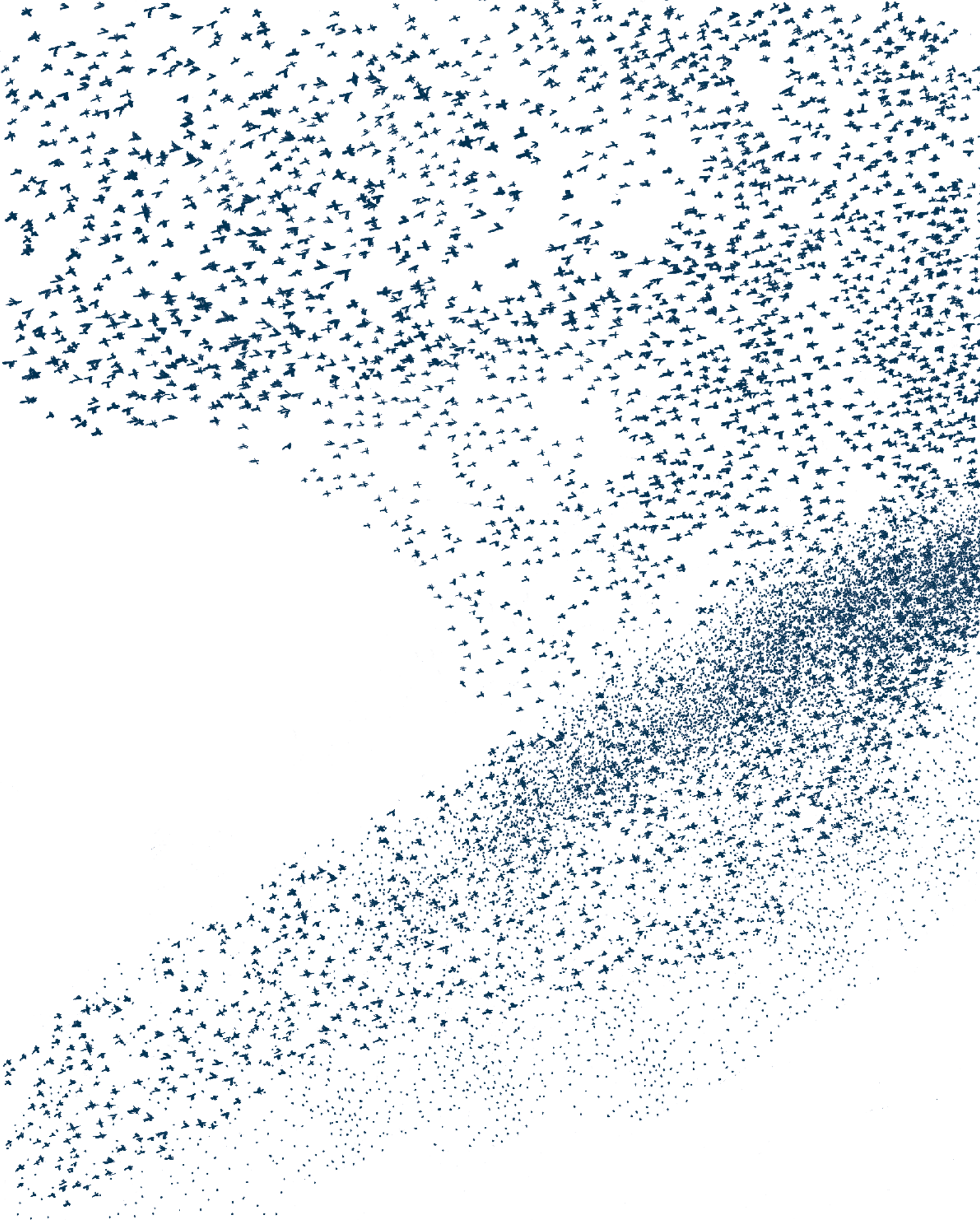
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