

Table of Contents

04	TUM President's Foreword	5 2 In Focus: Probing Perovs	kites
06	TUM-IAS Director's Message	6 2 Scientific Repo	rts
0 8	Actions, Awards, Events	 9 6 1 0 6 7 7 8 7 8 8 9 8 9 9 8 9 9<	es
22	Welcoming Our New Fellows	1 0 6 People	

3 6 Fellowships for Ukrainian Scientists

TUM President's Foreword

TUM is focusing specifically on clarifying the major unanswered questions of today's science and on developing future-oriented fields of technology.

More than ever complex scientific challenges require the dynamic, cross-border interaction of disciplines. This way science and technology can become game changers. They led us out of the pandemic and pointed us in the right direction to a sustainable way of living and economy in the major crises in recent years. This shows that science and technology are essential parts of the solution to various challenges. They can lead us to resource efficiency and energy conservation, which are important elements of sustainability.

Therefore, the TUM Sustainable Future Strategy 2030, which we recently adopted, is a historic step. Our university wants to contribute to overcoming the biggest challenges currently facing humanity: climate change and the necessity of resource efficiency and energy conservation. Focusing on the goal of sustainability in research, teaching, campus operations and university community requires enormous innovation, not just in the sense of technology, but also in our teaching and research content, in our organization, in our management and in our founding activities.

The first TUM Sustainability Day in October 2022, with significant participation from our TUM Institute for Advanced Study, showed the enormous range and diversity of sustainability activities at all TUM locations. Just three examples: In TUM SEED CENTER (Sustainable Energies, Entrepreneurship and Development) we research, teach and innovate on sustainable and affordable energy solutions for the global south. In our TUM Mission Network Circular Economy, we pool our resources for the realization of a sustainable circular economy. At TUM-IAS are not only half of its 70 Focus Groups working on scientific projects directly connected to the UN Sustainable Development Goals, the TUM-IAS is also responsible for selecting the international awardees of the Nobel Sustainability Trust.

Our university community consisting of students, researchers, alumni and business partners is the driving force behind the change towards more sustainability. As heads of the university, it is our task to create and support structures and initiatives realizing this.

New Schools

The new structure of our university serves exactly these purposes. The traditionally disciplinary oriented faculties are being transformed into seven schools with a broader subject focus, between which interdisciplinary research centers are located. Intensive cooperation across disciplinary boundaries, orientation toward the major research topics and professional fields of the future, modern governance structures. With its schools, TUM is creating future-proof units that break away from the small-scale faculty structure of German universities, are positioned more broadly, and can thus take up and establish newly emerging complex fields more quickly, e.g., Data Science, Biogenic Materials, or Mobility Systems Engineering. Through system-integrative networking via the interdisciplinary research institutes at the interfaces of the disciplines, we create a matrix organization, which enables innovative research and teaching. This restructuring is the most radical reform in the more than 150-year history of our university.



Expansion of TUM Campus Heilbronn

The TUM Campus Heilbronn, which was founded in 2018, is turning into a center of force for the form of digital transformation. The Dieter Schwarz Foundation is raising its long-term engagement at TUM by ten to a total of 41 professorships. These additional professorships are focused on Data Science and Artificial Intelligence. Part of the unique expansion program of the Dieter Schwarz Foundation are also two new Fellowships for the TUM-IAS, which are building a bridge between Heilbronn and the TUM location Garching.

TUM-IAS Fellowships for Ukrainian Scientists

Immediately after the Russian invasion of the Ukraine in February 2022, TUM initiated a comprehensive program. Students from the Ukraine and Russia should be supported. Furthermore, the TUM-IAS immediately accepted ten Ukrainian researchers, which were forced to leave their homes. Thanks to major private donations, we were able to act quickly and give the Ukrainian scientists a new academic home. They are integrated in our community and have benefited TUM and our research.

What also enriches and pleases us is that the IAS Fellows have again received top prizes and awards in the past year, proving once again that our IAS has always been a thought incubator.

Lecus, F. Clopa

Prof. Thomas F. Hofmann President

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TUM-IAS Director's Message

Times of upheaval provide chances for new ways, new approaches, and new connections. The TUM Institute for Advanced Study takes this opportunity particularly with its Focus Groups, the core of our institute.



The Focus Groups are research collaborations between outstanding scientists from international universities and business enterprises and professors as well as PhD candidates from our university of excellence. The groups are funded by TUM and its partners in science and business and create new knowledge and stable partnerships on a global level.

"Risking Creativity" and the development of innovative research fields are part of the institute's philosophy. The topic of sustainability is currently particularly urgent. Therefore, initiatives dedicated to sustainability are very important to us. And for this reason, half of our Focus Groups are currently working on topics related to the UN Sustainable Development Goals.

Due to the academic freedom allowed by the TUM-IAS, we are supporting our TUM scientists in building successful international collaborations and in shaping their careers. Numerous awards received by members of the TUM-IAS community in the previous year are prove for the continuing top-class work at our institute. In 2022, we were able to initiate further future-oriented projects and launch new Fellowship lines. We included the still young TUM campus Heilbronn, which has its focus on economics and digital transformation, into our funding with additional resources. Additionally, we increased our engagement in Eastern Europe and established new connections. With 7.5 million euros in newly acquired funds, we will be able to continue existing successful programs in the coming years and realize others that reflect the extensive, interdisciplinary research portfolio of the entire TUM in terms of content. With one Fellowship, we are breaking new ground: "Philosopher in Residence" is intended to build a bridge between natural sciences, engineering, medicine and health sciences on one hand and philosophy on the other hand, in order to reflect on and classify the rapid and complex scientific and technological change in depth and to provide reliable orientation.

Other important milestones in recent months are that the TUM-IAS will be responsible for the selection of the international awardees of the new Nobel Sustainability Trust Awards in the coming years. This way, TUM and Nobel Sustainability Trust together will further strengthen the idea of sustainability. In addition, the TUM-IAS will act as the interface between TUM and Alexander Humboldt Foundation, the most important German institution for international exchange of scientists.

Furthermore, the TUM-IAS was able to provide ten Ukrainian scientists, who were forced to leave their homes due to the Russian invasion a shelter and an academic home with the "Fellowship for Ukrainian Scientists," which was established on short notice. This was made possible by generous private donations, for which we would like to express our sincere thanks.

Siemens AG, TÜV SÜD Foundation, and Dieter Schwarz Foundation are both longstanding and new trustful supporters, who help us to realize our ideas in creative research programs, including sustainability research. I would like to express my special thanks to them!

Maly

Prof. Michael Molls Director

Actions, Awards, Events

The TUM-IAS has strengthened and expanded its portfolio with new projects and programs in 2022. We congratulate our Fellows on prestigious prizes and awards.







Actions

Recommendations of the German Science and Humanities Council

Germany's most important science policy advisory body, the German Science and Humanities Council, which advises the federal and state governments on the further development of the German higher education and science system in terms of structure and content, has conducted a systematic review of Institutes for Advanced Study in recent years in order to formulate recommendations for institutions of this kind in Germany. They have been published under the title "Development Perspectives of Institutes for Advanced Study (IAS) in Germany." Ten characteristics are defined in it and it recommends their design for the future. The TUM-IAS is already close to implementing the recommendations and is working on further performance in terms of content and structure. Unlike most

IAS Characteristics	Future Development/Demands	TUM-IAS
Orientation	Multi-, Inter- and Transdiscipli- narity	+
Geographic Orientation	Global South, East and South East Europe	+ Regional Fellowships
Funding Model	Tandem Model, Coupling Digital and InPerson Formats	-
Funding Period	Fellowships exceeding 1 year, i.e. for early career scientists	+ Fischer Fellowship, Mößbauer Fellowship
Extension/Connection	Regional and transnational partnerships, transcontinental partnerships, Programs for Collegial Networks	+
Professional Focus/Integration	Integration of Natural, Life, Engineering Sciences and Medicine	+ TUM-IAS founding principle
Integration of Social Sciences	Cooperation with Natural and Technical Sciences as well as the Humanities	+
Early Career Scientists	Young Academy	+ Mößbauer Fellowship, Fischer Fellowship, Struppler Clinician Scientist Fellowship
National Top Funding	Programs supporting national top-level funding	+ Linde Fellowship
Science and Knowledge reflection	Support for Science and Knowledge reflection,	+ Philosopher in Residence

German IASs, the TUM-IAS is home to international Fellows for up to three years after a competitive selection process and supports their research with up to 300,000 euros. It also participates in initiatives with other German IAS.

"Philosopher in Residence" program

Thanks to the support of the TÜV SÜD Foundation. the TUM-IAS 2022 was able to initiate a new program that is unique in Germany - the "Philosopher in Residence" Fellowship. It was launched against the backdrop that innovative research in natural sciences and technical disciplines raises numerous questions - of an internal nature, but also of societal scope. This requires deeper reflection and classification in the context of future-oriented social developments, not least under the aspect of sustainability and resilience. Philosophy has the possibility and the tools to meet these challenges and to shed light on them - especially from the point of view of responsibility towards people and nature. It promotes transdisciplinary discourse and makes fundamental contributions to making innovative scientific approaches effective in a democratic, inclusive and sustainable way in order to successfully and beneficially shape the upcoming transformations.

The new program is aimed at high-level international philosophers interested in philosophically engaging with and embedding the latest research and innovative approaches in the natural, engineering, life and health sciences. During the one-year Fellowship, a scientific project is carried out with a TUM Host in extended presence at the IAS.

Siemens funding for IAS Fellowships

Last year, the TUM-IAS was able to win over Siemens AG to once again fund six

Hans Fischer (Senior) Fellowships with over 2.4 million euros. Over the next few years, international experts will work together with TUM professors in the area of the Industrial Metaverse, focusing on "Token Economics," "Web3 Architecture," "Digital Twin," "Autonomous Systems" and "Trustworthy Artificial Intelligence." With the help of the funding from Siemens AG, TUM is thus strengthening its focus on digitalization, artificial intelligence and robotics, as well as computer simulation. In the industrial metaverse, technical plants, buildings, cities or even energy networks and transport systems and their functions can be simulated, including the behavior of operators and users. In this digital world, problems can be anticipated, errors found and processes improved without risking damage in the real world.

Cooperation with Nobel Sustainability Trust

The Nobel Sustainability Trust (NST) and TUM will jointly award three new prizes for international research and initiatives on sustainability. The prize money totalling 1.3 million Swedish kronor (currently approx. 120,000 euros) comes from the Nobel Sustainability Trust. The awards are given in three categories: for outstanding research and development in the fields of water and energy, and for leadership in implementing relevant sustainability projects. The award winners are selected by a jury of international experts and professors from TUM. The TUM-IAS is responsible for the entire selection process.

Hans Fischer Fellowship of the Georg Nemetschek Institute

Conceiving, designing and maintaining the built environment is one of the greatest challenges of the 21st century. The use of stateof-the-art computer technologies, artificial intelligence (AI), and machine learning offers completely new possibilities for ecologically and economically sustainable solutions. Thanks to a generous donation from the Nemetschek Innovation Foundation, TUM has founded the "TUM Georg Nemetschek Institute Artificial Intelligence for the Built World" to conduct research on this forward-looking technological focus. To this end, it also funds Fellowships at TUM-IAS with a corresponding thematic focus. Prof. Shioban Rockcastle is the first scientist to be appointed a Fellow in this new program in 2022. She is an Assistant Professor of Architecture at the University of Oregon, Director of the Baker Lighting Lab and co-founder of OCULIGHT dynamics, a company offering daylight design support to promote healthy indoor occupation.

TUM-IAS Fellowships of the Dieter Schwarz Foundation

The Dieter Schwarz Foundation (DSS) is increasing its long-term commitment to the further expansion of the TUM Campus Heilbronn. The expansion provides for ten additional professorships with a focus on data science and artificial intelligence. At the same time, it is establishing the new "Dieter Schwarz Fellowship" to attract excellent international professors to Heilbronn who will build a bridge to the TUM Campus Garching as Fellows of TUM-IAS. In addition, the "Dieter Schwarz Courageous Research Grant" will be established as an IAS Fellowship to promote courageous project ideas. In global competition, internationally outstanding scientists will be given the opportunity to carry out potential "High Risk - High Gain" research projects on the topics of digitalization and sustainability in collaboration with TUM. The first calls for proposals will be issued in 2023.

Fellowships for Ukrainian Scientists

Immediately after the Russian invasion of Ukraine, TUM launched an ad-hoc program for students and scientists. A Fellowship program was set up at TUM-IAS for established researchers, which awarded Fellowships for an initial six-month research stay at TUM. We were able to award ten of these Fellowships from March 2022 and also extend some of them until 2023. More on pages 36–51.

Carl von Linde Fellowships

The previous Carl von Linde Senior Fellowship of the TUM-IAS will in future be used more in terms of university strategy and has been awarded for the first time in its further developed form under the name Carl von Linde (CvL) Fellowship. It is aimed at TUM professors who have achieved excellent, internationally recognized achievements in research and who wish to pursue research work of particular originality and a high degree of innovation, preferably in an interdisciplinary team with other TUM-IAS Fellows. Up to two CvL Fellowships of 250,000 euros each can be awarded each year for a period of two years. In 2022, Prof. Eugénia da Conceição-Heldt, TUM School of Social Sciences and Technologies, became a Carl von Linde Fellow with her project "A multidisciplinary analyses of disruptions in politics and technology."

Bundling TUM activities in AvH programs at the TUM-IAS

Over the years, the award winners and Fellows of the Alexander von Humboldt Foundation (AvH) have contributed thematic initiatives to TUM and opened up new research perspectives. They are automatically also members of the TUM-IAS. In order to strengthen the cooperation between TUM and the Alexander von Humboldt Foundation, to better connect guests and award winners at TUM and to deepen interaction with the TUM-IAS Fellows, the TUM-IAS will in future be the central administrative point of contact for Humboldt Award winners and AvH Fellowship programs at TUM. The aim is to achieve closer interaction between TUM-IAS Fellows and AvH programs.

Innovation Networks

With interdisciplinary TUM Innovation Networks (each with ten Principal Investigators plus PhD students), the Technical University of Munich aims to create even more scope for scientific creativity and groundbreaking developments. As an institute for excellence and creative research, the IAS is involved both in the selection process and in the organization and implementation of so-called "Exploratory Workshops," from which the Innovation Networks emerge if successful.

After a successful start of the TUM Innovation Networks eXprt (Exoskeleton and wearables enhanced prevention and treatment) and NextGenDrugs (Next generation drug design) the TUM Board of Management selected three new promising concepts in the fall of 2022, for which TUM-IAS officially kicked off the initiatives and hosted the "Exploratory Workshops" dedicated to structuring the networks. With the new Innovation Networks CoConstruct, EarthCare, and GoTransTech, TUM fosters transdisciplinary research in specific fields from construction engineering, geodesy to economics and social sciences, and targets on a midterm perspective the development of Excellence Clusters.

Collaborative Construction (CoConstruct)

Coordinated by Prof. Christoph Gehlen (Materials Science and Testing), CoConstruct brings together researchers from the fields of civil engineering, mechanical engineering, material science, computer science, and architecture. They explore novel collaboration concepts between humans and machines for a sustainable transformation of the architecture, engineering, and construction domain.

Governing Transformative Technologies (GoTransTech)

Prof. Sebastian Pfotenhauer (Innovation Research), Prof. Hanna Hottenrott (Economics of Innovation) and Prof. Holger Patzelt (Business Administration and Entrepreneurship) are coordinating GoTransTech. Researchers from the TUM School of Social Sciences and Technology, and the TUM School of Management associate experts in engineering in order to address the ambivalence and impacts of transformative dynamics and technologies from the perspective of individuals, organizations, and societies.

Twin Earth Methodologies for Biodiversity, Natural Hazards, and Urbanization (EarthCare)

Coordinated by Prof. Xiaoxiang Zhu (Data Science in Earth Observation), EarthCare is composed of engineers, life scientists and data scientists. The project will merge innovative methodologies such as Al for Earth Observation and Earth System Modelling for use cases in biodiversity and forestry, the urban domain, and natural hazards. In total, since 2021, eight TUM Innovation Networks are funded under the Excellence Strategy of the Federal Government and the Länder (ARTEMIS, RISE, NEUROTECH, eXprt, NextGenDrugs, CoConstruct, EarthCare, and GoTransTech).

Sustainability Goals of the United Nations

The 2030 Agenda for Sustainable Development, adopted by all United Nations Member States in 2015, is a common approach to peace and prosperity. At its core are the 17 Sustainable Development Goals (SDGs), which represent an urgent call to action by all countries in a global partnership. They recognize that eradicating poverty and other deprivations must go hand in hand with strategies to improve health and education, reduce inequality and boost economic growth - all while combating climate change and working to protect our oceans and forests. From these goals, TUM has identified six priority themes to which it can make a particular contribution based on its portfolio of subjects: Health (SDG 3), Energy (SDG 7), Urban Systems (SDG 11), Circular Economy (SDG 12), Climate Protection (SDG 13) and Biodiversity (SDG 15). Of the currently 70 active Focus Groups of the TUM-IAS, almost half worked thematically in these areas in 2022, thus supporting the sustainability strategy of the TUM and contributing to the realization of the UN SDGs.

Future lab Green hydrogen in the IAS

Hydrogen produced in a climate-neutral way is considered one of the most important energy sources of the future. That is why an international future lab is being set up at TUM with researchers from 13 countries. The Federal Ministry of Education and Research (BMBF) is providing up to five million euros over three years. The research project "RE-DEFINE Hydrogen Economy" is coordinated by Prof. Hartmut Spliethoff, head of the Chair of Energy Systems at the TUM School of Engineering and Design. The special feature of the future laboratory "REDEFINE H2E" is the combination of innovative technologies such as high-temperature electrolysis, innovative gasification processes and the synthesis of basic chemicals and energy carriers. The researchers come to TUM from renowned institutions around the globe, including Australia, Brazil, Germany, Canada, Lithuania, Sweden, the USA and the UK, to jointly lay the foundations of a future hydrogen-based circular economy. The group will work at TUM-IAS and hold international workshops and conferences there.

TUM-IAS Fellowship Call

The TUM-IAS has awarded 28 Fellowships in 2022, more than ever before. Ten of these are part of the ad hoc Fellowships for Ukrainian Scientists program. 13 Fellowships are distributed among the various categories Carl

von Linde Fellowship, Hans Fischer (Senior) Fellowship, Anna Boyksen Fellowship for scientific illumination of issues in the field of gender, equality, diversity, Rudolf Diesel Industry Fellowship and Albrecht Struppler Clinician Scientist Fellowship. The newly appointed Fellows come from Germany, Israel, Poland, Sweden, Spain and the USA.

For more than ten years, TUM has been appointing promising talents as Tenure Track Assistant Professors (W2), after a thorough selection process organized by TUM-IAS. The TUM Faculty Tenure 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 researches the best start in their career possible, they are equally affiliated with the TUM-IAS as Fellows. In 2022, new Rudolf Mößbauer Tenure Track Assistant Professors have been appointed. For details on our new Fellows, please see Chapter "Welcoming Our New Fellows" from page 22.

¹ Awards

We are delighted and proud that our Fellows and partners have again received top-class awards in 2022:



European Research Council Established by the European Commission

ERC Grants

TUM-IAS Fellows and Rudolf Mößbauer Tenure Track Assistant Professors **Angelika Harbauer** and **Laura Leal-Taixé** received an ERC Starting Grant. IAS-Member **Prof. Jia Chen** and **Prof. Matthias Feige** were awarded the prestigious ERC Consolidator Grants.

Prof. Jia Chen has also been awarded the Arnold Sommerfeld Award 2021. The Bavarian Academy of Sciences honours Professor Chen's fundamental contributions to research on climate change and urban pollution.

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 2011 and 2021. Researchers who are cited particularly often in different fields are listed in the Cross-Field category. In total, the list comprises around 6,900 people in no particular order, including the following TUM-IAS Fellows

Prof. Ib Chorkendorff (Chemistry), DTU Copenhagen | Prof. Naomi Halas (Material Science), Rice University | Prof. Laura Herz (Cross-Field), University of Oxford | Prof. Bernhard Küster (Cross-Field), TUM | Prof. Peter Nordlander (Material Science), Rice University | Prof. Robert Schmitz (Cross Field), University of Georgia | Prof. Yang Shao-Horn (Chemistry), MIT

Prof. Eugénia da Conceição-Heldt, TUM-IAS Carl von Linde Fellow, has been invited to become Visiting Research Scholar at Princeton University's School of Public and International Affairs in 2022.

For developing light-powered "antenna-reactor" catalysts that can substantially lower the temperatures required for industrial-scale hydrogen production, **Prof. Naomi Halas** and **Prof. Peter Nordlander**, both from Rice University, have received the prestigious ENI Energy Transition Award 2022. It is endowed with 200,000 US dollars. Halas, a chemist, physicist and engineer, and Nordlander, a theoretical and computational physicist, were recognized for leading the development of commercially viable light-activated nanoparticle catalysts that can insert energy into chemical reactions with surgical precision.

Laura Herz, Hans Fischer Senior Fellow and Professor for Physics at Oxford University, has been awarded the Environment, Sustainability & Energy Division mid-career Prize of the Royal Society of Chemistry. She is honored for her pioneering work advancing the development of solar cells through fundamental understanding of electronic, structural and chemical properties of next-generation light-harvesting materials.

The Italian Knowledge Leaders prize 2022 was awarded to **Dr. Sara Lucatello**, former TUM-IAS Anna Boyksen Fellow.

Hans Fischer Fellow **Dr. Luca Magri** (Imperial College) has secured funding within the extremely competitive New Horizon program by the British Engineering and Physical Sciences Research Council EPSRC. Each project focuses on high risk, speculative engineering or information and communication technologies research with a potentially transformative impact. His aim is to create a framework and toolbox to marry over 60 years of high-performance computing with quantum computing to revolutionize understanding, modelling, and simulation of fluid mechanics.

Prof. Matthias Senge, Hans Fischer Senior Fellow, won a five years research grant of over 1.2 million euros from the Science Foundation Ireland for his project "Re-engineering Porphyrins – From Shape to Function."

For his scientific work on imaging techniques to improve image quality and for his algorithms for data storage in DNA, IAS-Fellow and Rudolf Mößbauer Tenure Track Assistant Professor **Reinhard Heckel** received the Young Scientist Honor from the Werner von Siemens Foundation.

TUM Distinguished Affiliated Professor and new IAS Member

Alan Irwin, Professor in the Department of Organization at Copenhagen Business School, will be appointed Distinguished Affiliated Professor at the Technical University of Munich and as such will become a Member of the IAS. His research focuses on issues of science and technology policy, scientific governance, environmental sociology and science-public relations; he is currently working on research and innovation policy. Alan Irwin was the Vice-President of Entrepreneurship and Innovation and Dean of Research at CBS. He was in addition Acting President during 2011. Previously, he was Professor at the University of Liverpool, and he has held appointments at Manchester and Brunel University. He is a Fellow of the Academy of Social Sciences, a foreign member of the Royal Danish Academy of Sciences and Letters, and an Honorary Fellow of the British Association.

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With a weakening pandemic and the end of numerous travel restrictions in many countries around the world, more workshops and meetings with personal participation could take place again. In addition to its own events, the IAS hosted over 100 other TUM workshops and conferences.

TUM-IAS General Assembly

For the first time in two years, our General Assembly could take place in person at the Institute with over 140 participants. A variety of lectures, presentations and poster sessions brought together Fellows, Hosts, PhD candidates and guests. To name but a few: Barbara Solenthaler talked about AI Revolution for Physics-Based Simulation, Daniela Pfeiffer presented latest research on Advanced X-ray and CT Techniques for Improved Lung Imaging, and Hydrogen-Fueled Gas Turbines for Decarbonizing Power Generation were presented by Mirko Bothien.

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 pioneer in cooling technology. The 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.

Maja Horst, TUM-IAS Hans Fischer Senior Fellow and Professor for Responsible Innovation and Design at Danish Technical University, DTU, Copenhagen, opened with her Linde Lecture the 2022 General Assembly. Her talk on "Responsibility, Science Communication and Social Cohesion" made a plea for co-creation and demanded co-creation, in which the collaboration of diverse actors, e.g. companies, universities, policymakers and members of the public gives an opportunity for making innovation processes more socially inclusive and responsible.

The 2022 General Assembly concluded with an exclusive sneak preview of the documentary "Rivers above the canopy," which the French-German station "arte" broadcasted later on November 12, in its program. Dr. Anastassia Makarieva, Anna Boyksen Fellow of the IAS and member of the International Expert Group on Earth System Preservation (IESP), was one of the scientific contributors. ►



Meike Schalk, Anna Boyksen Fellow

Sustainabiliity day

On October 27, 2022, TUM celebrated the launch of its Sustainable Futures Strategy 2030 with the first university wide TUM Sustainability Day. To this end, the IAS hosted a highlight event with presentations, lectures and public discussion, including speakers and students from TUM Campus Straubing on Biotechnology and Sustainability.

Events of Fellows

On October 1, 2022, **Prof. Pierluigi D'Acunto**, TUM-IAS Fellow and Rudolf Mößbauer Tenure Track Professor, and colleagues initiated the TUM innovation network CoConstruct (Collaborative Construction). The research group, coordinated by Prof. Christoph Gehlen, focuses on the topic of human-machine interaction in architecture and construction and started their project with a kick-off meeting at TUM-IAS.

Prof. Lothar Hennighausen, Hans Fischer Senior Fellow, and Dr. Markus List, TUM School of Life Sciences, organized a Bioinformatics Symposium at Freising-Weihenstephan on October 20. Hans Fischer Senior Fellow **Susan Park**, Professor of Global Governance at the University of Sydney, has a long standing commitment to Global Environmental Politics. Her research focuses on the global governance of the shift to renewable energy as well as on the examination if and how international grievance mechanisms operate to provide justice for communities harmed by international energy and development projects funded by multilateral development banks. In 2022, there were two events with her as part of her Fellowship:

A workshop on "China's Role in Global Economic Governance workshop" on November 4–5, 2022, co-organized by Prof. Eugénia da Conceição-Heldt, Chair of European and Global Governance at Technical University of Munich and TUM-IAS Carl von Linde Fellow.

Second was her book presentation "The Good Hegemon – US Power, Accountability as Justice, and the Multilateral Development Banks" on November 11, 2022.

Prof. Eitan Yaakobi, TUM-IAS Hans Fischer Fellow, and his Host Prof. Antonia Wacher-Zeh, organized the Munich Workshop on Coding and Cryptography in 2022.

Prof. Karin Nachbagauer, TUM-IAS Hans Fischer Fellow, hosted the IUTAM-Symposium on Optimal Design and Control of Multibody Systems – Adjoint Methods, Alternatives, and Beyond, at the TUHH in Hamburg, Germany, on July, 18–21, 2022.

Prof. Daniela Pfeiffer, Albrecht Struppler Clinician Scientist Fellow at TUM-IAS, was in charge IMXP 2022, the International Symposium on Medical Applications of X-ray, phase-contrast & photon-counting, at TUM-IAS in August 2022. ■

 A detailed report of the IESP starts on page 96.



TUM-IAS team (from left to right): Agnes Limmer, Susanne Wagenbauer, Annette Grötler, Sigrid Wagner, Morwenna Joubin, Katharina Frank, Anna Kohout



Barbara Solenthaler, Hans Fischer Fellow









PARIS













SYDNEY

RIO DE JANEIRO Welcoming Our New Felows

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

Fellowship Programs



Anna Boyksen Fellowship

two years for oustanding top-level female professors who intend to explore gender- and diversityrelevant themes in the context of the TUM subject portfolio



Rudolf Mößbauer Tenure Track Assistant Professorship six years for outstanding, highpotential early-career scientists



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



Albrecht Struppler Clinician Scientist Fellowship

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



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

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



Carl von Linde Fellowship two years for excellent TUM faculty members

Prof. Mats Alvesson

Lund University | University of Queensland

Prof. Johannes Betz

TUM School of Engineering and Design





Fellowship: Hans Fischer Senior Fellowship | Host: Prof. Claudia Peus (TUM School of Management) | TUM-IAS Focus Group: Training in companies: sensemaking of obligatory courses | TUM-IAS Research Area: Organizations, Management, and Leadership

The research investigates the motives, legitimation, meaning, perceived relevance and reception of obligatory courses on diversity, ethics and values and similar, non-technical topics, within professional service companies. It explores both managerial and employee views. A central topic is how various organizational levels interact – top down, negotiations, initiatives and feedback from lower level employees – and what are the effects of these courses. These may range from insights and ethical awareness to disinterest and cynicism, from clarity to and uncertainty and confusion.

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | TUM-IAS Focus Group: Autonomous Vehicles Systems (AVS) | TUM-IAS Research Area: Control Theory, Systems Engineering and Robotics

The Focus Group is interested in the algorithmic foundations of robot motion planning, control, and learning. The research of the AVS lab is aiming to create the next generation of intelligent autonomous vehicles. These vehicles will be able to interact with each other, including humans, while acting safely, efficiently, and with high performance. The group's vision is to enable safe and trustworthy autonomy for a broad range of high-integrity robotic applications. They are achieving this by designing adaptive dynamic path planning and control algorithms, developing decision-makers that can work under uncertainty in multi-agent environments, and validating the algorithms on real-world robotic systems.



TUM School of Natural Science

Prof. Eugénia da Conceição-Heldt

TUM School of Social Sciences and Technology





Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | TUM-IAS Focus Group: Quantum Sensing | TUM-IAS Research Area: Surface, Interface, Nano- and Quantum Science

Fellowship: Carl von Linde Fellowship | TUM-IAS Focus Group: Disruptions in Politics and Technology | TUM-IAS Research Area: Political, Social and Technological Change

The Focus Group is interested in the application of quantum sensors in chemistry. For this purpose, they use color centers in diamond, which have proven to be outstanding atomicscale sensors for magnetic fields. With these spin defects in diamond – more precisely nitrogen-vacancy (NV) centers – nuclear magnetic resonance (NMR) signals from a few cubic nanometer sample volumes or even single molecules can be detected, unreachable with conventional sensors. The applications of this new technology range from single-cell analysis in microfluidics to the characterization of surfaces and novel materials in the field of e-conversion. Rapid advances in technology - e.g., artificial intelligence, the rise of the world's largest technological companies, and autonomous driving - are leading to unprecedented changes in politics, society, and economics. At the same time, shocking events in politics - e.g., the Brexit, the backlash against globalization, the rise of populism, the pandemic, and the Russian invasion of Ukraine - are challenging liberal democracies and the global order. Against this background, the Focus Group "Disruptions in Politics and Technology" investigates how disruptions happen in the national, European, and global spheres from an interdisciplinary perspective. The main objectives of the project are to: a) provide a typology of disruptions; b) elaborate a theoretical framework to study disruptions from a multidimensional perspective; c) explain how, why and with what consequences political and technological disruptions occur on national, European and international levels. The insights gained from the empirical analysis will enable us to map different patterns of disruptions from a multidisciplinary perspective and to learn the consequences of disruptions.

Prof. Andrea Erhardt

University of Kentucky

Prof. Gregory D. Erhardt

University of Kentucky

Fellowship: Hans Fischer Senior Fellowship | Host:

Fellowship: Anna Boyksen Fellowship | Hosts: Prof. Martin Elsner (TUM School of Natural Sciences), Prof. Rolf Moeckel (TUM School of Engineering and Design) | TUM-IAS Focus Group: Removing Institutional Roadblocks for Inclusion in Science | TUM-IAS Research Area: Gender and Diversity in Science and Engineering

Despite recognition of the negative impact of low gender and ethnic diversity in science, barriers and misconceptions persist. Workplace dynamics, institutional impediments, and limited advocates all contribute to the reduced retention of diverse populations. This Focus Group will investigate different intervention programs to understand and address institutional issues with increasing diversity. They will focus on creating a better advocates program with the aim of training male advocates how to promote gender diversity. Additionally, a regular workshop series will identify impediments to diversity in Germany, and TUM specifically, with the final goal of providing recommendations for policy changes. The group is hoping to illustrate how implicit bias and workplace culture contribute to reduced gender diversity while providing encouragement for change. This program will be run concurrently in Germany and the USA, providing cultural comparisons and identifying the most impactful modules.

Prof. Rolf Moeckel (TUM School of Engineering and Design) | TUM-IAS Focus Group: Travel Behavior | TUM-IAS Research Area: Environmental and Earth Sciences, Building Technology

In the Focus Group Travel Behavior, former Hans Fischer Senior Fellow Prof. Kelly J. Clifton (University of British Columbia), Hans Fischer Fellow Prof. Greg Erhardt (University of Kentucky) and their Host former Rudolf Mößbauer Tenure Track Assistant Prof. Rolf Moeckel (TUM School of Engineering and Design) are concentrating on integrated modeling of land use and transport, as well as travel behavior research. This includes model development of land use, transport, and related models, such as environmental impact models, health models, and fiscal impact models. It also includes the spatial analysis of travel behavior and location choice of households and firms. The interaction between land use and transport is of special interest. Ultimately, models and spatial analyses should improve policy analysis by extending scenario capabilities and by improving model sensitivities. The Focus Group Travel Behavior emerged from the former Focus Group Modeling Spatial Mobility.



Prof. Julian Grünewald

TUM School of Medicine and Health



Bar-Ilan University | Exeter University



Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | TUM-IAS Focus Group: Gene Editing |

TUM-IAS Research Area: Bio-Engineering & Imaging

Fellowship: Anna Boyksen Fellowship | Host: Prof. Claudia Peus (TUM School of Management) | TUM-IAS Focus Group: He for She: Understaning men's allyship to promote gender equality | TUM-IAS Research Area:

Gender and Diversity in Science and Engineering

The first CRISPR therapy is heading for approval in 2023. This will herald a new era of medicine. CRISPR 2.0 gene editing tools, such as base and prime editors, can precisely modify DNA sequence without the need for DNA double-strand breaks. Delivery of these complex geneediting machineries to target tissues in the human body is another exciting frontier. In clinical trials, the first patients have received CRISPR intravenously, which led to robust in vivo editing in the human liver without substantial adverse events. The Emmy Noether group at the Department of Medicine I: Cardiology (TUM University Hospital rechts der Isar) is focusing on engineering CRISPR technologies for research and therapeutic applications, particularly in cardiovascular medicine. The group is aiming to apply the newest CRISPR 2.0 tools in stem cells and organoid systems as well. The lab is located at TranslaTUM and will also be part of the upcoming Center for Organoid Systems (COS).

The Focus Group is seeking to establish a broader understanding that lead to men's engagement for the promotion of women and gender equality in organizations with a special focus on hyper masculine fields and organizations (e.g., STEM fields). Using multimethods, that combine qualitative research methods (e.g. qualitative interviews) as well as quantitative methods (e.g. large-scale surveys, experiments) the Focus Group is aiming to unravel: 1) When men are likely to become allies by focusing on the ideology, motivations, emotions, opportunities and possible gains for men as allies in work organizations. 2) To uncover the challenges and possible drawbacks of men's allyship and how women (and other men) react to them. 3) To understand when they are likely to come across less barriers and backlash and when they will be successful in their actions. The group is also interested in offering more nuanced insights by adopting different contextual and social sensitive lenses and informing practical interventions designed to facilitate and improve men's allyship specifically in TUM and more at large within work organizations.

Dr. Dr. Kim **Melanie Kraus**

TUM University Hospital rechts der Isar

PD Dr. Philipp-Alexander Neumann

TUM University Hospital rechts der Isar





Fellowship: Albrecht Struppler Clinical Scientist Fellowship | TUM-IAS Focus Group: Clinical Translation of Microbeam Radiotherapy (MRT) | TUM-IAS Research Area: Medical Natural Sciences

Fellowship: Albrecht Struppler Clinician Scientist Fellowship | TUM-IAS Focus Group: Intestinal inflammation, anastomotic healing and fibrosis | TUM-IAS Research Area: Medical Natural Sciences

Dr. Dr. Kim Kraus and PD Dr. Stefan Bartzsch and his team are working in this Focus Group together with Prof. Markus Zimmermann from the TUM School of Engineering and Design. They are aiming to improve the therapeutic window of cancer treatment using microbeam radiation therapy (MRT) by the development of a clinically available compact source for MRT. MRT is a novel cancer treatment technique based on spatially fractionated radiation with the potential to reduce radiation induced toxicity. Several ten micrometers wide x-ray beams are spaced hundreds of micrometers apart. This unique beam profile has proven superior normal tissue sparing in preclinical experiments. The increase of the therapeutic window between tumor control and toxicity in organs at risk, promises a strong improvement in the treatment of tumors in radiation sensitive areas. This technique has only been applied preclinically and so far, large synchrotrons are required for beam production. At TUM we are combining cutting-edge medical and engineering expertise to translate MRT to a compact bench-top size source that can operate in any hospital. Thus, we are aiming to substantially improve cancer care in radiation oncology.

Dr. Neumann is a surgeon, clinician-scientist and PI of his group at the Department of Surgery, TUM University Hospital rechts der Isar. In 2009, he obtained his medical degree at TUM and started his career in surgery at the University of Muenster. Next to his clinical career, he has specialized on basic and clinical science of colorectal surgery with special interest in inflammatory bowel diseases (IBD) and intestinal wound healing following surgery. During a postdoctoral fellowship at Emory University, Atlanta/USA, he was part in numerous projects related to epithelial wound closure and inflammatory models in the gut. In 2016, he started his own group at TUM. His research is focusing on the role of anti-inflammatory proteins in intestinal inflammation, wound closure and fibrosis following surgery for IBD. During his Fellowship, he will further focus on delineating the impact of the gut's microbiome and the WNT-pathway on fibrosis development in Crohn's disease. A novel combination of classic intestinal inflammation models, combined with surgical procedures and molecular analysis, shall bring new insights into the mechanism behind intestinal anastomotic healing and fibrosis in IBD.

Prof. Natalia Perkins

University of Minnesota

Prof. Andreas Reiserer

TUM School of Natural Sciences





Fellowship: Hans Fischer Senior Fellowship | Host: Prof. Johannes Knolle (TUM School of Natural Sciences) | TUM-IAS Focus Group: Topology and Frustration in Spin-Orbit Coupled Quantum Magnets | TUM-IAS Research Area: Surface, Interface, Nanoand Quantum Science

Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | TUM-IAS Focus Group: Quantum Networks | TUM-IAS Research Area: Surface, Interface, Nano- and Quantum Science

This project is focusing on the theoretical understanding of quantum magnetic materials with strong spin-orbit coupling, nontrivial topology and correlations. This field has recently experienced a strong development both in theory and in experiment. A particular attention will be paid to quantum spin liquids (QSLs), which are fascinating magnetic states of matter characterized by long-range entanglement and fractionalized excitations. They are also technologically important as potential platforms for topological quantum computation. The group will focus on the development and analysis of effective super-exchange Hamiltonians describing novel Kitaev materials, which are believed proximate to Kitaev QSL and are realized in a variety of systems, such as transition metal oxides, rare-earths and halides. This Focus Group will compute the ground state phase diagrams of these models and identify the nature of possible quantum states and phase transitions between them. The group will also study the effects of disorder in these systems, as the competition of disorder, frustration and topology can potentially give rise to many unexpected phenomena.

Quantum networks will allow their users to implement tasks and communicate in ways that are not possible using present-day technology. As an example, they will enhance the computational power of quantum computers and allow users to safely connect to them. In addition, quantum networks enable the connection of distributed quantum sensors with unprecedented accuracy. In this context, the Professorship on Quantum Networks explores novel hardware platforms, in which stationary quantum systems are connected and entangled by the exchange of photons. In particular, the group investigates erbium dopants in silicon, which offer a unique potential for future devices that can be manufactured using established technologies of the semiconductor industry.

Dr. Felix Rempe

BMW Group, Autonomous Driving Division

Prof. Siobhan Rockcastle

University of Oregon





Fellowship: Rudolf Diesel Industry Fellowship | Host: Prof. Klaus Bogenberger (TUM School of Engineering and Design) | TUM-IAS Focus Group: Artificial Intelligence in Traffic Engineering and Control | TUM-IAS Research Area: Advanced Computation and Modeling

The development of connected and automated vehicles promises a profound change of current transportation systems. Using multiple sensors and fast transmission of data, significantly more information about the current traffic state, including all road users, can be gathered. Additionally, and most important, in an automated vehicle the human driver will be assisted or replaced with a computer system that acts in a deterministic and controllable way. The vehicle's speed and trajectory can be predicted and altered if necessary. Thus, foreseeable conflicts between road users can be avoided preemptively, inefficient stop and go movements can be suppressed and road space can be exploited better. Within this Focus Group novel approaches for traffic state estimation and control exploiting the technical opportunities of connected and automated vehicles are developed. Therefore, large amounts of data collected by current vehicle fleets are used to train machine learning algorithms to accurately infer current and future traffic conditions in transportation networks. On top of these, traffic control algorithms are designed, implemented and validated using the TUM testbed for automated driving and simulation environments.

Fellowship: Hans Fischer Fellowship | Host: Prof. Thomas Auer (TUM School of Engineering and Design) | TUM-IAS Focus Group: Human-Centric Building Performance | TUM-IAS Research Area: Environmental and Earth Science, Building Technology

The role of this Focus Group is to study the dynamic effects of visual and thermal conditions on human perception, health, and comfort indoors. Using controlled laboratory experiments and advanced computational methods, this group seeks to create dynamic predictive models that can inform the design of healthy buildings. Modelling human health and comfort across a holistic range of factors requires analysis of both physiological and subjective signals over time to understand biological adaptations and naturally occurring changes in the surrounding environment. Supported by the SenseLab (TUM) and through ongoing collaboration with the Baker Lighting Lab (University of Oregon), this Focus Group will evaluate visual and thermal conditions in an experimental setting to create a holistic dataset and reveal how indoor environments have an impact on shaping human health. This Focus Group will rely on regular collaboration from the Department of Informatics and the Department of Sport and Health Sciences.

Prof. Simon Thomas Schäfer

Prof. Yang Shao-Horn

TUM School of Medicine and Health





Fellowship: Rudolf Mößbauer Tenure Track Assistent Professorship | TUM-IAS Focus Group: Advanced Organoid Technologies for Mental Health Research | TUM-IAS Research Area: Medical Natural Sciences

As live human brain tissue is inaccessible. most studies of this organ have been restricted to the analysis of post mortem tissues or animal models, which bear a limited resemblance to the complexity of living human physiology. Organoids are emerging as novel technologies that allow to recapitulate the structure and function of various human organs in vitro, including the human brain. These tools have the potential to revolutionize the future of biomedical research. This group focuses on advancing these technologies to push the boundaries for personalized research on human brain disorders and to identify therapeutic strategies for facilitating brain repair. The lab is currently located at TranslaTUM and will also be part of the newly founded TUM Center for Organoid Systems and Tissue Engineering (COS).



Fellowship: Hans Fischer Senior Fellowship | Hosts: Prof. Aliaksandr Bandarenka, Prof. Roland A. Fischer (TUM School of Natural Sciences) | TUM-IAS Focus Group: Electrocatalysts based on or derived from crystalline coordination networks such as metal-organic frameworks and related materials | TUM-IAS Research Area: Fundamental Natural and Life Sciences

There are immense opportunities to make carbon-free or carbon-neutral energy carriers using low-cost electricity from renewable sources. Unfortunately, the efficiency of such processes is low, which is limited primarily by slow reaction rates such as the oxygen evolution reaction (OER), one universal step for making of energy carriers from water, carbon dioxide or nitrogen. Metal organic frameworks (MOFs) are a novel class of porous, crystalline inorganic/organic materials accessible by reticular chemistry, with promising activity and stability. The question arises whether MOFs present new perspectives for OER? The collaborating partners Prof. Bandarenka, Prof. Fischer, and Prof. Shao-Horn address the tunability of carboxylate linker-based MOFs under OER operando conditions, aiming to optimize their intrinsic OER performance. This Focus Group is aiming to leverage the potential of MOFs as precursors, taking advantage of the MOF metamorphosis into the active catalyst under OER. The major goals are characterizing the nature, distribution, and accessibility of the active sites and the evaluation of their tuneability by MOF design, including the MOF and the MOF-derived materials structural defect engineering.

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Prof. Piotr Tryjanowski

Poznań University of Life Sciences

Prof. Andreas Winter

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Fellowship: Hans Fischer Senior Fellowship | Host: Prof. Annette Menzel (TUM School of Life Sciences) | TUM-IAS Focus Group: Citizen Science Nature Watch | TUM-IAS Research Area: Fundamental Natural and Life Sciences

Citizen Science (CS) is popular to involve the public in nature watch and environmental education and has been providing necessary data to the scientific community. Based on complementary scientific expertise on animals and plants, our project aims at identifying phenological match-mismatch by merging corresponding CS sources and at analysing whether spatial variability and food webs are capable to buffer negative impacts. The novel aspect of this project will be to set in value CS also for a human-centred approach risking creativity with (so far) atypical applications. CS observations in combination with other social media data will be used to study spatial-temporal patterns of human activities in nature, modelled as a sort of "digital twin." This complex relationship between humans and nature/wildlife will reveal critical aspects and thus support the sustainable provisioning of ecosystem services, such as recreation and biodiversity. Recent publications have provided first single examples how government policies adopted in response to the COVID-19 pandemic were visible in altered CS observations. This project aims at going beyond this anecdotal evidence and will study on the global scale if and how COVID-19 related CS change patterns can be related to conservational status of species.



Fellowship: Hans Fischer Senior Fellowship | Hosts: Prof. Holger Boche (TUM School of Computation, Information and Technology), Prof. Gerhard Kramer (TUM School of Computation, Information and Technology) | TUM-IAS Focus Group: Quantum Information Theory | TUM-IAS Research Area: Surface, Interface, Nano- and Quantum Science

Nowadays, secure data transfer is largely based on complexity assumptions that might be rendered unreasonable by future quantum computers. Quantum communication opens up the possibility of physically verifiable privacy. It offers, however, many other potential applications and challenging theoretical problems. The standard approach to communication focuses on message transmission, and the notion of privacy is very much settled on a composable definition of statistical quality of secret keys. At the same time, few-user settings, such as Wyner's wiretap channel, can be analysed using only the classic inequalities for the entropy in correlated systems. This Focus Group will branch out beyond the standard paradigm by considering security criteria in quantum communication that are less demanding and more realistic than the standard setting. Likewise, the group will develop a focus on identification via quantum channels, going beyond the Shannon paradigm, which offers many exciting open questions to work on. Finally, they will further quantum entropy inequalities beyond strong subadditivity; such inequalities have long been known for the Shannon entropy, but are only conjectured for the von Neumann entropy.

Prof. Manuel Spitschan

TUM Department of Sport and Health Sciences



Fellowship: Rudolf Mößbauer Tenure Track Assistant Professorship | TUM-IAS Focus Group: Chronobiology & Health | TUM-IAS Research Area: Medical Natural Sciences

The Focus Group Chronobiology & Health investigates how the environment controls our inner biological clock. The light-dark cycle is a crucial influence on our circadian rhythm set by the activity of light-sensitive cells in the eye connecting to the structure in the brain housing the circadian clock. With the advent of electric lighting, light has become ubiquitous and available 24/7, leading to circadian disruption. The Focus Group Chronobiology & Health employs state-of-the-art methods to examine how light influences our physiology and behavior, ranging from wellcontrolled laboratory studies with carefully designed lighting scenarios to field studies in the real world. Our approach is to go from mechanisms to interventions to modify light exposure in a personalized fashion to support health and well-being optimally. In addition to answering these core translational research questions, three additional areas of interest are developing an open-source ecosystem for digital interventions in the field of sleep and circadian science, developing effective science communication strategies, and working within standardization organizations related to light and lighting.



Fellowships for Ukrainian Scientists

Immediately after the Russian invasion of Ukraine, TUM launched an ad-hoc program for students and scientists. A Fellowship program was set up at TUM-IAS for established researchers, which awarded ten Fellowships for an initial six-month research stay at TUM from March 2022 on. **Our sincere thanks go to the donors from the environment around TUM, who made this support possible.**


Olga Popovych, Julia Yamnenko, and Oksana Chernova experienced the Russian attack on their homeland, Ukraine, in different ways, at different locations, with different people. Popovych, Yamnenko, and Chernova were all scientists working at universities in Ukraine. Popovych and Yamnenko are engineers, and Chernova is a mathematician. They fled to Munich in the spring of 2022 from the Russian war of aggression and have found a place at TUM where they can continue their academic activities. How did these three women make their way to Munich? Why TUM of all places, and what do they do there? Here is their story.

By Fabian Dilger and Matthias Kirsch

On February 24, 2022, Thomas Hofmann, President of TUM, read and heard about the attack on Ukraine in the morning. One of his first thoughts was: Is there anything that we, as TUM, can do to help?

Thomas Hofmann: Every morning I confer with the press spokesperson; I immediately addressed the topic, and we started thinking about what we ourselves could do. Not just sit here and watch; what could we immediately do within the bounds of our possibilities, the options open to us.

Thomas Hofmann and his spokesperson Ulrich Meyer considered: Who might have contacts in Ukraine? And who might have an idea about how the university would be able to help? Ulrich Meyer sent out an e-mail to two colleagues at 8:14 a.m.: "Dear Uli, I was just developing an idea with the President about how we could offer Ukrainian researchers support in case they have to flee from their home country. He thought of the IAS and the TUM Global Visiting Professor Program as possible frameworks for something like that. What do you think?" The person whom Meyer addressed in this e-mail was Ulrich Marsch, Managing Director of the TUM Institute for Advanced Study. Marsch and the IAS already have some experience in bringing scientists to TUM from foreign countries.

Ulrich Marsch: I immediately said we should consider a program for receiving Ukrainian scientists and integrating them into the TUM world, even on a longer-term basis, since the war looked as if it would go on for quite some time.

Suddenly everything moved very quickly. Marsch presented his plan to Meyer.

Marsch: So that was my idea, and he said he'd take it along to the President. He called back about an hour later and said: Yes! Great idea! Please work out the details. Please outline how this could work and how much money would be needed to implement the plan. I was finished with my sketch by noon.



Ukrainian scientists fleeing the country. To do so it would create a grant program, to be run through the IAS. The support campaign should be developed and implemented as quickly as possible. The aim would be to to bring Ukrainian researchers from Ukraine to Germany and to TUM so that they are in a secure environment and can continue their research. Thomas Hofmann, TUM President, wanted to take action and would not be satisfied with simply issuing statements of position. That, Hofmann said, would not be in keeping with the spirit of TUM.

Hofmann: This is central to the DNA of our university: When we identify challenges, we try to take concrete measures to solve them. Whether these measures succeed or not is then a completely different question; you can never be sure. But I have to say: The university is basically an experimental space, and we have to try things out. If things work, that's fine; if they don't work, then we approach it differently next time, but it's better to try things in many different ways than to try nothing at all.

On the morning of February 24, 2022, Popovych was in the city of Ivano-Frankivsk in southwestern Ukraine. She woke to see her husband with his telephone in hand.

Olga Popovych: It was still night outdoors, and I woke up because my baby was crying, and I saw that he was just reading the news. And I said: "Why are you not sleeping? It's only four o'clock." He told me: "No, the war has started." - "No, you are joking, maybe it's some misinformation." - "No, several bombs have already hit Kyiv." On February 24, 2022, Julia Yamnenko was traveling on business in Chernivtsi, in western Ukraine.

Julia Yamnenko: It was four o'clock in the morning, and my husband called me. "We are being bombed," he said. "I am in the car, and I am going to your father. I will take your father, and we will come to you in Chernivtsi, and we will decide later what to do." In the evening, my husband and my father, as well as my sister and her husband, arrived in Chernivtsi. We all gathered there and started to think what to do.

Oksana Chernova: I was in Kyiv. It took me maybe two seconds to realize that something had gone wrong, and I immediately took my phone, checked the latest news, and understood what had just happened. Next I started to collect my documents and put some important items in my backpack. War has started.

Popovych: The whole day we were thinking: What should we do next? Where should we go? At night, when we again received lots of news, that something will be expected in the night, we decided to move. We just put all of what we saw in that moment in our suitcase, searched for the most important documents. I still remember, I took my PhD diploma. I was thinking it was the most important document that I had up to that moment, and I should take it.

Yamnenko: On February 26th, my husband said that I should go abroad. He wanted us to be in a safe place. In this situation, I, my father, my son, and my sister with her



"Everything was happening simultaneously. First I was just trying to find a place to stay for the night, second to find a job. I was not thinking only about me. I was also thinking about my brother and my husband, who were going with me."

OLGA POPOVYCH

two children crossed the border to Romania, just by walking. There was a huge crowd on the border. Romania accepted us and made us feel very welcome. I was crying, because I thought of my husband and I realized I didn't know when I would see him again. It was difficult to leave him, and to leave my country, and on the other hand I didn't know where to go and how to help these people who were with me and whom I was responsible for.

Olga Popovych and her family quickly decided to flee to another country where their two small children would be safer, considering Poland and Germany. While fleeing, Olga Popovych constantly scoured the Internet looking for aid programs for scientists and possible jobs abroad.

Popovych: Everything was happening simultaneously. First I was just trying to find a place to stay for the night, second to find a job. I was not thinking only about me. I was also thinking about my brother and my husband, who were going with me. I found the advertisement from TUM, just a small notice; I think it was on a web page saying the university was in solidarity with Ukraine. And there was only the contact of Dr. Marsch, to whom I just sent a direct message: "Hello, my name is Olga Popovych, I'm from Ukraine."

This reference on the TUM website was the first official mention of the Fellowship program that President Thomas Hofmann, Ulrich Marsch and TUM had discussed on February 24. But before the Ukrainian scientists could actually come to Munich, Hofmann and Marsch would have to resolve a substantial difficulty: Where would the grant funding come from? **Hofmann:** Of course TUM is dependent on external funding, since we're not allowed to fund a grant program directly from our budget. Budgetary constraints make this impossible. The only way we can issue grants like these is by acquiring external funding.

Marsch: Installing someone in an academic employment situation means officially announcing a vacancy, waiting for applications, scheduling interviews, calling in the Employee Council ... that takes weeks. A grant, based on donations, can be quickly issued. And when it comes to war, you just can't wait that long. You have to act and act quickly.

So now Thomas Hofmann had to raise a large amount of money. The calculations said: 3,000 euros per month for each individual. For ten people over a period of six months, that would amount to at least 180,000 euros in advance. Hofmann began the search for donors. He was counting on Susanne Porsche, a film producer and investor.

Susanne Porsche: I have very close ties to TUM, because it is such an incredibly good and interesting and leading-edge institution. Our university is simply fantastic. Thomas said: "Hello Susanne, Thomas here. We have to do something; what can we do? Do you think we could handle the financing, and what do you think of receiving the families as a partner university? We want them to be able to bring along their children; they can bring along the husband if they have three children or more." I instantly thought the idea was tremendous, and I was on bord immediately. I got on the phone right away to find out who would help. And I encountered a lot of compassion. My son also helped out. It was unbelievable how willing people were to help.

The idea of bringing Ukrainian scientists to TUM found many supporters. Susanne Porsche looked for additional donors within her network. TUM President Thomas Hofmann made more calls and met with potential sponsors.

Hofmann: You can only convince individuals to sponsor something when the right idea is brought to the right person. This matching of topics and individuals is decisive to success, since after all money can be used for a number of purposes. We have to make sure that people know the money is well-placed with us, going to a good cause. Most of all for measures that would never be possible without the support of the donors. Within less than ten days, we had the 250,000 euros that we needed in order to support ten grant recipients.

An impressive amount of money raised by Hofmann, Porsche and their associates. But there was hardly a shortage of potential applicants: Even before the grant program was officially advertised on the TUM website, people from every imaginable stage in their academic career contacted Ulrich Marsch at the IAS on their own, independent initiative.

When Oksana Chernova heard of the TUM aid program for the first time, she was still in western Ukraine. A colleague told her about the program by e-mail, and Chernova reacted immediately.

Chernova: The first time I heard about this program, I prepared a CV and sent it immediately.

Julia Yamnenko's first destination was not TUM, but rather Germany. She had a friend

here, a professor who went to Bayreuth in 2014 after the occupation of the Donetsk region. "Come to Bavaria, I'll help you," he said. Julia Yamnenko and her family traveled from Romania to Hungary and took a train from Budapest to Munich.

Yamnenko: I just started to search for information about universities, about possibilities for Ukrainian researchers, for Ukrainian professors and so on.

At the same time, Ulrich Marsch of the IAS was actually occupied with nothing except organizing the grants.

Marsch: I did nothing else for four weeks. I was exclusively dedicated to this topic, from dawn to dusk.

Marsch received more and more applications. The fleeing Ukrainians spread the word among themselves about aid campaigns such as the TUM program. Marsch received well over 400 applications. Like the other Fellows at the IAS, the Ukrainian scientists should have a host professor at TUM with whom they would work closely on a scientific project.

Marsch: This meant the Fellow would not be sitting alone in isolation in some random building, but instead would be closely integrated into our university. From there they'd be able to work up to a position from which they could publish, might acquire subsequent funding, and would be able to continue to work in their usual field. That is the reason for the close connection to an existing professorship at TUM and integration at the professorship, including a desk, online services, and laboratory access. ►



This also meant Marsch had to find the professionally appropriate professors and then select matching Fellows from among the considerable number of applicants. He needed criteria he could follow.

Marsch: The Fellows would have to be research personalities that fit the TUM profile. There were certainly ten to twenty possible choices for each Fellowship, but the filter I applied was, for example: Is this someone who has just completed a dissertation? Or is it someone who has already held an academic leadership position? The IAS is not an entity for promoting postdoctoral researchers, but rather for promoting personalities who have already held higher-ranking academic positions, for example professors or department heads.

In some cases, the host professors directly contacted the applicants or received direct inquiries from them. Constantinos Antoniou, Professor for Transportation Systems Engineering at TUM, worked together with Julia Yamnenko to formulate her application for the Fellowship.

Yamnenko: A friend told me about Constantinos. He is working on topics similar to mine, so I asked him for support, and he agreed enthusiastically, very quickly. So we just prepared this application together on a joint topic that is connected with intelligent control of road traffic.

Ulrich Marsch had to piece the puzzle together, with the Ukrainian scientists forwarding the necessary documents while still fleeing their home country.

Marsch: They were writing e-mails to all kinds of institutions on the fly while in cars



"It was very fast, maybe less than seven or ten days. I got an e-mail, and even before this Fellowship was confirmed, my host professor wrote to me that I could come immediately because he has some funding for a visiting researcher."

OKSANA CHERNOVA

and trains. Then they sent on the documents, CVs, diplomas, certificates. I also asked all of them to submit a brief description of a program they intended to work on with us. Everyone submitted a project proposal. I had the proposals reviewed by two other professors, not only by the respective Host: Is this a reasonable plan? Does it meet our standards? The response, without exception, was always: yes.

As early as the beginning of March, just over a week after the beginning of the Russian invasion, Marsch was already prepared to make the decision, a tough call. He would have to turn down many more people than he would be able to accept. Ultimately, a total of ten candidates were selected.

Popovych: In that moment I didn't believe that I would get a position. Even after he sent me confirmation that I am already a Fellow at the TUM-IAS, it was still for me something unbelievable.

She talked it over with her husband, who was not permitted to leave the country during the

first weeks of the war. He told her: "Take the kids and your father and head for Munich!"

Popovych: I was going by car, and the car was full of packages. I was going with my mother, my father, and my kids. It was 1500 kilometers.

While Oksana Chernova looked for offers of support in other countries, she left Ukraine for Poland, where she arrived in Warsaw. It was there, not quite a week and a half after the beginning of the war, that she was notified of her acceptance at TUM.

Chernova: It was very fast, maybe less than seven or ten days. I got an e-mail, and even before this Fellowship was confirmed, my host professor wrote to me that I could come immediately because he has some funding for a visiting researcher. I just came to Munich immediately, in mid-March, then I got confirmation that my host professor can support me with accommodation, and then at the end of March I got confirmation that I now had a TUM-IAS Fellowship. My trip from Warsaw was probably the longest trip I ever had. It took more than 12 hours, because of some train delay, and because trains were full of Ukrainian refugees like me. It was mostly women and children.

Julia Yamnenko was already in Germany when she received word of her acceptance. Traveling with her son, her father, her sister, and her sister's children, she found the search for a place to live difficult. On May 1, she began work as the last of the ten scientists participating in the IAS Fellowship program.

Yamnenko: And at last I received the invitation that I could come and sign the agreement for this Fellowship, so I started it in May, and it continued until the first of September. By then, I had obtained another formal grant, the Philipp Schwartz Initiative Fellowship of the Alexander von Humboldt Foundation. Now Olga Popovych, Oksana Chernova, and Julia Yamnenko were back to their scientific routines. And what are these everyday routines like? Oksana Chernova is a mathematician.

Chernova: I was fortunate to find my host professor Mathias Drton, who works in statistics. We are doing regression modeling and non-parametric statistics. It is not far from what I was doing. I was very lucky to join TUM and the Department of Mathematics because it is well known for its high-quality research groups. Especially my host professor Mathias Drton is a star in our statistical world. Now I have a favorable environment to work in.

The Ukrainian scientists fled to Germany under great duress. In their new research teams at TUM, they are in some cases filling existing gaps, according to Ulrich Marsch.

Marsch: As far as I can judge the results, this has all been very productive. In several cases I have received statements from professors saying: "This young woman is exactly the puzzle piece that has been missing from my project." There have been substantive synergies: In one project the Ukrainian scientist added a further component that had been missing before. It has really all worked very well, also, in substantive, scientific terms. It was very useful to have had an advance look at, for example, whether the candidate had a certain number of international publications, had a certain amount of experience in the respective field. Otherwise this wouldn't have worked out so well.

Popovych: Last week I came back from Egypt, where we tried to scan the pyramids in the hope of finding some interesting things there. We were making measurements during the whole week of the field trip. It was very exciting for me because it was the first time that I was inside the pyramids. I was investigating all the chambers, all the tunnels, and the parts where usually visitors are not allowed to go. I was using my nondestructive testing technique, and using it specifically for a cultural heritage project, so it was very fascinating.

Julia Yamnenko was formerly head of her department and as such responsible for students and researchers. She attended conferences, held lectures, and supervised degree projects. She will have to adapt to her new role at TUM.

Yamnenko: I love to learn something new. For me it's a challenge, but I hope I will overcome it. There is a language barrier of course, and there are also other circumstances like new, different demands and techniques for the teachers. But it's interesting just to discover for myself something new and try to improve myself, maybe to change myself in some areas. Why not?

Conceived on the day war broke out, February 24, in the office of TUM President Thomas Hofmann, the Fellowships were originally planned to last six months. In the meantime the scientists have been here much longer. What lies ahead for them? The scientists were expected to organize research funding for themselves. For example, refugees can submit additional applications to Germany's largest research support organization, the German Research Foundation (DFG), so that they can be integrated in ongoing projects. Oksana Chernova's TUM Fellowship has been extended for the time being in order to support her.

Chernova: The First Fellowship was for six months, and then in September it was extended for six more months. During this time I can apply for some grants at a research program. That is what we are doing now.

In the meantime, top management at TUM has already decided: We'll keep providing support and will find financial resources in case someone can't immediately find a follow-up project.

Hofmann: Many have already been integrated into subsequent projects at the professorships. That's wonderful, and we've also found additional funding for a number of them so that they can stay even longer. The idea was always not to cut off support after six months, but rather to take a long-term perspective, to maintain networks even after the Ukraine crisis has passed, the war is over and the people can return to their home country.

Julia Yamnenko has already found a follow-up project, financed with funding from the German Research Foundation, where she will be able to concentrate on an aspect of her work that she is especially enthusiastic about: promoting talented young researchers.

Yamnenko: Actually I had already started to work with one TUM student here. Thanks to the university's grant program, I am able to hire this student, so we are working together already. He is a Master's student and very talented. I have a huge plan for him and for our joint work. Also I plan to start working with another student later.

But in spite of all the big plans, it's hard for Yamnenko to forget all she has encountered in recent months, the outbreak of war, escape, and a new beginning. Her husband is still in Ukraine. As a result, she doesn't want to make any long-term plans.

Yamnenko: For me it's very hard to say for the



4 5

moment, so I prefer just to put up a plan for a week, for a couple weeks, maybe for a month.

Her colleague Olga Popovych on the other hand is planning farther into the future. She has also found research funding for a project and as a result has received a follow-up contract at her new university chair. She gets along well with her team, she enjoys her work, and most of all she has a feeling: I'm contributing something here, and if everything works out, I'll be here for a long time.

Popovych: I decided to stay here. Actually, I hope that after this project ends, I will continue my work here in Germany. At the moment the war has not ended. I overcame a lot of hurdles to come here and to settle down, and I think maybe there is a chance for me to stay in Germany and to work. I would like to contribute on the Ukrainian side with new possibilities of coordination between Ukraine and Germany. Actually that is my task for the future. My host professor and I have decided to do it together. That will create a lot of proposals aimed at supporting cooperation between Ukraine and Germany.

TUM wants to be sure to continue promoting this side-effect of the Fellowships. The relationships between Ukrainian scientists and the university absolutely have to be maintained. President Thomas Hofmann doesn't think this would result in a lack of scientific resources in Ukraine.

Hofmann: No, I don't really consider that to be "brain drain." That's how science works. Science means dealing with one another openly, transparently, sharing knowledge. And by sharing knowledge we create more knowledge and not less, and I think that's the benefit here. And this is also exactly the way "I feel optimistic about the future, mainly because I have this feeling that I belong here. So I have friends, mainly Ukrainian friends, also colleagues who support me since I'm living in Garching. I found some friends there as well."

OKSANA CHERNOVA

the TUM Institute for Advanced Study works. This is exactly the reason why in the meantime hundreds of Fellows have been here at TUM. They learn here, return to their universities, and of course take along a lot. This leads to a global network in which researchers meet up again and again at certain occasions, jointly acquire projects, and send us talented young researchers. So this is a win-win situation for all involved.

Chernova: I feel optimistic about the future, mainly because I have this feeling that I belong here. So I have friends, mainly Ukrainian friends, also colleagues who support me since I'm living in Garching. I found some friends there as well. All of this together contributes to my optimistic feeling and keeps me from feeling that I am not alone. I feel the support. For me it feels like a new beginning of life. I think of it this way: My new life began in March 2022 in Munich.

The interviews were conducted in October 2022.

Our Fellows from Ukraine

Fellow	Institution	Expertise/Project	TUM School/Faculty Host	Future Funding
Oksana Chernova	Taras Shevchenko National University of Kyiv	Mathematics	Mathematics Prof. Mathias Drton	Continuation from donation program until end of March 2023
luliia Yereshko	lgor Sikorsky Kyiv Polytechnic Institute	Enterprise Economics	School of Management Prof. Hanna Hottenrott	Research Staff posi- tion at TUM School of Management since January 1, 2023
Oksana Koshulko	Alfred Nobel Univer- sity, Dnipro	Economics	School of Social Sci- ences and Technology Prof. Ruth Müller	Fellow at IAS Hamburg from October 1, 2022 on
Sofiia Lahutina	Bogomolets National Medical University	Medicine	Department of Sport and Health Sciences Prof. Manuel Spitschan	Continuation from donation program until end of March 2023
Liudmyla Lisova	E.O. Paton Electric Welding Institute, National Academy of Sciences	Metallurgy	Department of Me- chanical Engineering Prof. Wolfram Volk	Research Position of German Science Foundation with Prof. Wolfram Volk since November 2022
Olga Popovych	Ivano-Frankvisk Na- tional Technical Uni- versity of Oil and Gas	Engineering, Material	School of Engineering and Design Prof. Christian Große	Research Staff position with Prof. Christian Große from October 1, 2022 on
Yuliia Semenova	Institute of Geo- physics, National Academy of Sciences	Earth Sciences	Aerospace and Geodesy Prof. Florian Seitz	Continuation from donation program until end of March 2023
Olena Streinyk	Taras Shevchenko National University of Kyiv	Sociology	School of Social Sci- ences and Technology Prof. Ruth Müller	Mercator Fellow of German Science Foundation from Oktober 2022 on
Dmytro Sytnyk	Institute of Mathe- matics, National Academy of Sciences	Computational Mathematics	Mathematics Prof. Barbara Wohlmuth	Staff position with Prof. Barbara Wohlmuth
lulia Yamnenko	lgor Sikorsky Kyiv Polytechnic Institute	Electrical Engineering	School of Engineering and Design Prof. Antoniou Constantinos	Funded from September 2022 onwards by Philipp Schwartz Initiative of Alexander von Humboldt Foundation

Dr. Oksana Chernova

Taras Shevchenko National University of Kyiv

Prof. Oksana Koshulko

4 7



Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Mathias Drton (TUM School of Computation, Information and Technology)

Our project is concerned with a problem in shape-constrained density estimation in the area of statistics. Density estimates help to visualize data, reveal its features, and make inferences. In this setting, there are two main reasons for imposing shape constraints, e.g., monotonicity and convexity. First, such shape constraints may be directly motivated by the problem under investigation. Second, methods built around shape constraints often allow one to derive an estimator that does not depend on a tuning parameter.

The class of log-concave functions can be considered as a natural infinite-dimensional generalization of Gaussian densities and lies at the heart of modern nonparametric inference, due to both the modeling flexibility and its attractive statistical properties. However, the inefficiency of existing computational algorithms remains an obstacle to more widespread adoption of this approach by practitioners.

We develop methodology for efficient logconcave density estimation, creating tools to be used by practitioners to solve modern data challenges. Our approach for higher-dimensional cases is to apply an exponential series method combined with a score matching procedure. Alfred Nobel University, Dnipro



Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Ruth Müller (TUM School of Social Sciences and Technology)

The scientific project was carried out from March to September 2022. The project was designed to explore motives, goals, issues, and strategies of the behavior of Ukrainian war refugees in the host countries Germany and Poland.

During the project, qualitative methods of research were used. Among these were case studies, semi-structured interviews, and fieldwork. To collect data and conduct volunteer jobs for the war refugees in Poland and Germany, I collaborated with Caritas and Münchner Tafel.

According to the results of the project, the majority of the refugees in the host countries were mothers with children. In the earlier stages, they needed different types of help, protection, and support in the countries. Later, some of them needed employment. After a while, some of them returned to Ukraine.

Using the results of the project, scientific articles for academic journals in Indonesia, Romania, the UK, and Turkey were written. Also, conference presentations in Italy, Sweden, Turkey, Germany, the UK, Morocco, and Poland were made.

Dr. Sofiia Lahutina

Bohomolets National Medical University



Fellowship: Fellowship for Ukrainian Scientists | **Host:** Prof. Manuel Spitschan (TUM Department of Sport and Health Sciences)

The war in Ukraine is a traumatic event on a global scale. Increased levels of stress due to psychological trauma negatively affect sleep quality. In turn, poor sleep negatively impacts our psychological functioning. The use of online interventions in the field of mental health has enormous potential. Digital interventions have proven to be effective for correcting sleep problems in particular. The use of chatbots in messengers to influence mental health is a fairly new format for providing assistance. Creating a chatbot may represent a good solution in the context of the current situation in Ukraine. Chatbots can present information in the form of a dialogue and imitate a conversation with a person using short messages. These dialogues will be designed in such a way to take into account the cross-cultural aspect of Ukrainian population. A sleep health chatbot may help to influence the quality of sleep of people affected by the war and could make this help as accessible as possible. In this research project, we will deploy a chatbot targeted to individuals affected by the war in Ukraine and examine its effectiveness.

Dr. Liudmyla Lisova

The E.O.Paton Electric Welding Institute, National Academy of Science of Ukraine



Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Wolfram Volk (TUM School of Engineering and Design)

I am working on a project for near-net-shape production of steel molds using indirect additive manufacturing. This project aims to develop fundamental concepts for the implementation of indirect additive manufacturing of high-quality steel molds and to implement them practically on a laboratory scale. Steel molds are usually machined by the toolmaker from steel blocks, which inevitably leads to large material and energy consumption. Alternative concepts, such as direct additive manufacturing of molds, are also being used, but due to the high cost of the metal powders and the energy input, such approaches are used only for inserts. So the idea is to make a steel mold by sand casting. I am investigating the metallurgy and properties of the steels that could be used for the production of steel molds. It is important to choose the right steel, which will have sufficient characteristics for casting and further use of the finished steel mold. The casted steel molds only require a small amount of machining to the final mold contour. In this way, it should be possible to efficiently combine the advantages of casting and additive manufacturing.

Dr. Olga Popovych

Ivano-Frankivsk National Technical University of Oil and Gas

Dr. Yuliia Semenova

Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Christian Große (TUM School of Engineering and Design)

The Fellowship supported the project "Development of an ultrasound-based fouling-monitoring solution for in-situ detection and prediction of scaling and biofilms in geothermal power plants and open cooling circuits."

The detection of cracks and other deteriorations in tubes and pipes is an important task in many fields, and in particular in the transport of gases and fluids in the energy sector. One prominent example is non-destructive testing (NDT) to detect scaling (calcitic deposits) in geothermal power plants; another is the need to ensure high accuracy in the wall thickness of new pipes made of tungsten fibers infiltrated with liquid copper. In order to evaluate the detectability of scaling in places with limited accessibility, guided waves can be used.

An advanced approach to deal with quality control tasks is to use numerical simulations of wave propagation in such materials to help in selecting the best setup, sensor type, measurement frequency, and so on. Appropriate numerical simulation tools are available at the chair, including full-waveform inversion using the software Salvus (https://mondaic.com/). This tool can also be applied to other problems in materials testing. Mastering this tool will be one of the key points for successful NDT applications. Institute of Geophysics, National Academy of Science of Ukraine



In her research, Dr. Yuliia Semenova studies the nonlinear ground behavior under seismic loads. Key elements of the joint study with DGFI-TUM are (a) to develop an approach to identify, in time series of permanent GNSS observing stations, nonlinear effects that occur in ground during and after earthquakes and (b) to analyze and model the characteristics of the manifestation of these effects. DGFI-TUM is responsible for the realization of the International Terrestrial Reference System (ITRS) as one of three ITRS Combination Centers of the International Earth Rotation and Reference System Service (IERS) worldwide - along with JPL/NASA (USA) and IGN (France). The ITRS is the global coordinate system of highest accuracy and the basis for global positioning and navigation, e.g., when using GPS. Better understanding of nonlinear ground behavior under observation stations during and after earthquakes will improve the analysis, interpretation, and modeling of postseismic deformations at GNSS stations. This in turn will lead to significantly increased accuracies of station coordinates and their temporal changes and thus improve the accuracy and long-term stability of the ITRS realization.

Annual Report 2022



Dr. Olena Strelnyk

Taras Shevchenko National University of Kyiv



Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Ruth Müller (TUM School of Social Sciences and Technology)

As a sociologist and researcher of gender issues, Dr. Olena Strelnyk reformatted the subject of her research with the beginning of Russia's full-scale war against Ukraine. Currently she studies various aspects of the impact of the war on gender roles and expectations, and on women's rights in Ukraine.

During the Fellowship Program at TUM-IAS, she worked on the topic of cultural and media representations of women in the context of war. The focus of the research is how ideas on women's roles and "femininity" are (re)constructed. Using examples of different (social) media images of women, Dr. Strelnyk demonstrated how these representations – including stories of women's coping strategies, resistance, and agency during the war that become more visible in the Ukrainian media space – form a contradictory and complex picture.

She also used the program as an opportunity to strengthen the position of Ukrainian studies in Germany, gave several public lectures, participated in many conferences and public discussions, and wrote several blogs about the gender aspects of the war in Ukraine. Dr. Strelnyk also coordinated a special Ukrainian panel at the 41st Congress of the Sociological Association of Germany. Institute of Mathematic, National Academy of Sciences of Ukraine



Dr. Dmytro Sytnyk

Fellowship: Fellowship for Ukrainian Scientists | Host: Prof. Barbara Wohlmuth (TUM Department of Mathematics)

Our research was focused on the development of novel analytical and numerical tools for mathematical modeling of fractional phenomena.

Fractional calculus is an emerging field of study that deals with the extension of classical calculus, operating with integrals and derivative of integer order, to the case when the order parameter might be non-integer.

In many applications the use of fractional calculus leads to more accurate models than those constructed using ordinary integer calculus. Among such applications are diffusion in porous media, phase transition and separation in mixtures of liquids or polymers, wave propagation and energy dissipation in geology, and dumping and crack propagation in structural mechanics. For certain classes of models, fractional order description is necessary to properly capture the essence of underlying phenomena. This is especially true for transient systems that involve some sort of "memory" effect, e.g., shape-memory alloys, self-assembling materials, information processing systems, and financial markets. Usually, such complex systems are modeled with the help of time-dependent fractional differential equations that require new tools for analysis and numerical solution. They constitute the main object of our study.

Prof. Iuliia Yamnenko

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"



Fellowship: Fellowship for Ukrainian Scientists | **Host:** Prof. Constantinos Antoniou (TUM School of Engineering and Design)

The project is called "Machine learning methods for traffic demand and supply prediction." We are working on the management of road traffic. Data about traffic flow and volume is to be collected and then processed to provide efficient monitoring, prediction, and control. Construction and validation of traffic simulation models is one of the basic activities in transportation system engineering. Thus, quality of data is a crucial element. We see an opportunity to use the prediction models to infer unknown data using readily available data. Diverse data could be obtained from open sources such as OpenStreetMap, open data portals, and publicly available data. For instance, open data platforms for Paris and Madrid provide archived as well as real-time traffic data. Private companies such as Uber, TomTom, and Google provide limited access to historical or even real-time traffic information. There is a huge potential for machine learning and deep learning here due to the scale and diversity of the data. The combination of machine learning methods, deep learning neural networks, and pre- and post-processing of data is a new and promising approach for traffic management.

Prof. Julia Yereshko

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"



Fellowship: Fellowship for Ukrainian Scientists | **Host:** Prof. Hanna Hottenrott (TUM School of Management)

The ongoing unprovoked russian invasion of Ukraine brings not only the horrors of war and a humanitarian crisis, but also an uncertain future for Ukraine and the global society. At least now, it appears that harsh times are coming for everyone. Or are they? Economic history has taught us that every crisis (or war) becomes the prerequisite for future active developments (both technological and economic ones). Hence, in order to contribute to said future developments, we are trying to understand: 1) What conditioned a commencement of the golden age of capitalism? That dramatic economic development is basically a legacy of depression and war. Similarly, the current situation is characterized by crisis, which is affected and deepened by war. 2) How are innovation cycles affected by war? We can elaborate that those cycles actually are of a dual nature: The vast majority of devices that are pervasive in our day-to-day activity as well as common commodities are actually rooted in previous wars: That includes the Internet, vaccines, instant coffee, and even vegan sausages. In other words, humanity tends to be creative in adopting "wartime" innovations to "peaceful" times. Already today we can observe some initial innovative efforts toward a brighter future.



In Focus

Probing Perovskites

Researchers from Munich and Oxford are exploring novel materials that could boost solar cell efficiency. Laura Herz, David Egger, and Thomas Bein form a dynamic "research triangle" combining expertise in condensed matter physics, theoretical physics, and physical chemistry to understand and optimize energy conversion. Can global, long-term environmental, economic, and security challenges be addressed, or at least mitigated, by probing artificial materials on a femtosecond time scale? The answer might be yes if this research contributes to a more rapid switch to energy production from renewable sources such as sunlight. Slowing global warming and adapting to its impacts will depend on drastically cutting greenhouse gas emissions while reducing dependence on fossil fuels. These same steps could make economies and nations less vulnerable to any disruption of gas and oil supplies.

The TUM Institute for Advanced Study Focus Group on Optoelectronic Properties of Perovskite Semiconductors is exploring the physics and chemistry of novel materials that have the potential to boost the efficiency of solar cells. The group is led by Hans Fischer Senior Fellow Laura Herz, a professor of physics at the University of Oxford, where she directs the Semiconductors Group at the Clarendon Laboratory and serves as associate head of Oxford's Mathematical, Physical, and Life Sciences Division. Her Munich collaborators are TUM-IAS Rudolf Mößbauer Tenure Track Assistant Professor David Egger and Professor Thomas Bein of LMU, both of whom are principal investigators in the DFG-funded Cluster of Excellence "e-conversion."

For an inside view of fundamental studies that could open the way for the development of more efficient solar cells – enabling further expansion of photovoltaics within the global energy mix – science journalist Patrick Regan spoke with Laura Herz via videoconference in February 2023. Their conversation has been edited for length and clarity.

Q: Photovoltaics technology, in real-world products, has come a long way in terms of cost, performance, reliability, and market acceptance, especially during these past two decades. That's roughly the same time in which researchers discovered and began exploring the potential of so-called perovskite materials for solar cells. Would development and commercialization of perovskite solar cells represent incremental progress or something more like a breakthrough?

People are now seeing solar energy in reality. They're installing solar panels everywhere. You can see how much electricity even Germany or the UK can generate from solar on a good day. Twenty or thirty years ago we were told this could not happen because the weather was awful, and it was too expensive. Now we're installing it and reaching a terawatt worldwide – and why is that? Partly because the cost of silicon solar panels has fallen massively over the past decades and keeps falling. A lot of that is caused by mass production. Manufacturing has moved to China, where they have ruthlessly cut costs and have been supplying us with ever cheaper panels.

So why perovskites at this stage? Because the cost of the actual silicon solar cell has fallen so much, what now matters most is the on-cost, everything that's needed to actually plug that cell into the grid. In a domestic installation that would mean putting it on your roof, reconstructing that roof. You also have to add electrical components, such as an inverter, because ultimately your solar cell gives you a DC low voltage, and you have to



Laura Herz (left) and Patrick Regan (right) in conversation via video conference.

plug it into the grid, which is 240-volt AC. All of that now forms most of the cost of the installation. This means that if you want to further reduce the cost of solar energy generated, it's not really about reducing the cost of the cell, but about increasing its efficiency. The way you need to look at cost is how much "watt peak" - a measure of peak power - you return on that whole investment. So if you're improving efficiency, you're returning something more across the whole installation. If you just lower the cost of the cell, you're lowering the cost of an element that's already not contributing much to that overall cost. And that's why solar cell research has now become all focused on efficiency.

And silicon has more or less peaked in terms of efficiencies and can't be improved much further. Silicon is a great material. It's made essentially from silicon dioxide, sand, so it's very abundant. But it's got what's called a fixed bandgap: you can't tune it. If you think of a semiconductor, you essentially have a material that absorbs light, photons that have a certain energy, and all the energy above that bandgap will be absorbed. The bandgap of silicon is just over one electron volt, and so every photon that has an energy above that will be absorbed, and anything below that will pass through.

Say there's a photon coming along, and it's got three electron-volt energy. And the bandgap of the light-absorber material is one electron volt. These two electron volts extra, that extra bit of energy, will be lost in the form of heat. So that's a waste, a huge waste.

To avoid such heat loss we move beyond solar cells with single absorber layers, by making multi-junction cells: We put one semiconductor absorber layer on top of another, with different bandgaps. The absorber layer facing the sun grabs the highest-energy photons first. Anything below that passes through, **>**

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Postdoctoral Researcher Marcello Righetto adjusting optical components to optimize measurements of light-induced conductivity in solar cell materials in Laura Herz's laboratory.

hits the next layer, which grabs the next lot, and the remainder passes through and is incident on the bottom layer. So if you go for a triple-junction stack, you can roughly double solar-cell efficiency with respect to silicon. That's because you're able to harvest energy now that otherwise would be lost as heat.

Q: And stacking cells with different bandgaps depends on creating new materials and understanding their behavior. Does this bring us closer to your research focus?

We look at the fundamental processes that underpin how these materials work. If you think about it, we start with sunlight, and turn that into electricity. My research is asking what's happening in between and how we can optimize that process. Light is not charged – it's made of these little particles called photons, and they're not charged – so how do you end up with moving charges, electricity? At first, the absorber material, the semiconductor, has to capture that photon efficiently. Then the initial excitation the photon has created has somehow to be turned from a neutral entity into a pair of positive and negative charges. That's the process. How does that happen?

If you excite this semiconductor, and you ultimately create something that's an electron and a hole – a hole is like a missing electron – those two attract each other. So how come they move apart to make that current? Are there any obstacles they encounter in their path out of the absorber layer? Are these obstacles fundamental in nature, for example, because these charges "bump" into the ions that hold the material together? How can we describe and understand these processes to then inspire the creation of even better absorber materials? These are the questions that we are trying to figure out.

Q: How do you probe such fundamental phenomena?

We have to simulate the whole process. We use ultrafast laser pulses to trigger absorption of photons, and then we ask: Is any neutral particle forming? Does it turn itself into charges? Are they moving freely? How fast are they moving? Do these charges maybe localize somewhere? Are they being trapped by some material defects? Do these charges make it out to collection contacts? And what fundamentally is underpinning each of these steps? Incrementally we can probe all of these processes and disentangle them. Ultimately, we can understand what makes a material work well in a solar cell.

Q: So you're probing these energy conversion phenomena from a lot of different angles, with some very sophisticated tools. Could you explain more about how you do it, and what kind of evidence comes out of these probes?

We do all of that work with advanced optical spectroscopy. It's very important to us that we can probe what's going on before people have even thought about optimizing their photovoltaic devices. My colleagues working on solar cell device fabrication work hard to try to figure out the best device architectures, the best extraction layers, and so on. If a new material just emerging is intrinsically incapable of producing a good solar cell, there's no point in anyone optimizing a device structure. For these reasons it makes perfect sense for us to go in there with non-contact probes that are capable of just taking a thin-film layer and determining whether or not it's a good candidate. And that means we're exciting materials and probing properties with just a set of very short laser pulses that simulates the sunlight and then reading out properties a little while later.

Q: How short are the pulses?

Typically around 100 femtoseconds in duration. After that light has been absorbed, we can probe a number of different processes. For example, I talked earlier about how some of the light is lost in heat. So, for example, we can probe that heat loss by exciting with photons whose energy is much larger than the bandgap, and then watch the charges as they relax right to that band edge while losing energy in heat. And that heat is stuck in the system for a while, for example in the electron gas, or in the vibrations of the ionic crystal. In theory the heat stuck in the electron gas could still be extracted to generate electricity, if it remains long enough for the charges to be extracted. So we can probe how hot these charges remain and for how long. This could ultimately lead to so-called "hot-carrier solar cells" with very high efficiencies. That's one of the measurements we can make at early times after photon absorption, for example, by measuring the energies of the photons that are emitted.

And then the next step might be to ask: How mobile are these charges? Can they move freely? The way we can probe this, again, is totally non-contact. We use another laser pulse to create what's called a single-cycle terahertz pulse. That is a little bit like an AC electric field. You can think of it as being analogous to the electricity supply in your home at 50 hertz. Only it's not 50 hertz, it's a terahertz electromagnetic pulse, and that is shuffling these charge carriers around, moving them around, interacting with them and saying: Are you here, and is there anything that's moving freely? Because that pulse is an electric field it interacts with charges, which modulates the terahertz pulse. So by reading out that terahertz pulse after it's passed through we ask: Hey, have you encountered any free charge carriers in there? Have they been mobile? It's a complex three-pulse experiment. We first have to generate that terahertz pulse with one short laser pulse.

"We look at the fundamental processes that underpin how these materials work. We start with sunlight, and turn that into electricity. My research is asking what's happening in between and how we can optimize that process."

LAURA HERZ

5 8 Then we have to read out that terahertz pulse with another short laser pulse. And then we're coming in with the simulated sunlight excitation pulse as well, in the visible part of the spectrum, and so we now have three laser pulses going.

Q: In the same experiment?

In the same experiment. They're all timedelayed in order for us to read all that out. It requires a very complex optical setup, homebuilt, home-thought-through. You can't buy it off the shelf.

Q: Is your optical setup hidden in a deep, quiet basement somewhere outside the city of Oxford?

No, it's right in the city, in an old heritagelisted building. One advantage is that the walls are one meter thick. Nothing moves, and we have very sophisticated vibration isolation mechanisms supporting the table, as well as an air conditioning unit that gives us precise control to keep the temperature stable.

Q: Let's move on to the material in the spotlight, usually referred to simply as perovskite. What is it, and what advantages does it bring to this business of energy conversion?

It's important to recognize that perovskite, in this context, is a material system rather than a single material. The name refers to a specific kind of crystal structure. The original perovskite is in fact one particular material (calcium titanate), but this label came to be used for all materials crystallizing in the same structure. When we talk about perovskite solar cells, we actually mean metal-halide perovskites. You can choose between different metals - it could be a bit of lead and a bit of tin - and between different halides, such as iodine or bromine. And you can mix them across these sites in the crystal structure, to have a random mixture of either iodine or bromine on a particular lattice point for example. This enables you to tune the bandgap of the semiconductor, which then allows you to tune the kind of photons that the material absorbs. For example, you could have a layer at the bottom of a multi-junction solar cell with a very narrow bandgap that has a mixture of tin and lead, and then you put another layer on top that's got a mixture of iodine and bromine, and that way you have stacks of varying bandgaps to reduce the heat loss in the system, as I mentioned earlier.

In this perovskite structure you have a series of octahedra that are connected, which gives

"It's very important to us that we can probe what's going on before people have even thought about optimizing their photovoltaic devices."

LAURA HERZ

a certain flexibility. You can twist these octahedra with respect to each other. Depending on which atoms you place on the structure, the octahedra will tilt to accommodate. That is partly why you can tune these materials so easily: For example, you might add some bromine even though it's smaller than iodine, and it will still fit in just as easily. The octahedra distort a bit differently, you get a different crystal structure overall, but the perovskite structure adapts. That allows bandgap tuning, and helps us access a wider, more flexible range of materials, which in turn allows the layering of materials with different bandgaps that makes it possible to reduce the heat losses in multi-junction solar cells.

You can't do that with silicon. With silicon you are stuck where you are, with the one bandgap that it has. You can improve a little bit by making it a nice uniform block, and that will improve efficiencies, but then after that, it is what it is.

Q: Are metal-halide perovskites "nice uniform blocks" as well?

Actually, we published a paper in Science in 2020 reporting how we imaged the microstructure of these systems on an atomic scale for the first time. That hadn't been done before because these materials tend to disintegrate under an electron beam. Our study showed that these materials can have beautifully periodic structures and that the interfaces are incredibly benign. We found really coherent grain boundaries, with atomic columns running towards each other in an almost perfect line right up to the interfaces. There's hardly any amorphous material there. It's beautifully formed.

This revealed one of the reasons why these materials work so well. The interfaces between individual crystal "bits," or grains, are incredibly benign. And that's perhaps relating back to the perovskite structure, because it is such a flexible structure that it alleviates strain. Normally you would see amorphous stuff forming, crystal lattice planes bending because of strain, dislocations and defects forming, but these grains and interfaces are beautiful. Another thing you often see in some materials is unwanted remnants of a precursor or formation of an oxide. One reason silicon is so successful is that silicon oxide forms such a benign interface with silicon. And in the Science paper we showed that metal-halide perovskite forms a fantastically benign interface with its precursor, lead iodide. No dislocations, just lattice planes merging straight into each other. That observation is probably a major reason why these materials work so well.

Q: That brings us to your TUM-IAS Focus Group, where your lab's experimental prowess is coupled to cutting-edge research in theoretical physics and physical chemistry. Could you talk a bit about the synergies? Do you find, in practice, that the complementary approaches are mutually helpful? ► It really is a very complementary assembly of expertise and exactly what you need to make progress quickly. On the one hand, Thomas Bein is synthesizing next-generation materials, some of which are perovskites, some perovskite-inspired. We're always looking out for even better materials that might deliver higher stability, better efficiency, easier casting, and so forth. So they're exploring a very wide space of materials with a very open mind. They are hard-core synthetic chemists who can make materials that perhaps no one else has made before.

On the other side, we have David Egger's group, who are at the forefront of trying to develop the next generation of theoretical models that allow us to understand and predict how easily charges can move through the material. As I said before, charges have to be mobile, but they may be held back by interactions with the underlying lattice of ions that makes up the solid. It's this ionic lattice that holds the crystal together, but of course the ions are charged, which will interfere with electrons and holes moving through. David has developed a new approach based on molecular dynamics simulations that explore such interactions, while being able to reflect properly this structural flexibility I talked about earlier, which really complicates matters in terms of making accurate predictions.

So my group is able to reveal experimentally the mobility of charges, and David Egger's group can make accurate calculations, and Thomas Bein will provide novel semiconductors. By feeding that expertise and these processes back in an interdisciplinary triangle, we can both improve understanding and, in the long run, through iterations, improve and invent new materials themselves.

"By feeding that expertise and these processes back in an interdisciplinary triangle, we can both improve understanding and, in the long run, through iterations, improve and invent new materials themselves."

LAURA HERZ

Q: Does David end up proposing experiments, or proposing things you might look for to test or confirm the theory?

Yes. We talk to each other frequently within this interdisciplinary triangle. He might say: I've got this theory, it predicts a particular trend, could you measure that? Or I might say: I've measured x, can your model explain that? And if that works, it's fantastic. If it doesn't work, then we'll have to think again. Because it might just be that I can't do those experiments, or that what I'm asking for would take so long to achieve computationally that we'll be retired by the time we receive an answer. And similarly with synthesis, of course, I might say: Could you just put that particular atom on that site please? I don't necessarily understand the intricacies of the synthesis, so they might have to tell me it's sadly impossible. So again, we have to go back to the drawing board. These conversations are really important to have on a regular basis, and they give us many new ideas.

Q: Can you give an example of how this works?

At the moment we're considering substitution on a specific site, for example a replacement of bismuth with antimony within a particular double perovskite. And so Thomas Bein's group may synthesize a series of compounds gradually going all the way across from bismuth to antimony. And then David Egger's group may calculate what this will do to the masses of the charges, which may predict whether they should be more mobile or not. Our experiments in my group may then examine whether that really reflects the truth. And the answer may be that it's not such a simple story, that it also could have something to do with how easily these materials crystallize. Then we might go back, passing it back to the synthetic chemists, and say hey, you have to find better ways of making that crystallization work. So that's an example of one particular feedback loop.

Q: I understand that device design, system development, manufacturing, and the electrical grid are outside your research focus, but you must have a sense of where these are heading with respect to perovskite solar cells. What can you say about the outlook?

I'd say it's now at the pilot plant stage. For example, the spin-out company Oxford Photovoltaics, which was founded in 2010, has bought and repurposed a factory in Brandenburg, Germany, to produce prototype perovskite solar cells. There are also companies in the United States trying hard to bring a product to market. I think the first product to market probably would be perovskite on silicon, because silicon is well established, and it would be seen as a booster layer on top of silicon. Such perovskite-silicon tandem cells have already demonstrated labbased power conversion efficiencies above 30 percent. So that is an exciting concept, and stability, another important aspect, is looking promising as well.



Q: How or why did researchers first decide to try using metal-halide perovskites for energy conversion? Was it a hint from theory or a hunt through libraries of materials?

I think it was more of a hunt through libraries of materials. Tsutomu Miyasaka in Japan tried to use this material, essentially as a sensitizer, in dye-sensitized mesoporous metal-oxide solar cells. He tried using lead iodide perovskite as a replacement for the dye, and it didn't work well for long. It showed some decent efficiency, but the perovskite quickly decomposed in the electrolyte forming part of this type of solar cell. Then Henry Snaith at Oxford talked to him, and they came up with the idea of using the perovskite to actually replace the electrolyte, to make an all-solidstate perovskite solar cell, still incorporating mesoporous metal oxides. Michael Johnston, here at Oxford, evaporated the material for the first time and showed that this thin-film layer works just as well, even without the metal oxide. In the beginning, it really was serendipity, but as usual, progress relied on many different contributions from researchers around the world.

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.





Prof. Marta C. Antonelli

Focus Group Early Biomarkers of Prenatal Stress

Prof. Marta C. Antonelli (University of Buenos Aires), Alumna Hans Fischer Senior Fellow | Ritika Sharma (TUM), Doctoral Candidate | María Sol Molinet (TUM), Dr. med. Candidate | Hosts: Prof. Marion Kiechle, PD Dr. Silvia M. Lobmaier (Women's Clinic at TUM University Hospital rechts der Isar)

Maternal stress affects the child neurocognitive and epigenetic outcome

Prenatal exposure to maternal psychosocial stress confers a lifelong risk for behavioral alterations that last beyond childhood. Our aim is to identify non-invasive biomarkers of the childdevelopmental outcome to offer a precise and truly personalized prediction and new possibilities for designing interventions to improve neurodevelopmental outcomes of pregnancy affected by prenatal stress.

Pregnancy is a significant time in women's lives but it can also be very challenging. During the gestational period, women like any other subject, can be exposed to endogenous and exogenous challenges that may be perceived as unpleasant, aversive or threatening in such a way that the homeostasis, wellbeing and overall health is threatened. This means that maternal stress during pregnancy and during early parenting can program physiological responses and lifetime trajectories of the infant, which in interaction with genetic liabilities and early-life challenges, will determine ultimate health status. Our main objective is to test the feasibility of identifying early non-invasive pre- and postnatal biomarkers of brain programming due to intrauterine stress exposure. To this end, we performed a prospective matched control study in stressed mothers with controls matched for parity, maternal age, and gestational age at study entry. Subjects were recruited for 36 months from a cohort of pregnant women followed in the Department of Obstetrics and Gynecology at "Klinikum rechts der Isar" of the Technical University of Munich (TUM). Maternal psychosocial stress was measured using the Cohen Perceived Stress Scale (PSS 10) to measure nonspecific perceived stress and was classified into stressed (SG) and control group (CG). Prenatal Distress Questionnaire (PDQ) was also administered to assess specific pregnancy worries. Two and a half weeks after screening, we performed a transabdominal ECG (taECG). Upon delivery, maternal hair strands were collected for cortisol measurements and newborns' saliva and cord blood samples were collected. Two years after delivery, infants' cognitive, language and motor development were assessed by Bayley Scale III of Infant Development (BSID) (Figure 1). >

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Figure 1, All pregnant women visiting the outpatient ward of Department of Obstetrics and Gynecology at "Klinikum rechts der Isar" of the TUM, in their third trimester were administered the Cohen Perceived Stress Scale questionnaire (PSS-10) attaching a short information brochure about the study. A score was obtained and a PSS-10 below 19 categorized them in the Control Group and a PSS-10 score equal or above 19 categorized them in the Stress group. **1)** Two and a half weeks after screening, obstetricians perform a transabdominal ECG (taECG) recording the data of which will be used for PRSA analysis. **2)** On the day of parturition, 3 cm of hair strands were collected from the posterior vertex region on the head. Based on an approximate hair growth rate of 1 cm per month, the proximal 3 cm long hair segment is assumed to reflect the integrated cortisol secretion over the three-month-period prior to sampling. Upon delivery a placenta sample was obtained as well as cord blood and a saliva sample of the newborn for the genetic studies. **3)** Two years later the mother is invited to come back to the clinic with her son/daughter to take a neurocognitive test called Bayley's Test (BSID: Bayley Scale of Infant Development) that evaluates the cognitive, motor and language skills of the infant. In the same visit a new saliva sample is taken for the epigenetic analysis. [1] Lobmaier, S. M. et al. (2020).

MAIN ACHIEVEMENTS:

In our quest for finding a prenatal measure that might have a preventive clinical significance we hypothesize that the coordinated roles of the ANS (Autonomic Nervous System) and the HPA (Hypothalamic Piuitary Axis) in the integrated stress response can be monitored non-invasively using electrocardiogram (ECG) and ECG-derived maternal and fetal heart rate (mHR, fHR). We propose a novel analysis method of coupling between mHR and fHR based on a signal-processing algorithm, first applied in adult cardiology, termed bivariate phase-rectified signal averaging (BPRSA) and applied to trans-abdominally acquired fetal ECG (fECG). Our first results show that PSS-10 shows a correlation with the coordination of fetal and maternal heart rate and fetal oxygenation at birth. The proposed BPRSA index (FSI) provides unique insights into the relationship between two

biological systems: mother and fetus. Interestingly, CG fetuses remained "stable" during these periods whereas fetuses of stressed mothers showed significant decreases of fHR. [1]

Our next goal was to quantify the levels of methylation across this entire genome in the newborn saliva employing EWAS (Epigenome-Wide Association Study) as a biomarker detector of epigenetic reprogramming in young infants. DNA was extracted from saliva samples and DNA methylation was measured using EPIC Bead-Chip array (850k CpG sites). To identify associations between PSSPDQ/FSI/Cortisol and methylation, linear regression models adjusting for confounders were run. We found epigenome-wide significant associations for 6 CpG sites in association with stress phenotypes (PDQ and cortisol). Annotated genes



prevent its long-term sequelae.

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to the CpGs were found to be enriched for development and growth in the hippo signaling pathway, organelle biosynthesis, and metabolism of proteins, cell proliferation and bone development. We report novel associations between DNA methylation and maternal stress phenotypes. We observe that the several associations are related to neurobiological disorders such as autism, schizophrenia, neural tube defects and atrophy [2]. Since this is a longitudinal study, we are assessing the neurodevelopmental outcome of the two years old infants and we will assess the differential methylation in saliva samples at that age. Detecting differences in methylation between the two ages will give a window of opportunity for early interventions.

Matching the rising need for iron during pregnancy is important to prevent an impairment of the growing child's neurodevelopment due to iron deficiency. Our next objective was to assess the influence of prenatal maternal stress (PS) on the neonatal iron homeostasis. Neonatal cord blood serum hepcidin, transferrin, and iron were determined. Transferrin saturation and iron were lower in male stressed neonates. SG reduces neonatal ferritin by 15.4% compared to controls. PS during the third trimester perturbs neonatal iron markers in a sex-dependent manner [3]. Early detection of PS can support early individualized pre- and postnatal iron supplementation and neurodevelopmental follow-up to prevent long-term sequelae.

As mentioned before, chronic prenatal stress results in entrainment of the fetal heartbeat by the maternal heartbeat, quantified by the fetal stress index (FSI). Deep learning (DL) is capable of pattern detection in complex medical data with high accuracy

[2] Sharma, R. et al. (2022).

[3] Zimmermann, P. et al. (2022).

- [4] Sarkar, P. et al. (2022).
- **[5]** Antonelli, M.C. et al. (2022).

in noisy real-life environments, but little is known about DL's utility in non-invasive biometric monitoring during pregnancy. A recently established self-supervised learning (SSL) approach to DL provides emotional recognition from electrocardiogram (ECG).

In collaboration with Dr. Martin Frasch (University of Washington, Seattle, USA) we hypothesized that SSL will identify chronically stressed mother-fetus dyads from the raw maternal abdominal electrocardiograms (aECG), containing fetal and maternal ECG. Our DL models accurately detect the chronic stress exposure group, the individual psychological stress score and FSI at 34 weeks of gestation, as well as the maternal hair cortisol at birth reflecting chronic stress exposure [4]. The final DL model can be deployed in low-cost regular ECG biosensors as a simple, ubiquitous early stress detection and monitoring tool during pregnancy. This discovery should enable early behavioral interventions.

Two years after delivery, infants' cognitive, language and motor development were assessed by Bayley Scale III of Infant Development (BSID). Cognitive and motor areas showed no significant variation between SG and CG toddlers even when accounting for sex. However, language composite scores showed a significant decrease in SG toddlers irrespective of sex and language spoken at home. When day care center attendance (DCA) was accounted for, this effect disappeared. PS affects the toddlers' language development in both sexes, regardless the language spoken at home. DCA seems to protect for this neurodevelopmental delay. These results confirm the importance of early stimulation through social interaction for reversion of language delays in toddlers exposed to PS.

In summary, we discovered how to detect the impact of chronic stress on mother and child during pregnancy non-invasively using several biomarkers combined with artificial intelligence techniques that could be employed as predictive biomarkers of the child neurodevelopmental outcome [5]. However, we believe that the best strategy lies in the preventive nature of the interventions that reduce stress during pregnancy and potentially avoid negative child outcomes. Based on our previous findings, we are now developing a project that brings together early detection and intervention yoga/mindfulness programs in a digital biofeedback paradigm compatible with today's challenges of pandemic and telemedicine (Figure 2). Our approach might lead to at-scale adoption of prevention of the detrimental effects of chronic stress on the child's potential.

In close collaboration with Dr. med. Camilla Zelgert, Dr. med. Peter Zimmermann (TUM).

Selected publications

Lobmaier, S. M. et al. Fetal heart rate variability responsiveness to maternal stress, non-invasively detected from maternal transabdominal ECG. *Archives of Gynecology & Obstetrics* 301(2), 405–414 (2020), https://doi.org/10.1007/s00404-019-05390-8.

Sharma, R. et al. Maternal-Fetal stress and DNA methylation signatures in neonatal saliva: An Epigenome-Wide Association Study. *Clinical Epigenetics* 14, 87 (2022), https://doi.org/10.1186/s13148-022-01310-x.

Zimmermann, P. et al. Prenatal stress perturbs neonatal iron homeostasis in a sex specific manner. *Scientific Reports* 12, 9341 (2022), https://doi.org/10.1038/ s41598-022-13633-z. Sarkar, P. et al. Detection of Maternal and Fetal Stress from ECG with Self-supervised Representation Learning. *Scientific Reports* 11, 24146 (2021), https://doi. org/10.48550/arXiv.2011.02000.

Antonelli, M.C. et al. Early Biomarkers and Intervention Programs for the Infant Exposed to Prenatal Stress. *Current Neuropharmacology* 20(1), 94–106 (2022), https://doi.org/10.2174%2F157015 9X19666210125150955.

For a full list of publications please see https://www.ias.tum.de/ias/antonellimarta-cristina/

Focus Group Understanding How Cancer Drugs Work

Prof. Bernhard Küster (TUM), Alumnus Carl von Linde Senior Fellow



Prof. Bernhard Küster

From understanding drug action to treating cancer patients

Most cancer drugs modulate the activity of malfunctioning proteins. However, it is often not clear how these drugs work and the molecular heterogeneity of tumors often render drugs ineffective. The goal of this Focus Group is to provide better treatment options to patients based on a detailed understanding of their tumor biology and exploiting the capabilities of existing targeted cancer drugs.

[1] Wilhelm, M. et al. Mass spectrometry based draft of the human proteome. *Nature* 509, 582–587 (2014); Giansanti, P. et al. (2022). Proteins execute and control practically every aspect of life. The human genome encodes for about 20,000 proteins, which, among many other functions, act as catalysts for anabolic or catabolic biochemical reactions inside cells, help to transmit signals via the network of neurons or control cell growth and division. Deregulated proteins can cause severe diseases including heart or liver disorders, neurodegenerative diseases or cancer to name a few. Therefore, most therapeutic drugs act on proteins with the goal to tone down or increase their activity in order to restore normal cellular function.

Despite a very long history of successful drug development, surprisingly little is known about how drugs impact the entirety of the human proteome or vice versa. Drugs sometimes do not work in humans even though the scientific rationale and pre-clinical data is strong. Often, drugs, have more than one effect, a phenomenon called polypharmacology, which may or may not be desirable. In part, this is due to an astounding molecular diversity of proteins in different cell types or organs and there is also strong heterogeneity in composition and dynamics of the proteome between (cancer) patients.

Understanding the complex interplay between a therapeutic compound and the cellular proteome and how this information may be used to make better choices for the treatment of cancer patients is the goal of this Focus Group. Our unique approach to this challenge builds on one of the world's most powerful proteomic technology platforms established by an interdisciplinary team of molecular oncologists, biochemists and bioinformaticians. A few highlights from published and ongoing work are provided in the following:

1. From our analysis of the human and mouse proteomes (Figure 1) [1], as well as hundreds of cancer patient proteomes, it has become very clear, that while the majority of all proteins is expressed in most organs or cancers, their quantities in these organs can be vastly

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Figure 1, Artist impression of the interplay of therapeutic drugs (chemical structures) and the human proteome as revealed by mass-spectrometry-based proteomics.

different. This is even more pronounced for the many chemical modifications with which proteins can be decorated and which strongly regulate their function. It should, therefore, no longer be surprising that drugs will encounter very different molecular environments when entering a particular cell.

We and others have screened hundreds of cancer cell lines against hundreds of cancer drugs to measure the ability of drugs to kill these cells [2]. Reflecting the aforementioned heterogeneity of cancer proteomes, most cancer drugs do not work in most cancer cells. Still, using advanced bioinformatic analysis, we were able to show that the expression of certain proteins, or the levels of phosphorylation modification on certain proteins, are predicative of response or resistance to certain cancer drugs. We exemplified the utility of such biomarkers of drug response by i) improving the stratification of breast cancer patients for anti-hormonal therapy and ii) suggesting higher doses of Cytarabine for the treatment of acute myeloid leukemia patients with high expression levels of the protein Adenylate Kinase 1.

3. One key element in understanding how drugs work is to identify the target proteins they engage and we have investigated hundreds of cancer drugs (mostly kinase inhibitors (KI) and histone deacetylation inhibitors (HDACi) for their ability to engage cellular proteins and pathways (Figure 2) [3]. This work not only provided systematic information on drug:target interactions, it also uncovered several unexpected targets that could only be discovered in a proteome-wide approach. The biological function of some of these so-called "off-targets" are not yet clear but for others, these additional target proteins explained toxic side effects of the drug, or suggest additional uses of the same drug for a new target and in new indications (a concept known as drug re-purposing). The same line of work also identified the targets of the drug lipoic acid which has been used in humans for decades in the absence of knowing how it exerts its therapeutic effects.

4. In ongoing work, we have extended our efforts to the direct measurement of the phospho-proteome of cancer cells in response to cancer drugs. The scale of these experiments is unprecedented and we have already accumulated millions of dose-response measurements with the aim to understand the details of the cellular mechanism of action (MoA) of these drugs. Important learnings have emerged from this work already. For instance, we could show that the classic breast cancer drug Herceptin is not a signaling drug. We could also demonstrate that the therapeutic **>**

[2] Frejno, M. et al. (2020).

[3] Klaeger, S. et al. The target landscape of clinical kinase drugs. *Science* 358, pii: eaan4368 (2017); Lechner, S. et al. (2022). antibody Rituximab kills cancerous B-cells by overactivating a particular intracellular signaling pathway, thus clarifying the MoA of a 25 year old and successful drug.

All the above research areas serve a common long-term goal: to provide better treatment options to cancer patients based on a detailed understanding of their individual tumor biologies and the molecular capabilities of molecularly targeted cancer drugs (Figure 3). We are in the process of pulling together the above lines of work as part of an ERC Advanced Grant as well as our participation in the German Consortium for Cancer Research (DKTK). We have already measured the phosphoproteomes of hundreds of cancer patients and these are analyzed and thousands more are to come. This will place the molecular profile of every patient into context of tumor heterogeneity and identify features that are characteristic for this particular patient. We then pair this information with data for the cancer drugs regarding which of an aberrantly regulated protein in a patient, matches the modulation profile of a drug. We have already begun to use this concept for treatment recommendations in molecular tumor boards and will incorporate it in retrospective and prospective clinical trials in order to learn, if the proteomic profiles and recommendations derived provide any benefit to the lives of patients.

In close collaboration with Prof. Dr. Mathias Wilhelm, Dr. Maria Reinecke, Dr. Matthew The, Dr. Stephanie Wilhelm, Dr. Patrick Allihn, Dr. Chen Meng, Dr. Chien-Yun Lee, Dr. Guillaume Medard, Dr. Jana Zecha, Dr. Patroklos Samaras, Dr. Svenja Wiechmann, Dr. Martin Frejno, Florian Bayer, Julian Müller, Nicola Berner, Nicole Kabella, Severin Lechner, Stefanie Höfer, Stephan Eckert, Yun-Chien Chang (TUM).



Figure 2, How drugs impact cancer biology. Left panel: network of therapeutic drugs and the proteins they target. The line width represents how strong a particular drug inhibits the target protein. Middle panel: network of drugs and the signaling pathways it engages in cancer cells. Right panel: QR-code leading to the web site of ProteomicDB where the data for thousands of drug:protein interactions can be interactively explored.


Figure 3, Translation of research results into clinical care. Molecular profiling of cohorts of cancer patients (middle panel) is already used today to identify molecular sub-types of cancer that aims for better-informed treatment decisions (right panel). Our work takes this a step further in that we are measuring the activity status of cancer proteomes to make molecularly guided treatment recommendations for individual cancer patients (left panel).

Selected publications

Lechner, S. et al. Target deconvolution of HDAC pharmacopoeia reveals MBLAC2 as common off-target. *Nat Chem Biol* 18, 812–820 (2022), https://doi.org/10.1038/ s41589-022-01015-5.

Giansanti, P. et al. Mass spectrometry-based draft of the mouse proteome. *Nat Methods* 19, 803–811 (2022), https:// doi.org/10.1038/s41592-022-01526-y.

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Reinecke, M. et al. Chemoproteomic selectivity profiling of PIKK and PI3K kinase inhibitors. *ACS Chemical Biology* 14, 655–664 (2019), https://doi.org/10.1021/ acschembio.8b01020.

For a full list of publications please see https://www.ias.tum.de/ias/kuester-bernhard-1/



Focus Group Dynamic Vision and Learning

Prof. Laura Leal-Taixé (NVIDIA and TUM), Alumna Rudolf Mößbauer Tenure Track Assistant Professor | Dr. Aljosa Osep (CMU, Carnegie Mellon University), Dr. Ismail Elezi (TUM), Postdoctoral Researchers | Qunjie Zhou, Tim Meinhardt, Maxim Maximov (TUM), Doctoral Candidates

Dynamic scene understanding for autonomous agents

[1] Bergmann, P., Meinhardt, T. & Leal-Taixe, L. (2019).

Prof. Laura Leal-Taixé

- [2] Xu, Y. et al. How To Train Your Deep Multi-Object Tracker. Conference on Computer Vision and Pattern Recognition (CVPR) (2020).
- [3] Meinhardt, T., Kirillov, A., Leal-Taixe, A. & Feichtenhofer, C. TrackFormer: Multi-Object Tracking with Transformers. Conference on Computer Vision and Pattern Recognition (CVPR) (2022).
- [4] Seidenschwarz, J. et al. Simple Cues Lead to a Strong Multi-Object Tracker. Conference on Computer Vision and Pattern Recognition (CVPR) (2023).
- [5] Sattler, T., Zhou, Q., Pollefeys, M. & Leal-Taixe, L. Understanding the Limitations of CNN-based Absolute Camera Pose Regression. Conference on Computer Vision and Pattern Recognition (CVPR) (2019).

We work on dynamic scene understanding for autonomous agents, i.e., enabling mobile robots to understand the world around them primarily from image sensors. Our core topic is computer vision such as multi-object tracking, video panoptic segmentation, or visual localization. We also have exciting projects in the areas of brain signal analysis, image generation, and earth observation.



Figure 1, We compare TrackFormer [Meinhardt, T., Kirillov, A., Leal-Taixe, A. & Feichtenhofer, C. (2022)] segmentation results with the popular Track R-CNN on selected MOTS20 (MOTChallenge) test sequences, showing an observable improvement in pixel mask accuracy.

Research Area: Advanced Computation and Modelling

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Since the start of the Fellowship in 2018, the Focus Group has produced a total of 52 publications in the main venues of computer vision, machine learning and robotics. I will highlight the huge advances that we have made in the three core areas multi-object tracking, visual localization, and benchmarking for video understanding in the last 4 years.

Multi-object tracking

Tracking-by-detection has long been the dominant paradigm for multi-object tracking, but in the last years, we have been able to propose two new paradigms that have been the dominating state-of-the-art.

We first introduced Tracktor [1] as a new tracking-by-regression paradigm, which efficiently merged the detection and the tracking tasks. We were able to train our model end-to-end by computing derivatives through tracking metrics [2].

After the success of Transformers for various image classification tasks, we were able to formulate multi-object tracking as a set prediction problem with Transformers [3], effectively presenting a new tracking-by-attention paradigm, with an unprecedented level of integration between detection and tracking.

Nonetheless, our current research is suggesting that simple tracking-by-detection trackers, if properly designed [4], can achieve even better results. Our goal for the future is to understand which parts of modern vs classic trackers are crucial to create a robust and efficient solution.

Visual localization

Deep learning is dominating almost all tasks in computer vision, and it recently started tackling the 3D domain and tasks such as visual localization as well. In our study [5] we show the pitfalls of using machine learning for visual localization, effectively showing that current solutions are not applicable to real world scenarios. After that, we proposed several state-of-theart solutions for visual localization based on relative pose estimation [6].

We also opened entirely new visual localization tasks, such as text to pose localization [7], which computes the exact location from a verbal description of the place.

All the above methods are based on visual features and a pre-computed map with such features stored. This has several issues, most notably: (i) privacy issues, as one can reconstruct a scene based on the visual features, and (ii) storage, as visual features take up terabytes for relatively small scenes. Therefore, we recently proposed a novel localization paradigm [8] only based on geometric features, a much harder problem, but without the privacy or storage problems. We strongly believe this will be the localization paradigm of the future.

Benchmarking for video understanding

One of the key ingredients for the success of machine learning in computer vision has been the creation of datasets with ground truth annotations, starting from the famous ImageNet. We contributed our part to the community by creating MOTChallenge [9], the now de facto benchmark for multi-object tracking.

We have enriched the benchmark in recent years with new challenges, such as temporally-dense pixel semantic annotations [10], synthetic-to-real multi-object tracking [11], and open-world tracking [12].

One of the most exciting new research lines is the study of how we can anonymize video data after recording. This is extremely important >

- [6] Zhou, Q., Sattler, T., Pollefeys, M. & Leal-Taixe, L. To Learn or Not to Learn: Visual Localization from **Essential Matrices.** IEEE International Conference on Robotics and Automation (ICRA) (2020); Zhou, Q., Sattler, T. & Leal-Taixe, L. Patch2Pix: **Epipolar-Guided Pixel-**Level Correspondences. Conference on Computer Vision and Pattern Recognition (CVPR) (2021).
- [7] Kolmet, M., Zhou, Q., Osep, A. & Leal-Taixe, L. Towards crossmodal pose localization from text-based position descriptions. Conference on Computer Vision and Pattern Recognition (CVPR) (2022).
- [8] Zhou, Q., Agostinho,
 S., Osep, A. & Leal-Taixe, L. (2022).
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- [10] Weber, M. et al. STEP: Segmenting and Tracking Every Pixel. Proceedings of the Neural Information Processing Systems Track on Datasets and Benchmarks (2021).
- [11] Fabbri, M. et al. MOT-Synth: How Can Synthetic Data Help Pedestrian Detection and Tracking?. International Conference on Computer Vision (ICCV) (2021).

- **[12]** Liu, Y. et al. Opening up Open-World Tracking. Conference on Computer Vision and Pattern Recognition (CVPR) (2022).
- [13] Maximov, M., Elezi, I. & Leal-Taixe, L. CIAGAN: Conditional Identity Anonymization Generative Adversarial Networks. Conference on Computer Vision and Pattern Recognition (CVPR) (2020).
- [14] Maximov, M., Elezi, I. & Leal-Taixe, L. Decoupling identity and visual quality for image and video anonymization. Asian Conference on Computer Vision (ACCV) (2022).

to comply with privacy laws such as GdPR. Since our multi-object tracking videos often contain hundreds of pedestrians, it is impossible to obtain express permission from everyone before filming. Therefore, we propose to modify the recorded video and replace the observed identities with synthetic counterparts. This research was started in 2020 [13] and further explored and improved in 2022 [14]. We will continue to improve the video output quality and push towards making this anonymization tool a priority for all benchmarks containing humans.

In close cooperation with: Aysim Toker, Franziska Gerken, Jenny Seidenschwarz, Andreas Roessler, Patrick Dendorfer, Guillem Brasó, Mark Weber, Orcun Cetintas (TUM), Doctoral Candidates



Figure 2, We propose GoMatch [Zhou, Q., Agostinho, S., Osep, A. & Leal-Taixe, L. (2022)] to tackle visual localization w.r.t. a scene represented as a 3D point cloud. By relying only on geometric information for matching, GoMatch allows structure-based methods to achieve localization solely using keypoints, sidestepping the need to store visual descriptors for matching. Keeping only the minimal representation of a 3D model, i.e., its coordinates, leads to a more scalable pipeline towards large-scale localization that bypasses privacy concerns and is easy to maintain.



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Figure 3, A set of triplet images generated by our framework [Maximov, M., Elezi, I. & Leal-Taixe, L. (2022)]. In every triplet, the leftupper image is the original image in 128x128 resolution, the left-lower image is the anonymized version of it in 128x128 resolution, and the large image in the right is its anonymized version in 512x512 resolution. We present cases of different gender, skincolor, pose, and illumination.

Selected publications

Bergmann, P. Meinhardt, T. & Leal-Taixe, L. Tracking without bells and whistles. IEEE International Conference on Computer Vision (ICCV) (2019).

Braso, G. & Leal-Taixe, L. Learning a Neural Solver for Multiple Object Tracking. Conference on Computer Vision and Pattern Recognition (CVPR) (2020).

Dendorfer, P. et al. MOTChallenge: A Benchmark for Single-camera Multiple Target Tracking. International Journal of Computer Vision (IJCV) 129, 548–578 (2020). Zhou, Q., Agostinho, S., Osep, A. & Leal-Taixe, L. Is Geometry Enough for Matching in Visual Localization?. European Conference on Computer Vision (ECCV) (2022).

Toker, A. et al. DynamicEarthNet: Daily Multi-Spectral Satellite Dataset for Semantic Change Segmentation. Conference on Computer Vision and Pattern Recognition (CVPR) (2022).

For a full list of publications please see https://www.ias.tum.de/ias/leal-taixe-laura/ **Focus Group Quantum Electronics and Computer Engineering**

Prof. Kai Müller (TUM), Alumnus Rudolf Mößbauer Tenure Track Assistant Professor



Prof. Kai Müller

Engineering photonic quantum technologies

In the framework of the TUM-IAS Rudolf Mößbauer Tenure Track Assistant Professorship, the Professorship for Quantum Electronics and Computer Engineering was established in 2019 and promoted to W3 Associate Professorship in 2022. The group's research focuses on quantum engineering of photonic quantum systems.

Introduction to photonic quantum technologies

The emerging area of quantum technologies holds the promise to revolutionize our world by exploiting fundamental quantum physical effects for technological applications. For example, the European Union's "Quantum Flagship" mission has identified the four core areas quantum communication, quantum computation, quantum simulation and quantum sensing/metrology as areas where quantum physics will enable new technologies with capabilities far beyond existing technologies. Examples are ultra-secure communication where the security is guaranteed by physical principles, or powerful computers, which can solve specific tasks many orders of magnitude faster than classical computers. This is based on the peculiar properties of quantum mechanics, in particular the ability to control and exploit quantum coherence and quantum entanglement. To this end, photons are a unique type of quantum bits, so-called qubit as, in contrast to all other qubit systems, they do not suffer from decoherence. Moreover, they can be used to transmit quantum information over large distances.

History of the Focus Group

The Professorship of "Quantum Electronics and Computer Engineering" at the Department of Electrical and Computer Engineering, was established in 2019 with the appointment of Kai Müller as Rudolf Mößbauer Tenure Track Assistant Professor. It emerged from a junior research group that he previously established at the Walter Schottky Insititut of TUM funded by a highly-competitive BMBF "Quantum Futur" grant (4.5 million euros for 5 years). Due to the success of the group, Kai Müller obtained early tenure in 2022, after three years as a tenure-track professor. Within the tenure-track period, the group contributed to more than 25 publications (key publications below), grew to a size of more than fifteen doctoral candidates and postdoctoral researchers and acquired several third-party funded projects with a total volume of more than 13 million euros. Among those are multiple collaborative projects where the group's leader is the coordinator, including the BMBF project "Photonic-Integrated Quantum Computer (QPIC-1)," the DFG major instrumentation initiative "Munich Quantum Communications Laboratory (MQCL)" and the project "6G and Quantum Technologies" funded by the Bavarian Ministry of Economic Affairs.

Research of the Focus Group

The research of the group focusses on the quantum engineering of building blocks and devices that are essential for all areas of photonic quantum technologies. These building blocks are sources of non-classical light such as single-photons or entangled photons, spin-photon interfaces, quantum memories and single photon detectors. Overall, the group's research spans the entire range from engineering light-matter interactions to demonstrator experiments, which enable systems engineering, and can be divided into three interlinked areas (Figure 1):

optical techniques. Specific properties that are investigated are quantum-optical and spin coherence properties. Since every quantum material has specific advantages and disadvantages and future systems are likely to be hybrid quantum systems, the group works on a variety of materials, including semiconductor quantum dots, color centers in diamond, rare-earth ions in crystals, atomically-thin transition metal dichalcogenides and superconducting nanowires. Quantum-optical techniques developed by the group are techniques for the coherent-optical control of electronic excitations and spin states, as well as techniques for the generation and detection of non-classical light.

Area A

Research area A addresses the investigation of novel optically-active quantum materials and the development of novel quantum-

Area B

Research area B addresses the engineering of modular building blocks and quantum photonic-integrated circuits for photonic quantum technologies. Embedding opticallyactive quantum systems into nanophotonic ►



Figure 1, Research of the Quantum Electronics and Computer Engineering Focus Group.

resonators allows to enhance the light matter interaction thus increasing operational rates. Moreover, tailored nanophotonic resonators allow for efficient photonic interfacing. For modular building blocks, photonic in-coupling and out-coupling efficiencies are key parameters. In addition to working with many different quantum materials, the group also works on a large number of different nanophotonic structures, such as micropillar resonators, photonic crystals and bullseye resonators to use for each application the best suitable nanophotonic resonator. In addition, different building blocks can be integrated on a chip to form scalable quantum photonic-integrated circuits.

Area C

Research area C addresses the realization of demonstrator experiments to obtain feedback for the device engineering and to enable systems engineering. Here, the techniques developed in area A and the devices engineered in area B are combined to realize demonstrator experiments such as quantum communication (quantum key distribution and quantum networks), optical one-way quantum computing and quantum simulation (Boson sampling). Results from these experiments give feedback for the device engineering, i.e., which parameters turn out to be particularly important in real-world settings. In addition, the demonstrator experiments enable systems engineering and allow developing protocols for photonic quantum technologies, such as techniques for quantum key distribution, remote entanglement generation and quantum error correction.

In close collaboration with Dr. Matteo Barbone, Dr. Björn Jonas, Dr. Viviana Villafane (TUM), Postdoctoral Researchers | Stefan Appel, Fabian Becker, Katarina Boos, Beatrice Costa, Jan Flaschmann, Lukas Hanschke, Sang Kyu Kim, Marko Petric, William Rauhaus, Friedrich Sbresny, Bianca Scaparra, Christian Schmid, Fabian Wietschorke, Lucio Zugliani (TUM) Doctoral Candidates

Selected publications

Villafañe, V. et al. Three-photon excitation of quantum two-level systems. *arXiv*:2202.02034 (2022).

Sbresny, F. et al. Stimulated generation of indistinguishable single photons from a quantum ladder system. *Physical Review Letters* 128, 093603 (2022).

Petrić, M. M. et al. The Raman Spectrum of Janus Transition Metal Dichalcogenide Monolayers WSSe and MoSSe. *Phys. Rev. B* 103, 035414 (2021). Hanschke, L. et al. Origin of Antibunching in Resonance Fluorescence. *Physical Review Letters* 125, 170402 (2020).

Klein, J. et al. Site-selectively generated photon emitters in monolayer MoS2 via local helium ion irradiation. *Nature communications* 10, 2755 (2019).

For a full list of publications please see https://www.ias.tum.de/ias/mueller-kai/

Focus Group Pollutants and Sustainability Governance

Prof. Henrik Selin (Boston University), Alumnus Hans Fischer Senior FellowProf. NoelleSelin (Massachusetts Institute of Technology), Alumna Hans Fischer Senior FellowFionaKinniburgh (TUM), Doctoral CandidateHost: Prof. Miranda Schreurs (TUM)

Advancing pollution governance for sustainability

The Focus Group aimed to inform sustainability governance through a better understanding of how people and technology interact. Research developed new multidisciplinary analysis methods and examined empirical cases of pollutants, including mercury and pesticides. Results illuminated underappreciated dynamics of environmental and societal pollutant flows and trade-offs between governance approaches.

Human activities and technologies have fundamentally altered the Earth in ways that have both facilitated the development of modern societies and challenged the ability to protect and improve human well-being in the long term. In this Focus Group, we built and tested theories about how humans, technology, and the environment interact in the context of institutions and knowledge, to help advance sustainability governance. We did this by constructing richly described empirical cases of distribution and management of pollutants over time, applying interdisciplinary methods from across social sciences, natural sciences, and engineering. The research drew lessons for policy-making and practice on hazardous substances and other sustainability challenges.

The intentional and unintentional mobilization of large amounts of material substances into the environment and human societies provides rich data through which to analyze historical and present-day implications for sustainability. Some of these substances are naturally occurring elements, like mercury and carbon, while other chemicals are synthetic. Substances can be local, regional, and/or global pollutants that have severe negative impacts on human health and the environment. Management efforts involve both public and private governance, which may interact in complex and unexpected ways. Major empirical cases involved mercury pollution and pesticide uses, both of which pose health and environmental risks locally and through long-range trade and atmospheric dispersion. Mercury is emitted from a variety of sources globally, including coal burning, industrial processes, and use in artisanal and small-scale gold mining. These are all addressed by the global Minamata Convention on Mercury. Many pesticides are subject to global governance under the Stockholm Convention on Persistent Organic Pollutants and the Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and Pesticides in International Trade. Pesticide governance has historically focused on managing human health



Prof. Henrik Selin



Prof. Noelle Selin



Fiona Kinniburgh



Prof. Miranda Schreurs



Figure 1, Historical trends in mercury production and consumption, emissions, releases, and future scenarios from 1972 to 2072. Colored bars on timeline indicate data availability, noting key milestones on global mercury policy and sustainability.

risks, but mounting evidence of biodiversity loss highlights these chemicals' chronic environmental impacts.

A key Focus Group achievement was the development and application of a new Human-Technical-Environmental (HTE) systems framework, a structured and comprehensive method for assessing sustainability issues. [1] The HTE framework provides analysts from different disciplines a common way to advance systems-focused sustainability research. Focusing on mercury, we used the HTE framework to identify insights for systems analysis for sustainability, sustainability definitions and transitions, and sustainability governance. Related empirical research documented mixed global 50-year trends in mercury production, consumption, and discharges (see Figure 1). [2]

Because mercury is emitted from coal burning, it connects closely to global and regional efforts on climate change and energy transitions. This links the Focus Group's work to larger efforts in Miranda Schreurs' research group on understanding climate and energy governance in the European Union and beyond. Topics explored through collaborations and conversations with the Focus Group included comparative politics of energy transitions, nuclear waste disposal, ►

- [1] Selin, H. & Selin, N.E. (2020); Selin, H. & Selin, N.E. (2022b).
- [2] Selin, H. & Selin, N.E. (2022a).

[3] Kinniburgh, F., Selin, H., Selin, N.E. & Schreurs, M. (2022).

[4] Kinniburgh, F. (2023).

and phase-outs of legacy technologies and substances.

Work by the Focus Group on pesticides examined how private-sector led efforts to reduce pesticides use can interact with multilateral governance, using an empirical case of the listing of new substances under the Rotterdam Convention (see Figure 2). We documented "confounding interactions" that occur when private agricultural standard-setting bodies use the Rotterdam Convention's pesticide list to develop their own lists of banned substances, and unintentionally undermine the potential for international statebased governance to become more stringent. [3] This highlighted the need for scholars and policymakers to more fully consider complex interactions among actors in the context of global sustainability governance. Research also focused on linkages between pesticide regulation and biodiversity loss in the context of challenges to expand pesticide governance. Using an empirical case of pesticide regulation on a national level, we examined how the French government developed a new regulatory instrument for the most widely used pesticide worldwide, restricting its use based on the availability and costs of alternatives, rather than on health or environmental risks alone. Our analysis highlighted governance implications of decisions made in the commissioning and design of scientific expertise used by national governments as a basis for pesticide governance, demonstrating how expertise design plays a key role in defining the scope of policy options. [4]

Engagement of relevant research communities occurred through conference presentations, workshops, and collaborations. Conference presentations were made across multiple disciplines and professional organizations, including at the International Studies Association, the American Meteorological Society, the Earth Systems Governance Conference, the International Conference on Mercury as a Global Pollutant, and the International Sustainability Transitions Conference. Fiona Kinniburgh co-organized an emerging scholars' workshop at TUM. Miranda Schreurs co-organized a Jean Monnet Network on EU-Canada Relations Workshop, attended by Fiona Kinniburgh and Noelle Selin.

Focus Group participants engaged with policy-makers to gather data and disseminate findings. Henrik Selin and Noelle Selin attended the third Conference of Parties to the Minamata Convention on Mercury. Fiona Kinniburgh participated in meetings of the Stockholm Convention and the Rotterdam Convention. Results of the Focus Group's work informed graduate-level teaching at TUM and at Fellows' home institutions Boston University and the Massachusetts Institute of Technology. Henrik Selin and Noelle Selin gave multiple guest lectures in TUM's Politics and Technology Master's program. The HTE framework was used to develop open-source case studies for teaching, available online at http://mercurystories.org.



Figure 2, Processes for pesticide nomination and addition to the Rotterdam Convention Prior Informed Consent (PIC) list. The numbers in parentheses (n) refer to the number of pesticides listed under each category as of early 2022.

Selected publications

Kinniburgh, F., Selin, H., Selin, N.E., & Schreurs, M. When private governance impedes multilateralism: The case of international pesticide governance. *Regulation and Governance* (2022).

Kinniburgh, F. The politics of expertise in assessing alternatives to glyphosate in France. *Environmental Science and Policy*, in press (2023).

Selin, H. & Selin, N.E. *Mercury Stories: Understanding Sustainability through a Volatile Element.* Cambridge, MA: MIT Press (2020). Selin, H. & Selin, N.E. From Stockholm to Minamata and Beyond: Governing Mercury Pollution for a More Sustainable Future. *One Earth* 5(10), 1109–1125 (2022a).

Selin, H. & Selin, N.E. The Human-Technical-Environmental Systems Framework for Sustainability Analysis. *Sustainability Science* (2022b).

For a full list of publications please see https://www.ias.tum.de/ias/selin-henrik/ https://www.ias.tum.de/ias/eckley-selin-noelle/

Focus Group Visual Computing

Prof. Angel X. Chang (Simon Fraser University), Alumna Hans Fischer Fellow | Dave Zhenyu Chen (TUM), Doctoral Candidate | Host: Prof. Matthias Nießner (TUM)



Prof. Angel X. Chang

Grounding natural language to 3D scenes

We study the emerging research problem of connecting natural language describing objects and scenes to 3D data representations of the objects and scenes. We address resolving textual references of objects to 3D localizations of those objects, dense captioning of 3D scenes, and unified approaches that can both localize and describe objects in 3D scenes by leveraging a speaker-listener model.

- Dai, A. et.al. ScanNet: Richly Annotated 3D Reconstructions of Indoor Scenes. Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) (2017).
- [2] Chen, Z., Nießner, M. & Chang, A. X. (2020).
- [3] Chen, Z., Gholami, A., Nießner, M. & Chang, A. X. (2021).

This project is focused on connecting natural language to 3D representations of objects in real scenes. This interdisciplinary area involves methodology from natural language processing, 3D computer vision, and machine learning and is of increasing importance due to the increasing ubiquity of 3D data representing objects and scenes in the real world. With this increase of available 3D data, it is particularly important to enable the use of natural language for searching, describing, manipulating, and eventually generating 3D representations.

The project involved the investigation of a series of research problems that require connections between natural language and 3D scenes. The beginning of the project relied on recent prior work that the project team members had carried out to collect ScanNet [1]: a large-scale dataset of RGB-D scans of real scenes that was richly annotated with semantic information about the objects present in each scene. The first focus of the team was on collecting a set of natural language text descriptions of distinct objects observed in each of the ScanNet scenes. This correlated text and 3D data allowed us to address the problem of resolving references in text to objects in the 3D scan in our ScanRefer [2] paper. We found that this is a challenging research problem with much space for future work on improving 3D localization performance given natural language descriptions of objects.

In a follow up paper called Scan2Cap [3], we focused on the "inverse" direction of generating text descriptions of a given input 3D scene. Here, the focus was on generation of dense captions that refer to objects in the scene, their appearance, and spatial relations. During this work, we again observed that generation of natural language descriptions for 3D scenes is quite challenging, due to the complexity of spatial relations between objects and the diversity of objects observed in the real world. ►





Figure 1, We introduce the task of object localization in 3D scenes using natural language. Given as input a 3D scene and a natural language expression, we predict the bounding box for the target 3D object (right). The counterpart 2D task (left) does not capture the physical extent of the 3D objects.

- [4] Chen, Z., Wu, Q., Nießner, M. & Chang, A. X. (2022).
- [5] Chen, Z., Hu, R.,
 Chen, X., Nießner, M.
 & Chang, A. X. (2022).

The third major stage in our project attempted to tackle the two previous research problems by using a unified neural architecture we called D3Net [4]. This architecture leveraged the speaker-listener methodology to enable for 3D dense captioning and grounding of natural language descriptions to 3D objects using the same architecture. A key focus of this approach was to allow the use of unannotated 3D scene data for which natural language descriptions were not available. Leveraging such data for training in a semi-supervised fashion enabled improvements in both the captioning and localization tasks. Most recently, we investigated how the more powerful transformer neural architecture can enable further improvements in the unified setting with both captioning and localization. The resulting UniT3D [5] architecture that we developed establishes state-of-the-art performance for these tasks.

In addition to the publication output referenced above, we engaged with the emerging community of researchers interested in this area of connecting language with 3D scenes through the organization of two workshops and associated benchmark challenges. The first workshop and challenge was at CVPR 2021 (virtual) and named "Language for 3D Scenes." It involved invited talks by five research leaders in associated areas of research, as well as two benchmarks for natural language grounding tasks. The second workshop and challenge had the same title and was held at ECCV 2022 (virtual). In addition to six invited talks, we hosted a panel discussion by researchers with backgrounds in computer vision, machine learning, natural language processing, and cognitive science. We also expanded the benchmark component of the workshop by introducing a third dense captioning task. These workshops and associated challenges have helped to bring together the 3D language research community and to measure research progress in a systematic way.

The outcomes of this project can enable applications in assistive robotics, autonomous driving, and democratization of 3D content creation. All these domains and related industry sectors stand to benefit immensely from computational systems that can better understand how natural language connects with 3D data.



Figure 2, D3Net is an end-to-end neural speaker-listener architecture that can detect, describe and discriminate. D3Net also enables semi-supervised training on ScanNet data with partially annotated descriptions.

Selected publications

Chen, Z., Hu, R., Chen, X., Nießner, M. & Chang, A. X. UniT3D: A Unified Transformer for 3D Dense Captioning and Visual Grounding. *arXiv* 2212.00836 (2022), https://arxiv.org/pdf/2212.00836.pdf.

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Chen, Z., Gholami, A., Nießner, M. & Chang, A. X. Scan2Cap: Context-aware Dense Captioning in RGB-D Scans. *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)* (2021), https://arxiv.org/pdf/2012.02206.pdf. Chen, Z., Nießner, M. & Chang, A. X. Scan-Refer: 3D Object Localization in RGB-D Scans using Natural Language. *Proceedings of European Conference on Computer Vision (ECCV)* (2020), https://arxiv.org/ pdf/1912.08830.pdf.

Avetisyan, A. et al. Scan2CAD: Learning CAD Model Alignment in RGB-D Scans. *In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) (2019)*, https://arxiv.org/ pdf/1811.11187.pdf.

For a full list of publications please see https://www.ias.tum.de/ias/chang-angel/

Focus Group Electrochemical Interfaces in Batteries

Dr. Filippo Maglia (BMW Group), Alumnus Rudolf Diesel Industry Fellow | Lennart Reuter (TUM), Doctoral Candidate | Host: Prof. Hubert Gasteiger (TUM)

Dr. Filippo Maglia

- [1] Egbue, O. & Long, S. Barriers to widespread adoption of electric vehicles: An analysis of consumer attitudes and perceptions. Energy Policy 48, 717-729 (2012).
- [2] Peled, E. The Electrochemical Behavior of Alkali and Alkaline Earth Metals in Nonaqueous Battery Systems-The Solid Electrolyte Interphase Model. J. Electrochem. Soc. 126, 2047-2051 (1979).
- [3] Miura, T., Cotte, S. & Masanori, K. Lithium-Ion Battery Formation Process 8 (2018).
- [4] Zhang, B. et al. Role of 1,3-propane sultone and vinylene carbonate in solid electrolyte interface formation and gas generation. J. Phys. Chem. C 119, 11337-11348 (2015).

Electrolyte-Interphase on Graphite Anodes

Formation of the Solid-

A deeper understanding of the solid-electrolyte interphase (SEI) formation process and its influence on the LiB performance and durability is needed. For that, we have coupled standard electrochemical techniques with the on-line electrochemical mass spectrometry to clarify the effect of temperature on the SEI characteristics and their effect on the durability of LiBs containing widespread electrolyte additives.





9 1

Major obstacles for battery electric vehicles (BEVs) to be competitive with internal combustion engine ones have been identified as the limited driving range, high cost of the battery system, extended charge period, and capacity fading. Thus, the Focus Group Electrochemical Interfaces in Batteries aims to improve the capability and lifetime of lithium-ion batteries (LiBs). [1]

Most performance indicators of lithium-ion batteries (LiBs), including charge / discharge efficiency, rate capability, and cycle life, heavily depend on the many competing processes that occur at the interphases between the electrodes and the electrolyte. The most investigated interface in LiBs is the so-called solid-electrolyte-interphase, which is the product of electrolyte decomposition occurring at the negative electrode (anode) during the very first operating cycles. [2] Most anode materials (including the most widespread, i.e. graphite) operate in fact outside the voltage stability window of commercially available electrolytes. A general working principle is displayed in Figure 1.

Being permeable towards Li⁺-ions diffusion but electronically isolating, the SEI acts as a passivating layer allowing normal LiB operation but preventing further electrolyte reduction. Understanding and improving the SEI formation process is of critical relevance to the LiB industry. To yield an effective SEI, commercial battery cells undergo extensive and time-consuming formation procedures directly after cell assembly, comprising multiple voltage holds and current steps at various temperatures. [3]

In more detail, the SEI is a chemically and morphologically complex layer containing inorganic and organic compounds. Most of these compounds are reduction products of the commonly used cyclic, e.g., ethylene carbonate (EC), and linear carbonate-based electrolyte solvents. Linear carbonates such as ethyl methyl carbonate (EMC), dimethyl carbonate (DMC), and diethyl carbonate (DEC) are widely employed in LiB applications due to their low viscosity, high salt solubility, and high conductivity. [4] Additionally, organic electrolyte additives are commonly added to form an SEI layer with increased cycling stability and reduced irreversible capacity loss during the first cycle. [5] Among a variety of additives, vinylene carbonate (VC) is the most prominent.

The decomposition reaction of carbonates, together with the formation of the solid species contained in the SEI, is accompanied by the evolution of gaseous species. The amount, composition, and time of evolution of such gases are indicative of the underlying chemical reactions and can be used to elucidate the effect of electrolyte additives, reveal substantial degradation processes within LiBs, and rationalize optimized formation strategies. [6]

The evolution of gaseous species is typically quantified in-situ by monitoring the cell pressure (e.g., via the so-called Archimedes principle) or by online mass spectrometry. [7] Concerning the latter, an on-line electrochemical mass spectrometer (OEMS) was developed for the application in LiB research and proved to be particularly powerful since it allows a quantitative analysis and the identification of the evolved and consumed gas during the operation of a battery. [8]

However, the application of an OEMS is challenging when the vapor pressure of the electrolyte is high, as it is the case with most LiBs electrolytes due to the presence of highly volatile linear carbonates. At elevated temperatures, in particular a significant share of the gas present in the head-space of the OEMS cell, will consist of electrolyte vapor whose components undergo fragmentation in the mass spectrometer. As a consequence, a large background signal is superimposed ►

[5] Taskovic, T. et al. Optimizing Electrolyte Additive Loadings in NMC532/Graphite Cells: Vinylene Carbonate and Ethylene Sulfate. J. Electrochem. Soc. (2021).

- [6] Jung, R. et al. Oxygen **Release and Its Effect** on the Cycling Stability of LiNixMnyCozO2 (NMC) Cathode Materials for Li-Ion Batteries. J. Electrochem. Soc. 164. A1361-A1377 (2017); Aiken, C. P. et al. An Apparatus for the Study of In Situ Gas **Evolution in Li-Ion** Pouch Cells, J. Electrochem. Soc. 161, 1548-1554 (2014); Schreiner, D. et al. Comparative Evaluation of LMR-NCM and NCA Cathode Active Materials in Multilaver Lithium-Ion Pouch Cells: Part I. Production. Electrode Characterization, and Formation. J. Electrochem. Soc. 168. 030507 (2021).
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- [10] Zhang, B. et al. Role of 1,3-propane sultone and vinylene carbonate in solid electrolyte interface formation and gas generation. J. Phys. Chem. C 119, 11337-11348 (2015).

on the relevant mass traces related to hydrogen, ethylene, carbon monoxide, oxygen, and carbon dioxide. [9] To mitigate this effect, we developed an elaborate method for signal normalization, a correction for the electrolyte background change, and a precise practice for signal quantification of evolved gas species with commercial electrolytes.

The method allowed us to interpret the temperature-dependent SEI formation for cells containing an additive-free (LP57: 1 M LiPF, i n EC:EMC 3:7wt / wt) and additive-containing (LP572: LP57 + 2wt% VC) electrolyte. For the former, we were able to determine how the formation temperature influences the gas evolution as well as how the bulk of the electrolyte degrades during formation. We were able to conclude that increasing the formation temperature from 25°C to 45°C significantly increases the overall amount of all relevant gases. More specifically, higher temperatures induce a rapid jump in the amount of the evolved ethylene indicating a change from lithium ethylene dicarbonate (LEDC) to lithium carbonate (Li₂CO₃) as the primary reduction product of EC in the SEI. Additionally, the trans-esterification of EMC to form DMC and DEC proved to be highly temperature dependent leading to a conversion of approx. 15 vol% EMC at 45°C (summarized in Figure 2).

The SEI formation in the presence of the electrolyte additive changes significantly. The reduction of VC initiates at higher reduction potentials compared to alkyl carbonate solvents (e.g., EC), and therefore it is reduced preferentially during the first charge. [10] We compared the formation temperatures in a range between 10-60°C by investigating the performance of both full-cells (i.e. graphite anode and a Ni-rich NCM cathode) as well as of graphite/Li half-cells. We could conclude that the formation at 10 and 25°C is most favorable due to the lowest initial Li-loss attributed to SEI formation, cell resistance over cycling (see Figure 3 (b)), lowest SEI-related gas evolution during formation, and a very similar capacity fade (see Figure 3 (a)) compared to cells formed at elevated temperatures. Consequently, the formation at lower temperatures is beneficial for a higher energy density of the cell and a higher rate performance.

This understanding will help to rationalize formation conditions in an industrial application and to extend driving ranges as well as optimize charging periods of LiBs in a BEV application.



Figure 2, Temperature dependence of the evolution of SEI related gases of a graphite / Ni-rich NCM with LP57: H_2 (green bars), ethylene (C_2H_4) (blue bars), and CO (red bars) as well as the amount of DEC originating from the trans-esterification of EMC to DEC (violet bars) in units of vol% of the electrolyte.



Figure 3, (a) Specific discharge capacity versus cycle number for 0.5C cycling at 45°C of a Graphite-NCM full-cells with LP572 electrolyte formed at 10 (black), 25 (blue), 45 (green), and 60°C (orange); (b) 2C direct current internal resistance (DCIR) pulse evaluated at 1s versus cycle number.

Selected publications

Strmcnik, D. et al. Electrocatalytic transformation of HF impurity to H2 and LiF in lithium-ion batteries. *Nat. Catal.* 1, 255–262 (2018).

Castelli, I. E. et al. The role of an interface in stabilizing reaction intermediates for hydrogen evolution in aprotic electrolytes. *Chem. Sci.* 11.15, 3914–3922 (2020).

Reuter, L. et al. Temperature-Dependent Gassing Analysis by On-Line Electrochem-

ical Mass Spectrometry of Lithium-Ion Battery Cells with Commercial Electrolytes. *Manuscript in preparation.*

Reuter, L. et al. Temperature Dependent Formation of SEI with Vinylene Carbonate (VC) Electrolyte Additive. *Manuscript in preparation.*

For a full list of publications please see https://www.ias.tum.de/ias/maglia-filippo/



Focus Group Computer Vision & Machine Learning

Prof. Daniel Cremers (TUM), Alumnus Carl von Linde Senior Fellow



Prof. Daniel Cremers

Novel Optimization Methods for Computer Vision and Shape Analysis

Within the Carl von Linde Senior Fellowship, we were fortunate to attract two outstanding reaserchers as temporary professors to TU Munich. These were Prof. Jörg Stückler (now Max Planck Institute for Intelligent Systems, Tübingen) and Prof. Florian Bernard (now University of Bonn). Rather than giving a complete account of respective research activities, in the following we will highlight two publications in the area of computer vision and shape analysis performed in collaboration with Florian Bernard.





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In [1], we developed a method for joint deep multi-graph matching and 3D geometry learning: Graph matching aims to establish correspondences between vertices of graphs so that both the node and edge attributes agree. Various learning-based methods were recently proposed for finding correspondences between image key points based on deep graph matching formulations. While these approaches mainly focus on learning node and edge attributes, they completely ignore the 3D geometry of the underlying 3D objects depicted in the 2D images. We fill this gap by proposing a trainable framework that takes advantage of graph neural networks for learning a deformable 3D geometry model from inhomogeneous image collections, i.e., a set of images that depict different instances of objects from the same category. Experimentally, we demonstrate that our method outperforms recent learning-based approaches for graph matching considering both accuracy and cycle-consistency error, while we also obtain the underlying 3D geometry of the objects depicted in the 2D images.

In [2], we developed a unified framework for implicit Sinkhorn differentiation: The Sinkhorn algorithm is a classical iterative algorithm for minimizing regularized optimal transport

problems. And optimal transport (also known as earth-movers distance) is a formalism for computing correspondence, a central component in many computer vision and shape analysis works. As a result, the Sinkhorn operator has recently experienced a surge of popularity in computer vision and related fields. One major reason is its ease of integration into deep learning frameworks. To allow for an efficient training of respective neural networks, we propose an algorithm that obtains analytical gradients of a Sinkhorn layer via implicit differentiation. In comparison to prior work, our framework is based on the most general formulation of the Sinkhorn operator. It allows for any type of loss function, while both the target capacities and cost matrices are differentiated jointly.

We further construct error bounds of the resulting algorithm for approximate inputs. Finally, we demonstrate that for a number of applications, simply replacing automatic differentiation with our algorithm directly improves the stability and accuracy of the obtained gradients. Moreover, we show that it is computationally more efficient, particularly when resources like GPU memory are scarce.

- [1] Ye, Z., Yenamandra, T., Bernard, F. & Cremers. D. Joint Deep Multi-Graph Matching and 3D Geometry Learning from Inhomogeneous 2D Image Collections. AAAI (2022).
- [2] Eisenberger, M., Toker, A., Leal-Taixé, L., Bernard, F. & Cremers, D. A Unified Framework for Implicit Sinkhorn Differentiation. IEEE International Conference on Computer Vision and Pattern Recognition (CVPR) (2022).



Figure 2, In [2], we show that a number of challenges in computer vision such as point cloud registration, interpolation and shape analysis can be significantly improved with the help of the proposed implicit Sinkhorn differentiation.

In which environment do we want to live in the future?

Towards the end of five years the project "Agriculture – Water Management – Climate Change. New perspectives for agriculture and the environment" (granted by the Bavarian Ministry of Environment and Consumer Protection), special attention was paid to public outreach and documentation of results.

Sustainable water (re)use

Using and reusing resources efficiently was the top theme at the IFAT Munich Congress and Exibition 2022, world trade fair for water and waste management. Circular Economy as the overarching theme connecting supporting programs, exhibitions as well as the special areas, offered visitors a platform to discuss in a variety of settings the effects of climatic changes exacerbating in extended droughts and extreme heat waves. To address these challenges, changes in water (and waste) management will be necessary.

The IESP Forum Drought and Heat, held on the second day of the fair, May 31, 2022, focused on the sustainable (re)use of water resources. Prof. Wolfram Mauser from Ludwig-Maximilians-University Munich (LMU) gave an overview of the systemic interrelationships within the Water-Food-Energy Nexus of water supply, food cultivation and energy production in the Danube region. Using satellite data and models, he highlighted the potential of effective irrigation methods for intensified farming. It is thereby possible to double yields, yet at the risk of massive runoff of surface waters. An economic analysis shows that the gain in food production outweighs the loss in energy production along the river Danube by far. However, agricultural conversion could return land to nature as compensation areas. This would make a significant contribution to climate and biodiversity protection globally and locally. A multinational area, such as the Danube basin, poses considerable challenges to intergovernmental knowledge, data exchange, and cross-border state administration. At the same time, the necessary agro-structural transformation of the post-communist states enables far-reaching innovations to integrate measures of nature, environment and climate protection.

Prof. Jörg E. Drewes of the Technical University of Munich (TUM) used small-scale irrigation demand data to demonstrate the effectiveness and possibilities of



Wolfram Mauser on the necessity of integrated, transnational water management.



Stage discussion "Nutrition and Land Use" participants from left to right: Stefan Schwarzer, UNEP; Christine Röger, KErn; Georg Bayerle, BR; Martin Grambow, StMUV; Tobias Gaugler, TH Nürnberg.

using municipal waterwater effluents after advanced treatment for agricultural and landscape irrigation purposes. Multi-stage, modular purification processes are currently being researched within the framework of the BMBF-funded 'Nutzwasser' project with a demonstration-scale test site in Schweinfurt, Lower Frankonia. This region is already suffering from dwindling water supplies and resulting conflicts of use. Different quality levels and irrigation techniques are being tested in parallel to demonstrate a save reuse practice for the cultivation of crops eaten raw. This form of utilizing alternative water resources will become increasingly important as global temperatures rise. Regional climate change also result in weather extremes, which affect the availability of local ground and surface water supplies as well as their quality. Local water reclamation therefore offers a financially viable possibility for small and medium-sized entrepreneurs to become climate change resilient. Thus, the effective use of recycled water cannot only strengthen a local economy, but entire rural areas. At the same time, water reuse contributes to environmental protection and nature conservation in the respective region.

The lively discussion following a summarizing commentary by Dr. Klaus Arzet of the Bavarian Ministry for the Environment and Consumer Protection (StMUV) iterated the complex interrelationship between environmental, nature and climate protection, but also the challenges arising from comprehensive approaches to solutions and their implementation. The benefit of a direct comparison of large complex systems and small local initiatives was clearly evident. Positive feedback from representatives of farmers' associations as well as state and federal regulatory administration further expressed the necessity for open and continued dialogue between professionals of the sectors water management and agriculture in order to jointly develop sustainable solutions for the challenges posed by anthropogenic overuse of resources and climate change in an often lobby driven political environment.

Sustainable global supply chains

The "farmers' protests" of recent years made the challenges of domestic producers are facing in Bavaria, Germany, and Europe widely visible. Little political mitigation has been taken even though experts from the fields of agriculture and water management, nature and climate protection, and economy have been concerned about the impact of globally linked food production on biodiversity, environmental landscape, ►



Jürgen Geist, TUM, commenting on the 2019 Seeon workshop.

but also farmers for many years. With effect of January 1, 2023, the German federal government's Supply Chain Sourcing Obligations Act (LkSG) aims to bring attention to both the environmental and social effects of international trade connections.

In June 2022, the IESP workshop "Supply Chains of the Food Industry" looked into the global connections of agriculture, consumption, and food production, staged

at the premises of Schloss Blumenthal near Aichach under the patronage of the StMUV and the Bavarian State Institute for Agriculture (LfL). Participants of the workshop discussed the topic of supply chains in the food industry in general, and from the perspective of sustainable development. It not only considered economic and social, but also ecological aspects, against the background of the prospective implementation of the German Supply Chain Sourcing Obligations Act, and the ongoing EU activities to introduce a framework directive on "sustainability obligations of companies." Even before coming into effect, the law presented itself as a unique initiative for global sustainability.

The LkSG requires companies to make transparent their suppliers and ensure meeting certain social and environmental standards. The German law translated into respective national law can take international effect. Quite revolutionary is the clause that can hold company boards individually accountable. It has the potential to positively impact local agriculture and food production. It can strengthen the markets, individual producers, favor smaller enterprises and producers. With removing economic pressure from the local market and farmers, it removes environmental stress. The LkSG thereby supports the social transition to a future proof, sustainable 21st century agricultural system:

- Sustainability and fairness along global supply chains mutually enforce each other.
- Sustainability is not a state of affairs, but an ongoing process that requires everyone to take responsibility.
- Sustainability only works if the value of food is worth enough – when its true cost is accounted for people and the environment.

The workshop focused on the diverse, but specific aspects of the food industry and thus addressed a topic

that had been widely neglected so far. In the workshop context, the food economy included producers (farmers), processors (food industry), and distributors (discounters, retailers), and thus sometimes long, complex, and international supply chains. The presentations highlighted the legal, ethical and economic aspects of the LkSG and ongoing EU activities and dealt with questions of practical implementation using practical examples, including the example of a discounter. It was the last workshop in a series of events, which will be concluded by March 2023.

Nutrition and land use in the Anthropocene

Over the project term, it became increasingly obvious that food and nutrition - in consumption, distribution, and production alike - are crucial to the human community in adapting to a rapidly progressing climate change. Therefore, this topic framed the concluding project event on February 27, 2023, which attracted a heterogeneous audience from science, economy, political administration, and civil society. The IESP network presented their recommendations for action formulated in the course of three workshops, supported by online discussions surrounding the 2021 expert report for the Bavarian State Chancellery on the Free State's future water security. In the afternoon of the half-day event at Munich's Nymphenburg castle, invited comments on the workshop findings stressed the well-known discrepancy between well-researched, validated knowledge on problems arising at the nexus of agriculture, water management, and climate change; and the (political) implementation deficit of at least 25 years that drives today's climate protests. Here, another important issue to overcome is the communication between political and administrative departments' or "ivory tower conversations." This could hold the key to upscaling and synergizing departmental research, targeted towards the same direction, thereby including all those "in the field" concerned with implementing measures. In the evening, Prof. Hans Hauner, TUM, lectured about diet and nutrition influencing individual and public health, and the role of an unregulated Janus-headed industry of processed foods. A subsequent stage discussion on sustainable land and water use in (agricultural) food production concluded the event.

Sustainable landscape engineering

Further developing the topic of health-beneficial and healthy landscapes with resilient landscape hydrology, the IESP secured funding for a 2-year-feasibility study by the Bavarian State Chancellery. In collaboration with local partners in Tunisia, the project will generate insights on the possibility to stabilize local groundwater supplies by water reuse and reforestation. It builds upon the Tunisian Master Plans 2050 for Water Use and Reuse. Dwindling water resources in combination with increasing temperatures and extreme weather events are of global concern beyond the Mediterranean. The project also intends to learn from a country with 2000 years of experience in drought management. The interdisciplinary research team will be rooted at the TUM chairs for Ecoclimatology and Urban Water Systems Management as well as the TUM-IAS.

1 0 0

Where do the TUM-IAS Fellows come from?

USA

Prof. Andrea Erhardt Prof. Gregory Erhardt University of Kentucky

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. Natalia Perkins University of Minnesota

Prof. Siobhan Rockcastle University of Oregon

Prof. Robert J. Schmitz University of Georgia

Prof. Henrik Selin Boston University

Prof. Noelle 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

Ukraine

Dr. Oksana Chernova Dr. Olena Strelnyk Taras Shevchenko National University of Kyiv

Dr. luliia Yereshko Dr. lulia Yamnenko Igor Sikorsky Kyiv Polytechnic Institute

Prof. Oksana Koshulko Alfred Nobel University, Dnipro

Dr. Sofiia Lahutina Bogomolets National Medical University

Dr. Liudmyla Lisova E.O. Paton Electric Welding Institute, National Academy of Sciences

Dr. Olya Popovuch Ivano-Frankvisk National Technical University of Oil and Gas

Dr. Yuliia Semenova Institute of Geophysics, National Academy of Sciences

Dr. Dmytro Sytnyk Institute of Mathematics, National Academy of Sciences

Argentina

Prof. Marta C. Antonelli Universidad de Buenos Aires



Prof. Gustavo Goldman University of São Paulo

Canada

Prof. Angel X. Chang

Prof. Jihyun Lee University of Calgary

Simon Fraser University

1

United Kingdom

Dr. Ioannis Brilakis 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

Germany

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Dr. Filippo Maglia Dr. Felix Rempe BMW Group

Dr. Philipp-Alexander Neumann Prof. Daniela Pfeiffer Dr. Benedikt Zott TUM University Hospital rechts der Isar

Rudolf Mößbauer Fellows at TUM

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Prof. Maja Horst DTU Technical University of Denmark

Sweden

Prof. Meike Schalk KTH Royal Institute of Technology

Prof. Mats Alvesson Lund University

Hungary

Prof. Örs Legeza Wigner Research Centre for Physics

Poland

Prof. Piotr Tryjanowski University of Life Sciences in Poznań

Russia

Dr. Anastassia Makarieva Petersburg Nuclear Physics Institut

China

Prof. Lifeng Chi Soochow University

India

Prof. Shobhana Narasimhan Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)

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Prof. Susan Park University of Sydney

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Prof. Giuseppe Savaré Bocconi University

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Israel

Prof. Ronit Kark Bar-Ilan University

Prof. Eitan Yaakobi Technion



Dr. Elena del Valle Universidad Autónoma de Madrid

Prof. Andreas Winter Autonomous University of Barcelona

Facts and Figures

Excellence Strategy, Clusters of Excellence, and TUM Budget

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 (2006– 2012 and 2012–2019), the TUM-IAS became 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 contributes to 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. By 2022, a total of three Fellows had been appointed within this program.

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, which ended in 2022. In 2022, TÜV SÜD Foundation and TUM agreed on a new Fellowship called "TUM-IAS Philosopher in Residence." Each Fellowship runs for a full year. Three Fellowships can be awarded from 2023 on.

Siemens AG

Siemens AG provides funding for six Hans Fischer (Senior) Fellowships with over 2 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. In 2022, Siemens continued to provide six Hans Fischer (Senior) Fellowship, focusing on the Industrial Metaverse, starting in 2023.

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 has been awarded in 2022 (see Welcoming Our New Fellows), more will follow in 2023.

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Fellow Distribution by Fellowship Category in 2022



E	penditure per Fellows	ship Category in 2022				Total € 2,564,000 H
A				В	С	DEFG
A	€ 1,440,000	Hans Fischer Senior Fellowship	B 	€ 627,000	Hans Fische	r Fellowship
С	€ 259,000	Fellowship for Ukrainian Scientists	D	€ 84,000	Anna Boykse	en Fellowship
E 	€ 81,000	Albrecht Struppler Clinician Scientist Fellowship	F	€ 58,000	Rudolf Diese	el Industry Fellowship
G	€ 13,000	Carl von Linde Senior Fellowship	н	€ 3,000		oauer Tenure ant Professorship

Fellow Distribution according to TUM-IAS Research Areas in 2022

А	В	С	D	E F		G	H I JKL
A	Advanced Computation and Modeling	Surface, Interface, Nano- and Quantum Science		Fundamental Natural and Life Sciences	D	9	Bio-Engineering and Imaging
E	Environmental and Earth Sciences, Building Technology	Gender and Diver- sity in Science and Engineering	G	8 Medical Natural Sciences	н	3	Political, Social and Technological Change
I	2 Communication and Information	Control Theory, Systems Enginee- ring, and Robotics	к	1 Neuroengineering	L	1	Organization, Management and Leadership

Expenditure per TUM-IAS Research Area in 2022

Total € 2,305,000

									I			
А		В	С	D	Е		F	G	н	I	J	к
A	€ 730,000	Advanced Computation and Modeling	В	€ 364,00	0	Funda Scienc		l Nat	ural a	and L	.ife	
C	€ 321,000	Bio-Engineering and Imaging	D	€ 241,00	0	Enviro Scienc					ogy	
E	€ 174,000	Political, Social and Technolo- gical Change	F	€ 115,00	0	Surfac Quant				no- a	and	
G	€ 84,000	Gender and Diversity in Science and Engineering	н	€ 79,00	0	Contro Engine						
I	€ 79,000	Neuroengineering	J	€ 75,00	0	Comm	unicat	ion a	nd In	form	natio	n

K **€ 42,000** Medical Natural Sciences

Fellow Distribution by TUM School/Department in 2022

А		В	С	D	Е	F G H
A	School of Compu- tation, Information and Technology	в 19	School of Natural Sciences	C 14 School of Enginee- ring and Design	D	Department of Medicine
E	School of Life Sciences	f 6	School of Social Sciences and Technology	G School of Management	н	Department of Sport and Health Sciences

Expenditure per TUM School/Department in 2022

Total € 2,305,000

A	В		С	D	E	F	G
A	© 905,000 School of Computation, Information and Technology	В	€ 3	44,000	School of E	ngineering aı	nd Design
С	School of Natural Sciences	D	€ 2	31,000	School of L	ife Sciences	
E	221,000 School of Social Sciences and Technology	F	€ 2	18,000	Departmen	t of Medicine	9

G **© 77,000** School of Management

Board of Trustees

(status: December 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: December 2022)

The TUM-IAS Advisory Council is composed mainly 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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TUM-IAS Management Office

(status: December 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. (6.3 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 fulltime equivalents)



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Pages 5, 18-21, 26

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