# Annual Report

Technical University of Munich

Institute for Advanced Study

2019

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Institute for Advanced Study

2019

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# TUM President's Foreword



As I write these opening words for a report highlighting brilliant achievements of 2019, I must acknowledge the dark cloud of the coronavirus pandemic hanging over the present moment, which allows for only digital education of our students without their inspiring presence on campus. Already the Technical University of Munich (TUM) is engaging with the coronavirus pandemic on various research fronts, ranging from medicine and public health to economics and society, and on to environment and sustainability – and is doing so in a way that recognizes and harnesses the potential for synergies across TUM's portfolio of disciplines. As a forefront thinker of society, our university is being challenged not merely to weather the current storm, but to master it for the common good while grasping new opportunities and building toward a robust and sustainable future.

The full extent of the unfolding global health emergency and economic crisis may become clear only in retrospect. There are two things we already know for sure, however. Communities like ours can provide resilience against shocks and changes of any kind, on any scale. And one of the best hopes for tackling the challenges ahead is an interdisciplinary, international, and intergenerational approach to top-level research, education, and innovation. Such an approach determines the heartbeat of the TUM Institute for Advanced Study (TUM-IAS). The TUM-IAS was established as the core of the long-term development strategy of TUM in the first round of the Excellence Initiative (2006–2012). It provides outstanding scientific talents from all over the world with the necessary support to activate high-risk research ideas of the highest innovation potential together with the best people at TUM through our Fellowship program.

Honored once more as a University of Excellence in 2019, TUM has again received – with gratitude and a keen sense of responsibility – the strong endorsement and financial support of Germany's federal and state governments. TUM is the only technical university to prevail in all three rounds of the highly competitive Excellence Initiative. TUM shares the distinction of three consecutive wins from day one with only one other university nationwide. That is Ludwig-Maximilians-Universität München (LMU), our intimite partner in four Clusters of Excellence funded for the period 2019–2025 as well as in our ONE MUNICH strategy which, as a key measure of our TUM AGENDA 2030, is designed to jointly pioneer emerging research fields in Greater Munich through a cross-institutional approach and to accelerate the diffusion and adoption of innovations into business and society.

Our strategy going forward, under the banner of TUM AGENDA 2030, calls for ever closer alignment of our research, education and innovation processes with the values, needs, and expectations of society. With a deliberate focus on human-centered engineering, technology design, and responsible innovation, we are bringing a fresh impulse to "German engineering" – an engine of our economy and effectively one of the most admired brands in the world. And we have undertaken one of the largest reform initiatives in our university's history.

The most visible change will be the reorganization and incorporation of our traditional fifteen departments into seven TUM Schools: Engineering & Design; Computation, Information & Technology; Social Sciences; Management; Life Sciences; Natural Sciences; and Medicine & Health. Flanked by established as well as newly founded Corporate Research Centers, such as e.g. the Center for Quantum Engineering, transdisciplinary Integrative Research Centers like the recently initiated Munich Data Science Institute, and Higher Learning Institutes like the new TUM Institute for Life Long Learning (TUM IL3), the TUM Schools stand at the heart of an interwoven matrix structure designed to facilitate interactions and promote new directions in education, talent management, research, and innovation.

The TUM-IAS will have a number of special roles to play as we translate our strategy to reality. One aim of the TUM-IAS is to become a central catalyst for the implementation of the TUM Innovation Networks and serve as a hub and platform for realizing innovative ideas across departmental borders. We support teams of up to ten principal investigators, with up to ten doctoral candidates, who want to put their pioneer spirit to the test in high risk / high gain projects. Naturally, a seed-fund program like this carries some risk, but it is entirely in keeping with our university's entrepreneurial character. We are confident that some of these TUM Innovation Networks will expand the boundaries of knowledge and then form the basis for larger scientific enterprises, such as Collaborative Research Centers and Transregional Collaborative Research Centers. Those that eventually reach critical mass may give rise to “bottom-up” competitive focus areas and overarching centers geared toward system-wide challenges.

I do not want to close without expressing my deepest appreciation for my predecessor Wolfgang A. Herrmann, a truly effective scientist and supreme mover and shaker in academic management, who personifies our university's optimistic, entrepreneurial spirit, and by offering my heartfelt thanks to Ernst Rank, who has completed his term as TUM-IAS Director. One might say these two invented the TUM-IAS in the first place, and both have made enormous contributions to its success over the years. I look forward to fruitful collaboration with incoming Director Michael Molls, one of our highly distinguished researchers, emeritus professor of radiation therapy and radiological oncology and currently spokesman for the TUM Emeriti of Excellence.

As the TUM-IAS has become a great intellectual force-field, I look forward to welcome the talented scientists from all over the world to come together to exchange ideas, challenge each other and work together with us without being restricted by technical, institutional or intellectual boundaries.

*Prof. Thomas F. Hofmann*
President

# TUM-IAS Director’s Message



For the TUM-IAS as for the university community as a whole, the year 2019 was indelibly marked by the new round of the Excellence Initiative, now called the Excellence Strategy. The joy was overwhelming on July 19 when Anja Karliczek, the Federal Minister of Education and Research, announced that TUM had won the title of “Excellence University” for the third time in a row. This makes the two Munich universities, TUM and LMU, the only ones that have been consistently successful in the Excellence competition from the start in 2006.

Since the beginning of the Excellence Initiative, the TUM-IAS has played a central role in promoting TUM as an institution. The Institute has again taken on important tasks in the Excellence Strategy “TUM. THE ENTREPRENEURIAL UNIVERSITY – Innovation by Talents, Excellence, and Responsibility,” which has now been funded since November 2019. In addition to the proven Fellowship programs – Hans Fischer and Hans Fischer Senior Fellowships, Rudolf Mössbauer Tenure Track Professorships, Rudolf Diesel and Anna Boyksen Fellowships, and (with certain modifications) Carl von Linde Senior Fellowships – new initiatives are coming along. The most important will be the commitment to developing and organizing Exploratory Workshops, which are meant to serve as the starting points for TUM’s Innovation Networks. With this new workshop and network format, seminal research topics will be identified early on and taken up at our university. As in an entrepreneurial incubator, the Innovation Networks will then develop these research fields to the point where they can win their first external funding. Many of these topics will be multidisciplinary in nature and thus anchored in the university's new Schools structure. The TUM-IAS, with its broad, interdisciplinary approach and the network of Fellows at the best universities in this world, is thus destined to provide strong support for this initiative. So the prospects for the future are very interesting indeed.

At this point a bit of a retrospective view is in order. After five years, my term as Director of the TUM-IAS is coming to an end. Building on the already successfully established programs, the Institute team was able to set additional priorities. And so it became possible, through the TUM-IAS Focal Periods, to create a framework for the growing number of Alumni Fellows to maintain ongoing academic exchange with active Fellows. We were also able to develop novel models for cooperation with the private sector, which guarantee maximum benefit for both partners while ensuring 100% scientific independence for the TUM-IAS. A further expansion of our connections to the worldwide network of related institutes was also achieved, particularly within the framework of the UBIAS network (University-Based Institutes for Advanced Study).

For me personally, these were five satisfying years full of exciting encounters with outstanding scientists from TUM and from all over the world, with interesting workshops and symposia on topics that are not on the list of typical conference programs, and last but not least five years with staff who have always advanced our Institute with very special commitment and an approach to the work that goes far above and beyond the usual level. The abundant and always positive feedback from our Fellows speaks for itself. Especially close to my heart are two event series that my predecessor Gerhard Abstreiter had already launched – our weekly "Wednesday Coffee Talks" and the Sunday matinee, "What are our neighbors actually doing, these researchers in Garching?" The first series provided countless short presentations on the latest news about research at TUM, while the second offered the broader public introductions to major technological and scientific questions. Always particularly inspiring, for many of the speakers as well, were the discussions with non-experts who attended these events, which often opened up completely new perspectives.

Beginning with the summer semester 2020, management of the TUM-IAS will be in new hands. As Director, Prof. Dr. med. Dr. h.c. Michael Molls will continue to develop the Institute and will surely accentuate many aspects in his own way.
I myself would like to stay closely connected to the TUM-IAS as an "alumnus" while I go back to focusing more strongly on my own research questions.

*Prof. Ernst Rank*
Director, in March 2020

# Message from the incoming TUM-IAS Director

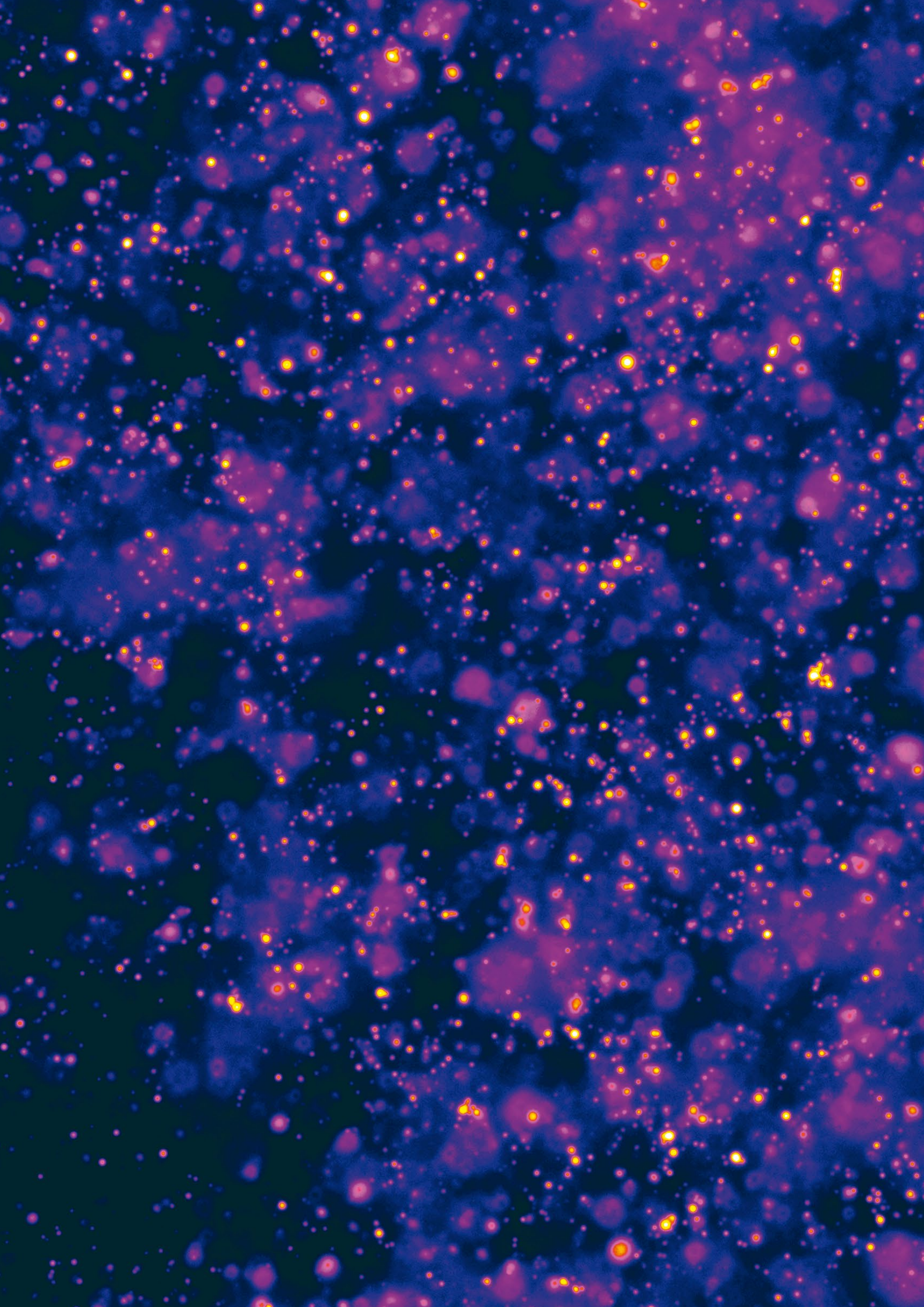


First of all, I would like to thank my predecessor Ernst Rank, the previous Directors Patrick Dewilde and Gerhard Abstreiter, and their teams for their excellent work. We have to preserve that excellence and maintain continuity as we move forward. As a member of the TUM family, I would like to help make TUM as a "scientific brand" even more highly visible internationally. That means, among other things, ensuring that the TUM-IAS contributes to realizing the goals set in the Excellence Strategy proposal: for example, working in alliance with TUM Forte and IGSSE to establish new TUM Innovation Networks through the organization of Exploratory Workshops. Within the TUM community, the TUM-IAS should be perceived and used even more than before as a hub and platform for the realization of creative ideas. The TUM-IAS enables a productive interplay between younger and more experienced researchers.

Modern research means interdisciplinarity, and that includes the humanities. As an oncologically oriented scientist (radiation biology) and physician (radiation therapy/radiooncology), I have a strong interest in the topic of "generation of evidence" for new procedures or therapies in medicine as part of our responsibility to society. The current coronavirus crisis underscores how much we depend on "hard" data, scientifically generated in a correct manner, to make appropriate political decisions regarding the health of people of all ages, a functioning economy, and social solidarity. The corona crisis also shows – sometimes easy to discern, sometimes less so – that a lack of seriousness can come into play in science: excessive ambition and an addiction to high-profile attention, greed for the big money, and so on. It is extremely important to consider in great detail and to understand precisely the mechanisms for generation of evidence, and also to develop new ideas and methods.

A second overarching topic in which I have a strong interest, and which I will promote at the TUM-IAS, is sustainability. In the next decade this will concern not only biodiversity, climate, and environment, but also the economy, biotechnology, design, risk management, and much more. Our collaboration with the International Expert Group on Earth System Preservation (IESP), which is based at the TUM-IAS, will continue. In recent years a fruitful cooperation has developed between the IESP and the Senior Excellence Faculty of TUM. Symposia were organized – drawing on the diverse, excellent competences of TUM and external scientists, and with participation by representatives of business, administration, and politics – where recommendations for science, business, and policy were developed. The TUM-IAS will continue to support these important activities in the future. Outstanding science is the sustainable motor for the healthy further development of civilization and a good future for societies in Europe, Africa, and other continents. We at TUM, as a community, must constantly convey this great idea to the outside world. In the future as in the past, the TUM-IAS will play a role in transmitting this message to the public.

*Prof. Michael Molls*
Director, in April 2020



People

## Board of Trustees

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.

## Members

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Technical University of Munich, President

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**Prof. Anders O. Bjarklev** Technical University of Denmark, President
**Prof. Martin Carrier** Bielefeld University, Faculty of History, Philosophy and Theology, Institute for Interdisciplinary Studies of Science, I²SoS-Head
**Prof. Michael J. Hannon** University of Birmingham, Chair of Chemical Biology and Director of the EPSRC Research and Training Centre in Physical Sciences for Health, Institute of Advanced Studies, former Director
**Prof. Heather Hofmeister, Ph.D.** Goethe University Frankfurt am Main, The Center for Leadership and Behavior in Organizations (CLBO), Scientific Director
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**Dr. Dorothea Rüland** German Academic Exchange Service (DAAD), Secretary General
**Prof. Reinhard Rummel** TUM, Institute for Astronomical and Physical Geodesy, TUM Emeritus of Excellence
**Prof. Hiroyuki Sakaki** The University of Tokyo, Professor Emeritus Toyota Technological Institute, former President
**Prof. Bert Sakmann** Max Planck Florida Institute, Inaugural Scientific Director Max Planck Institute of Neurobiology, Emeritus Research Group Leader, Nobel Prize for Physiology or Medicine 1991
**Prof. Londa Schiebinger** Stanford University, John L. Hinds Professor of the History of Science, Gendered Innovations in Science, Health & Medicine, Engineering, and Environment, Director
**Prof. Dr. med. Markus Schwaiger** TUM, University Hospital Klinikum rechts der Isar, Medical Director
**Prof. Henry Tye** The Hong Kong University of Science and Technology, Department of Physics, and Jockey Club Institute for Advanced Study, former Director, IAS Professor

# Advisory Council



The TUM-IAS Advisory Council consists of a member from the Max Planck Institute of Quantum Optics and TUM professors covering all major fields of the university. It functions as a standing advisory board to the TUM-IAS Director and his management team. 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 regularly, typically three times a year.

## Members

**Prof. Martin Bichler**
Decision Sciences and Systems
**Prof. Dirk Busch**
Medical Microbiology, Immunology and Hygiene
**Prof. Hubert Gasteiger**
Technical Electrochemistry
**Prof. Ulrich Heiz**
Physical Chemistry
**Prof. Florian Holzapfel**
Flight System Dynamics
**Prof. Katharina Krischer**
Nonequilibrium Chemical Physics
**Prof. Sabine Maasen**
Sociology of Science, Director of the Munich Center for Technology in Society (MCTS)
**Prof. Claudia Peus**
Research and Science Management
Senior Vice President Talent Management and Diversity
**Prof. Gerhard Rempe**
Max Planck Institute of Quantum Optics – Quantum Dynamics Group
**Prof. Ulf Schlichtmann**
Electronic Design Automation
**Prof. Chris-Carolin Schön**
Plant Breeding
**Prof. Daniel Straub**
Engineering Risk Analysis Group
**Prof. Barbara Wohlmuth**
Numerical Mathematics, Director IGSSE

# Management Office



Prof. Ernst Rank
Director

Tatjana Steinberger
Acting Managing Director

Dr. Ana Santos Kühn
Managing Director
(leave of absence)

Dr. Yves Vincent Grossmann
Program Manager

Anna Kohout
Program Manager
(leave of absence since 05/2019)

Dr. Agnes Limmer
Program Manager of IESP

Dr. Simon Märkl
Program Manager
(since 06/2019)

Eva Pettinato
Program Manager

Dr. Susanne Wahler
Program Manager

Sigrid Wagner
Senior Event Manager /
Web Coordinator

Simone Schmid
Assistant / Building
Coordination

Hanka Schmidt
Secretary / Guesthouse
Coordination

Jessica Westermayr
Assistant of IESP

# Fellows



## Anna Boyksen Fellows

2018 Dr. Sara Lucatello, Prof. Nina A. Mayr

## Carl von Linde Senior Fellows

2016 Prof. Hendrik Dietz
2017 Prof. Daniel Cremers
2018 Prof. Bernhard Küster

## Hans Fischer Senior Fellows

2016 Prof. Angela Casini, Prof. Krishnendu Chakrabarty, Prof. Johannes Lehmann, Prof. Bernhard Schrefler (awarded by the TÜV Süd Foundation)
2017 Prof. Kelly Clifton, Prof. Paolo Giommi, Prof. Maya Schuldiner, Prof. Takao Someya
2018 Prof. Marta C. Antonelli, Prof. Leonidas Guibas, Prof. Noelle Eckley Selin, Prof. Henrik Selin
2019 Dr. Ioannis Brilakis, Prof. Lifeng Chi, Prof. Gustavo Goldman, Prof. Susan Park, Prof. Giuseppe Savaré, Prof. Krasimira Tsaneva-Atanasova

## Hans Fischer Fellows

2016 Prof. Jochen Blumberger, Dr. Marc Janoschek, Prof. Melike Lakadamyali
2017 Prof. Camilla Hollanti, Prof. Hai (Helen) Li
2018 Prof. Angel X. Chang, Dr. Luca Magri, Prof. Robert J. Schmitz
2019 Dr. Christian Bick, Prof. Eleni Chatzi (awarded by the TÜV Süd Foundation), Dr. Barbara Solenthaler, Prof. Leila Takayama, Prof. Eitan Yaakobi

## Rudolf Diesel Industry Fellows

2017 Prof. Michael Bronstein
2018 Dr. Mirko Bothien, Dr. Filippo Maglia

## Rudolf Mößbauer Tenure Track Professors

2013 Prof. Kathrin Lang, Prof. Bjoern Menze
2014 Prof. Jia Chen, Prof. Matthias J. Feige, Prof. Franz Hagn, Prof. Michael Knap, Prof. Robert König
2015 Prof. Job Boekhoven, Prof. Frank Johannes, Prof. Rolf Moeckel
2016 Prof. Stephan Günnemann, Prof. Matthias Nießner, Prof. Menno Poot, Prof. Sebastian Steinhorst, Prof. Antonia Wachter-Zeh
2017 Prof. Laura Leal-Taixé, Prof. Kathrin Schumann
2018 Prof. Reinhard Heckel
2019 Prof. David Egger, Prof. Angelika Harbauer, Prof. Susanne Kossatz, Prof. Christian Mendl, Prof. Kai Müller

# Alumni Fellows



## Anna Boyksen Fellows

2014 Prof. Madeline Heilman
2015 Prof. Giovanni Boniolo, Prof. Regina Ensenauer, Prof. Sarah de Rijcke
2016 Prof. Nicola Lautenschlager

## Amalie Baur Fellow

2017 Prof. Lena Henningsen

## Carl von Linde Senior Fellows

2007 Prof. Andrzej Buras, Prof. Arthur Konnerth, Prof. Reiner Rummel
2008 Prof. Horst Kessler, Prof. Claudia Klüppelberg
2009 Prof. Axel Haase
2010 Prof. Ulrich Stimming, Prof. Gerhard Abstreiter
2011 Prof. Ingrid Kögel-Knabner
2013 Prof. Annette Menzel
2014 Prof. Martin Buss
2015 Prof. Franz Pfeiffer

## Carl von Linde Junior Fellows

2007 Prof. Adrian Jäggi
2008 Dr. Martin Gorbahn, Dr. Ulrich Rant, Prof. Robert Stelzer
2009 Prof. Kolja Kühnlenz, Dr. Marco Punta, Prof. Ian Sharp, Prof. Julia Kunze-Liebhäuser
2010 Prof. Wilhelm Auwärter, Dr. Vladimir García Morales, Prof. Alexandra Kirsch, Prof. Miriam Mehl, Dr. Christian Stemberger, Prof. Dirk Wollherr
2011 Prof. Angelika Peer, Prof. Dongheui Lee
2013 Dr. Peer-Hendrik Kuhn

## Hans Fischer Senior Fellows

2007 Prof. Gerhard Beutler, Prof. Walter Kucharczyk, Prof. Bert Sakmann
2008 Prof. Anuradha M. Annaswamy, Prof. Yasuhiko Arakawa, Prof. Douglas Bonn, Prof. Mandayam A. Srinivasan, Prof. David A. Weitz
2009 Prof. Matthew Campbell, Prof. Richard Davis, Prof. Gino Isidori, Prof. Shuit Tong Lee, Prof. Wolfgang Porod, Prof. Stanley Riddell, Prof. Peter Schröder, Prof. Zohar Yosibash
2010 Prof. Robijn Bruinsma, Prof. Markus Hegland, Prof. Michael Ortiz, Prof. Stefan Pokorski, Prof. Tim Sparks, Prof. Raman I. Sujith

2011 Prof. Silvio Aime, Prof. Polly Arnold, Prof. Daniel Gianola, Prof. Frank R. Kschischang, Prof. Christian Werthmann
2012 Prof. Stephen M. Goodnick, Prof. Dietmar W. Hutmacher, Prof. Josef P. Rauschecker
2013 Prof. Harald Brune, Prof. Zvonimir Dogic
2014 Prof. John S. Baras, Prof. Dirk Bergemann, Prof. Gregory D. Hager, Prof. Tamas Horvath, Prof. A. Lee Swindlehurst, Prof. Nicholas Zabaras
2015 Prof. Carl P. Blobel, Prof. Klaus Kästner, Prof. Yannis Kevrekidis, Dr. Thierry Lasserre, Prof. Jane A. McKeating, Prof. Anca Muscholl, Prof. Ayyalusamy Ramamoorthy

### Hans Fischer Fellows

2012 Prof. George Biros, Prof. Franz Hagn
2013 Prof. Matthias Batzill, Dr. Christian Hirt
2014 Prof. Yana Bromberg, Prof. Tsung-Yi Ho, Prof. Stuart Khan
2015 Dr. Kaye Morgan, Prof. Alessandro Reali, Prof. Dominique Sugny

### Hans Fischer Tenure Track Professors

2007 Prof. Thomas Misgeld
2010 Prof. Hendrik Dietz

### Rudolf Diesel Industry Fellows

2009 Prof. Khaled Karrai, Dr. Dragan Obradovic, Dr. Georg von Wichert
2010 Dr. Tsuyoshi Hirata, Prof. Gernot Spiegelberg, Prof. Matthias Heller, Dr. Chin Man W. Mok
2012 Dr. René-Jean Essiambre, Prof. Michael Friebe, Dr. Bruno Schuermans
2013 Dr. Thomas Koehler, Dr. Peter Lamp
2014 Dr. Norman Blank, Dr. Heike Riel
2015 Prof. Carlo Ratti

### Rudolf Mößbauer Tenure Track Professor

2013 Prof. Alessio Zaccone
2015 Prof. Carlo Camilloni

# Visiting Fellows 2019



Prof. Abhinav Bhatele | Lawrence Livermore National Laboratory
Prof. Charles Eesley | Stanford University
Prof. Mari Kobayashi | Université Paris-Saclay, Gif-sur-Yvette
Prof. Bert Roozen | Katholieke Universiteit Leuven
Prof. Jack Taunton | University of California, San Francisco
Dr. Gottfried Ungerboeck | Broadcom Inc.

# Honorary Fellows 2019



## Gottfried Wilhelm Leibniz Prizewinners

Prof. Brenda Schulman | Department of Chemistry, Honorary Professor at TUM
Prof. Sami Haddadin | Robotics Science and System Intelligence, TUM

## ERC Grantees

Dr. Jennifer Altomonte | Clinic and Polyclinic for Internal Medicine II, TUM
Prof. Job Boekhoven | Supramolecular Chemistry, TUM
Prof. Daniel Cremers | Computer Vision and Artificial Intelligence, TUM
Dr. Felix Deschler | Walter Schottky Institute, TUM
Prof. Mathias Drton | Mathematical Statistics, TUM
Prof. Sandra Hirche | Information-Oriented Control, TUM
Prof. Dimitrios Karampinos | Body Magnetic Resonance Research, TUM
Prof. Michael Knap | Collective Quantum Dynamics, TUM
Dr. Barbara Lechner | Physical Chemistry, TUM
Prof. Susanne Mertens | Experimental Astro-Particle Physics, TUM
Dr. Veit Rothhammer | Neurological Clinic, TUM
Prof. Ian Sharp | Walter Schottky Institute, TUM
Prof. Stephan A. Sieber | Organic Chemistry, TUM
Prof. Nils Thürey | Physics-Based Simulation, TUM
Prof. Gil Gregor Westmeyer | Molecular Imaging, TUM

## August-Wilhelm Scheer Visiting Professors

Prof. Haldun Aytug | University of Florida
Prof. Walter Baratta | Università degli Studi di Udine
Prof. Jeffrey Bennett | University of Colorado Denver
Prof. Andreas Hamann | University of Alberta
Prof. Mari Kobayashi | Centrale Supélec
Prof. Boris Kozinsky | Harvard University
Prof. Roland Krug | University of California, San Francisco
Dr. Tei-Wei Kuo | National Taiwan University
Dr. Torsten Lange | ETH Zurich
Dr. Rianne Lord | University of Bradford
Prof. Hrushikesh Mhaskar | Claremont Graduate University
Prof. Aimilios Michael | University of Cyprus
Prof. Kok Kwang Phoon | National University of Singapore
Dr. Saúl Ramos-Sánchez | Universidad Nacional Autónoma de México
Dr. Pierre-Francois Rodriguez | Université Paris-Saclay
Prof. Rui Wu | Shanghai Jiao Tong University

# Activities and Events


deep learning era
layer 1
layer 2
layer 3
learnable task-specific features

# TUM-IAS General Assembly



May 23–24, 2019

The venue for the General Assembly, which has already been held for the eleventh time, was the TUM Science & Study Center Raitenhaslach. For two days, the former Cistercian monastery Raitenhaslach was filled with Fellows and members of TUM-IAS who otherwise are spread all over the world. Over 100 participants from various disciplines took advantage of the opportunity to hear about progress in the Focus Groups and TUM-IAS projects, to engage in lively discussions, and to exchange experiences and ideas with new members and old acquaintances.

As always, the talks came from scientific areas that were as interdisciplinary as the TUM-IAS itself, including topics such a synchrotron light source, quantum optics, deep learning, the sex of chicken embryos, smart skin, and CRISPR engineering. Two poster sessions during which most of our doctoral candidates took part offered a colorful overview of the work of our Focus Groups, giving participants and visitors alike the chance to meet scientists from related fields as well as to learn more about developments and results in wholly different areas of research.

The arched hall (brew room) of the monastery inn served as the perfect location for our festive conference dinner. In his dinner speech TUM President and TUM-IAS Board of Trustees chair Prof. Wolfgang A. Herrmann emphasized once more the uniqueness of the TUM Science & Study Center Raitenhaslach: it is the ideal place for university, interdisciplinary and international interaction in historical surroundings. Thereby he also pointed out the important role the TUM-IAS plays in the sustainability of TUM's international strategy. Moreover, as has been tradition since the founding of the Institute, the new members of the TUM-IAS community were announced. TUM President Prof. Wolfgang A. Herrmann and TUM-IAS Director Prof. Ernst Rank presented the Fellowship certificates to our Fellows.

## Program

**SESAME – A Source of Light in the Middle East**
Eliezer Rabinovici | The Hebrew University of Jerusalem

**Quantum Optics on a Chip**
Menno Poot | Rudolf Mößbauer Tenure Track Professor

**The Universe in Multi Messengers: The High Energy Frontier**
Elisa Resconi | Chair for Experimental Physics with Cosmic Particles, TUM

**Geometric Deep Learning: From Astrophysics to Fake News**
Michael Bronstein | Rudolf Diesel Industry Fellow

**The Art of Modelling Fluids in the Age of Big Data**
Luca Magri | Hans Fischer Fellow

**Smart Skin**
Takao Someya | Hans Fischer Senior Fellow

**From Electronic Structure to Biological Function**
Ville Kaila | Associate Professorship of Computational Biocatalysis, TUM

**Non-invasive Bioimaging of Chicken Eggs to Detect the Sex of Embryos**
Axel Haase | Alumnus Carl von Linde Senior Fellows

**Perceived Maternal Stress During Pregnancy Alters Fetal Autonomic Nervous System**
Marta C. Antonelli | Hans Fischer Senior Fellow

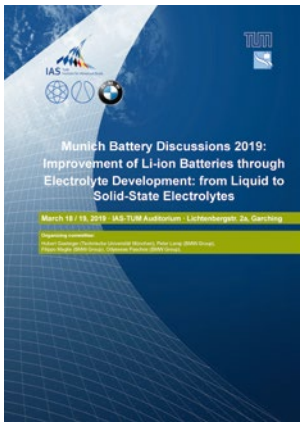
**From Mapping out the Human Proteome to Making Data- and Evidence-driven treatment Recommendations for Cancer Patients**
Bernhard Küster | Carl von Linde Senior Fellows

**CRISPR-Engineering Immune Cells for Experimental and (Future) Therapeutic Use**
Kathrin Schumann | Rudolf Mößbauer Tenure Track Professor


Analysis

# 7th Munich Battery Discussions

March 18–19, 2019
Organization: Focus Group Electrochemical Interfaces in Batteries




The development of e-mobility is at a tipping point, with increasingly optimistic forecasts regarding the future market share of electric vehicles. Nevertheless, the drive range-to-costs ratio is still far from what is required for mass-market penetration.

Near-future solutions will be based on the evolution of the present generation of Li-ion batteries through improvement of anode and cathode materials as well as electrode and cell design. Nevertheless, the energy density increase achievable with technologies based on liquid electrolytes is limited. In addition, pursuing higher energy densities through the implementation of high capacitive electrode materials (e.g., Ni-rich cathodes, Si-based anodes), higher operating voltages, and higher electrode loadings negatively affects both lifetime and safety.

A revolutionary approach, based on solid-state batteries and other new cell concepts, would offer the chance to extend the drive range far beyond 500 km, thanks to a broader choice of electrode materials – in particular lithium metal anodes – and a larger potential for cell / module / pack design optimization. In particular, the use of new-generation electrolytes (e.g., inorganic solid electrolytes) might be the only viable solution to combine high energy densities with the demanding safety requirements of automotive applications. However, a large number of scientific and technological challenges still need to be solved before all-solid-state batteries can reach a meaningful share of the electromobility market.

To address the hottest topics in the field of research and development of future battery materials and systems, BMW and the TUM Institute for Advanced Study have been jointly organizing, since 2013, the Munich Battery Discussions, an international conference held annually at the TUM-IAS. This 7th edition was dedicated to “Improvement of Li-ion Batteries through Electrolyte Development: from Liquid to Solid-State Electrolytes”. Eighteen international speakers from European, North American, and Asian universities and research centers presented their latest results on electrolyte development for high-energy and high-power battery propulsion systems in automotive applications. A select audience of around 150 participants, including numerous TUM students and faculty, BMW scientists and engineers, and national and international guests had the chance to engage in fruitful discussions with world-renowned experts from the field of electrochemical energy conversion and storage.

On the same topic, we also continued with our Speakers´ Series dedicated to “New Frontiers in Battery Science and Technology”. The purpose of these invited seminars is to offer to the BMW and TUM-IAS community a continuous update on the most exciting new findings in the field of battery research.

In 2019 we had the following eight presentations:

25.01. Prof. Sung-Soo Kim Thermal and structural stabilities of $Li_xCoO_2$ cathode for Li secondary battery studied by a temperature programmed reduction.

25.01. Prof. Zhumabay Bakenov High Performance Cathode Materials for Lithium-Sulfur Batteries.

10.05. Dr. Charles Delacourt Determination of parameters for physics-based models of Li-ion batteries.

19.07. Prof. Eric D. Wachsman Beyond Dendrites, Cycling Li-Metal Across Garnet at High Current Densities.

26.07. Prof. Boris Kozinsky Computational discovery of materials for energy conversion and storage from transport properties of ions, electrons and phonons.

06.09. Prof. Bor Z. Jang From Graphene to Graphene-Enabled Batteries for EV Application: A 17-Year Journey.

08.11. Dr. Jason R. Croy Development of High-Capacity, Manganese-Rich, Lithium-Ion Cells.

13.12. Prof. Harry Hoster From atomistic models to high-precision charge counting: reading tales told at tabs and how to convert them into pounds.

# TUM-IAS Focus Workshop

## Hot Carrier Dynamics in Advanced Concept Solar Cells

October 28–29, 2019
Organization: Focal Periods 2019 – Advanced Concepts for Ultrahigh-Efficiency Solar Cells

In the fall of 2019, the TUM-IAS hosted an interdisciplinary workshop on Hot Carrier Dynamics in Advanced Concept Solar Cells, which formed part of the TUM-IAS Focal Periods program for 2019. Organized by Gregor Koblmüller (TUM Junior Fellow and ERC Consolidator Grant awardee) from the Walter Schottky Institute (WSI) at TUM, the workshop brought together leading scientists worldwide to explore fundamental energy conversion processes in new types of photovoltaic materials and devices.

A particular emphasis was placed on promoting interdisciplinary and sustainable collaboration between world-renowned researchers in the field of “hot carrier” type solar cells and associated TUM-IAS Focus Groups. These included the Alumni Focus Group Nanoscience for Renewable Energy Sources (led by Prof. Stephen Goodnick, Arizona State University), the Focus Group Nanophotonics and Quantum Optics (led by Prof. Jonathan Finley, TUM-WSI), and the Focus Group Semiconductor Nanowires (led by PD Dr. Gregor Koblmüller, TUM-WSI).

The program consisted of about 20 keynote talks drawn from leading groups across Europe, the US, and the Asia-Pacific region, as well as local groups from TUM, Ludwig-Maximilians-University Munich and the new Cluster of Excellence “e-conversion,” all hosted in seven focus sessions. The workshop was opened by two pioneers in hot carrier dynamics of advanced solar energy conversion strategies, Dr. Victor Klimov from the Los Alamos National Laboratory (LANL) and Dr. Matthew Beard from the US-based National Renewable Energy Laboratory (NREL). Both illustrated recent examples of quantum-confined materials that enable bypasses in hot carrier cooling and, thus, significant enhancements in carrier multiplication and solar cell conversion efficiency.

The subsequent keynote talks focused on various aspects of hot carrier dynamics in low-dimensional semiconductors and their related solar energy conversion devices. The workshop also tried to strike a good balance between theoretical modeling and experimental investigations to develop rich understanding of non-equilibrium carrier relaxation dynamics as well as multi-exciton generation in a variety of nanostructured materials (quantum wells, dots, wires, perovskites, 2D materials, etc.). Thus the workshop provided a unique interdisciplinary forum for researchers to discuss the most important developments at the interfaces between multiscale modeling, engineering of sophisticated low-dimensional semiconductor materials, and characterization including ultrafast optical and electron/X-ray spectroscopy methods.

The participants in the TUM-IAS Focal Periods Workshop, with the three TUM-IAS Focus Group leaders in the front row: Prof. Stephen Goodnick (second from left), PD Gregor Koblmüller (third from left, workshop organizer), and Prof. Jonathan Finley (third from the right). Former TUM-IAS Director Prof. Gerhard Abstreiter (fourth from the left) also took part in the workshop.

Dr. Victor Klimov (Los Alamos National Laboratory) during his opening keynote talk.

Prof. Alexander Efros (Naval Research Laboratory, Alexander von Humboldt Awardee and TUM-IAS Honorary Hans Fischer Senior Fellow) with Prof. Gerhard Abstreiter (former TUM-IAS Director).

Poster session and discussions in the coffee breaks

TUM-IAS director Prof. Ernst Rank giving the welcome address

The talks were complemented by a poster session of more than 20 posters presented by students and young researchers, generating active dialogue to explore the forefront of this field. Overall, the workshop was a true success and saw large attendance by both TUM students and faculty members. The personal atmosphere of the TUM-IAS and the social dinner organized in a traditional Bavarian beer house in downtown Munich gave the participants ample opportunities to develop further ideas for future successful collaborations.

## Scientific Program

**Monday, October 28**

8:30 Registration
9:00 Opening Address
*Ernst Rank*, Director of TUM-IAS

### Session I – Advanced Solar Energy Conversion by Multi Exciton Generation

9:15 Novel Approaches to Photoconversion with Engineered Quantum Dots
*Victor I. Klimov*, Los Alamos National Laboratory (LANL)
9:45 Using Colloidal Quantum Dots to Overcome Hot-Carrier Relaxation Losses in Advanced Solar Energy Conversion Strategies
*Matthew C. Beard*, Natioal Renewable Energy Laboratory (NREL)
10:15 Coffee break

### Session II – Hot Carrier Solar Cells – Fundamentals and Device Aspects

10:45 Hot Carrier Photovoltaic Devices
*Ned Ekins-Daukes*, University of New South Wales (UNSW)
11:15 Hot Carriers – Dissipation and Work
*Jean-Francois Guillemoles*, CNRS & The University of Tokyo
11:45 Valley Photovoltaics: Towards the Realization of the Hot Carrier Solar Cells
*Ian Sellers*, University of Oklahoma
12:30 Lunch
13:30 Poster Session and Coffee

### Session III – Hot Carrier Scattering Dynamics I – Ultrafast Optical Spectroscopy

14:30 Electron-Phonon Coupling and Charge-Carrier Cooling in Metal Halide Perovskites for Photovoltaic Applications
*Laura Herz*, University of Oxford
15:00 Dynamics of Photocarriers and Excitons in Lead Halide Perovskites
*Yoshihiko Kanemitsu*, Kyoto University
15:30 Hot Carrier Scattering and Momentum Polarization in Hybrid Perovskites
*Felix Deschler*, Technical University of Munich (TUM)
16:00 Coffee break

Session IV – Hot Carrier Scattering Dynamics II –
Ultrafast Electron & X-ray Spectroscopy

16:15 Hot Carrier-Lattice Coupling in Nanostructures probed by Femtosecond X-ray and Electron Scattering Techniques
*Aaron M. Lindenberg*, Stanford University

16:45 Hot Carrier and Phonon Dynamics in Semiconductors Investigated with trARPES and Femtosecond Electron Diffraction
*Ralph Ernstorfer*, Fritz-Haber Institut (FHI) Berlin

17:15 End of Session

18:30 Conference Dinner

**Tuesday, October 29**

8:30 Registration

Session V – Dynamics of Bright Exciton States

9:00 Bright Triplet Excitons in Cesium Halide Perovskites
*Alexander Efros*, Naval Research Laboratory (NRL)

9:30 Carrier Dynamics in Size-Controlled Halide Perovskite Nanocrystals
*Alexander Urban*, Ludwig-Maximilians-University (LMU) Munich

10:00 Spatiotemporal Exciton Dynamics in Atomically Thin Materials
*Ermin Malic*, Chalmers University

10:30 Coffee break

Session VI – Carrier Multiplication in Diverse Materials / Experiment & Theory

11:00 Investigation of Materials for Hot Carrier Solar Cell Absorbers
*Gavin Conibeer*, University of New South Wales (UNSW)

11:30 A Decade of Carrier Multiplication in Delft
*Laurens Siebbeles*, Delft University of Technology

12:00 Simulation of Nonequilibrium Electron and Phonon Dynamics in Advanced Photovoltaic Devices
*Stephen M. Goodnick*, Arizona State University (ASU)

12:30 Lunch

Session VII – Non-Equilibrium Carrier Effects in Nanowire and Photonic Systems

13:30 Nonequilibrium Electron and Phonon Effects in Quantum Cascade Devices
*Christian Jirauschek*, Technical University of Munich (TUM)

14:00 Harvesting heat from electrons in nanowires
*Heiner Linke*, Lund University

14:30 Strong Hot Carrier Effects in a GaAsSb/InP Nanowire Heterostructure
*Leigh M. Smith*, University of Cincinnati

15:00 From Bulk-like to 1D-Quantum Confined InGaAs-based Nanowire Solar Cells
*Gregor Koblmüller*, Technical University of Munich (TUM)

15:30 End of Workshop / Coffee Break

15:45 Optional Lab Tour through WSI / ZNN

17:00 End of Lab Tour

# TUM-IAS International Workshop on Built Environment Digital Twinning

December 17–18, 2019
co-organized by TUM and Siemens

A great success, this workshop drew the attention of experts in building information modeling (BIM) from academia and industry alike. They had the opportunity to discuss the future of building information modeling in workshop sessions and on a more personal level during long coffee breaks. The presentations were aligned along the life cycle of the digital building model itself, from creating it to bringing it to market.

Since one major aspect of building twins is interoperability, standardization accounted for a significant share of the presentations. For example, an overview of standardization efforts was presented by RWTH Aachen, while the standardization of building systems from a company's point of view was introduced by Siemens. As of today, most buildings are still developed without BIM. Therefore introducing building twins into brown-field projects is an important topic. Most solutions presented in the sessions aim toward digitizing the as-built status by acquiring point clouds and analyzing them afterwards.

While this is the usual business of academia and big players like Bentley, start-ups and small and medium-sized enterprises are also in the front line of development. For example, the presenter from LocLab astonished the audience by showing how cheaply and easily a digital twin can be acquired from existing structures. In any case, the digital twin of a building would be useless if it cannot be connected to live data. How to achieve this in an efficient and effective way was demonstrated by Siemens and Oracle.

When it comes to use cases of digital building twins, the UK is one of the leading countries in promoting this topic from a government perspective, and this is supported by leading universities such as Cambridge. The presentation from the Centre for Digital Built Britain showed how important the careful design of regulations is in finding a good tradeoff between fostering best practices and leaving enough room for innovation. Last but not least, the evening event on site provided good opportunities for networking, particularly between academia and industry.


Leonhard Obermeyer Center


TUM

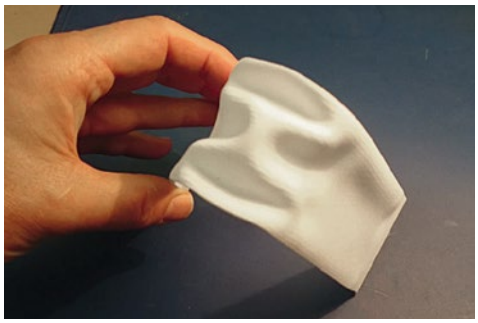
# The TUM-IAS “Neighbors” Lecture Series: So what exactly is it that you do in Garching?

## A peek behind the scenes at work being done by researchers in Garching


It all started in 2013 with a question the former Institute Director, Prof. Gerhard Abstreiter, was always getting from the area locals: “So what exactly is it that you do at the Garching campus?” In response to this, he came up with the new concept of the TUM-IAS “Neighbors” series, aimed at getting the local community and people living around TUM’s Garching campus more involved in the exciting research happening next door – and to encourage a real dialogue with them.

In this spirit, several times a year the TUM-IAS opens its doors to interested neighbors from the region for a “science Sunday matinee.” At this event we feature an informal talk (in German) by a well known scientist from the university or from one of our campus neighbors, with the aspiration of making their work accessible to the diverse, general-public audiences in attendance. In around 45 to 60 minutes, the listeners – consisting of a mix of people from nearby communities ranging in age from grade school to retirement age – are taken on a scientific journey during which they can gain new insight into the fascinating world of research and scientific advances. After the talks, audience members (usually a respectable crowd of around 80) have the possibility of asking follow-up questions and talking directly with the experts over a cup of coffee and fresh-baked pastries.

In 2019, the scope of topics ranged from gamified augmented reality to the molecular world of the good taste, as well as architecture to inspire and the interaction of engineering design and computer simulation.



Left: Work Report – Building to Inspire, Prof. Francis Kéré.

Right: Strength and Form – Form and Strength: About the Interaction of Engineering Design and Computer Simulation, Prof. Kai-Uwe Bletzinger.


The Molecular World of the Good Taste: From First Violins to Sensory Sound, Prof. Thomas F. Hofmann.

January 27 — Lecture Series Neighbors in Garching
**Gamified Augmented Reality: How to Better Connect the Real World with IT Using Elements of Computer Games and Location-Based 3D Displays**
Organization: TUM-IAS
Speaker: Prof. Gudrun Klinker (Chair for Augmented Reality, TUM)

May 19 — Lecture Series Neighbors in Garching
**The Molecular World of the Good Taste: From First Violins to Sensory Sound**
Organization: TUM-IAS
Speaker: Prof. Thomas F. Hofmann (Chair for Food Chemistry and Molecular Sensory Science, TUM)

July 21 — Lecture Series Neighbors in Garching
**Work Report – Building to Inspire**
Organization: TUM-IAS
Speaker: Prof. Francis Kéré (Chair for Architectural Design and Participation, TUM)

November 24 — Lecture Series Neighbors in Garching
**Strength and Form – Form and Strength: About the Interaction of Engineering Design and Computer Simulation**
Organization: TUM-IAS
Speaker: Prof. Kai-Uwe Bletzinger (Chair of Structural Analysis, TUM)

# Fellows' Lunches

An essential characteristic of the TUM-IAS is that it has Fellows, Honorary Fellows, Host professors, and other community members from all research areas in the TUM portfolio. With the aim of bringing our large community of talented people with many different specializations together, we regularly (typically once a month), host the TUM-IAS Fellows' Lunch. As the name already indicates, this event offers the possibility of getting to know each other at an informal lunch in connection with a talk by one of the members. This year, presentations ranged from microfluidic design automation to coding for DNA storage – including not only discoveries enabled by new technologies, but also critical insights into the techniques themselves. As always, talks were pointedly geared toward communicating new ideas with an audience of experts in fields other than the speaker's. When, after the lunch, we see vivid discussions and the formation of new, perhaps unexpected acquaintances, we know that once again, the Fellows' Lunch has fulfilled its purpose.

February 4
**Shape Differences and Variability**
Prof. Leonidas Guibas | Hans Fischer Senior Fellow

March 3
**From Inverse Design to Implementation of Practical Photonics**
Prof. Jelena Vuckovic | Alumna Hans Fischer Senior Fellow

April 11
**Image-Based Modeling of Tumors**
Prof. Björn Menze | Rudolf Mößbauer Tenure Track Professor

May 9
**Investigating the Properties of Quark-Gluon Plasma with Heavy-Ion Collisions at LHC**
Dr. Ante Bilandzic | ERC Grant Awardee

July 8
**Microfluidic Design Automation: Enabling Convergence between the Life Sciences, Microelectronics, and Computational Thinking**
Prof. Krishnendu Chakrabarty | Hans Fischer Senior Fellow

October 15
**Coding for DNA Storage**
Prof. Eitan Yaakobi | Hans Fischer Fellow

November 11
**PARP Inhibitor-Based Molecular Imaging for Diagnosis, Treatment and Monitoring of Cancer**
Prof. Susanne Kossatz | Rudolf Mößbauer Tenure Track Professor

December 12
**Why New Materials are Urgently Needed, and How Theory Helps Finding Them**
Prof. David Egger | Rudolf Mößbauer Tenure Track Professor

# Scientists Meet Scientists – Wednesday Coffee Talks




The Wednesday Coffee Talks seem to have become one of the best-known and most popular activities of the TUM-IAS: Under the responsibility of the Institute's Director Prof. Ernst Rank, the Coffee Talks are held weekly after lunch in the spacious atrium on the first floor of the building. They provide a platform for outstanding TUM publications, allowing their authors to present their work in a short, simple presentation that would be understandable to non-experts too. The audience, made up of scientists on all career levels from the various research fields of TUM, profits in turn from the possibility to gain insight into exciting projects currently happening at TUM and to get to know each other in a relaxed, informal atmosphere. What we especially like about this event, besides bringing together Fellows and guests who are currently in the area, is that it has brought in plenty of new faces with no prior relation to the TUM-IAS, often entering our building for the first time for this occasion. Again in 2019, we had very interesting talks with topics ranging from the Antarctic ice cap to molecular lego and hyperloop vision, followed by inspiring discussions and lively conversations. The Wednesday Coffee Talks are thus certainly adding to the TUM-IAS's standing as a center for intellectual exchange and discourse on campus.

| | |
|---|---|
| January 9 | Prof. Roland Pail on the Antarctic Ice Cap Melting Faster and Faster |
| January 16 | Prof. Robert König on the First Proof of Quantum Computer Advantage |
| January 23 | Dr. Joachim Reichert on Switching with Molecules |
| January 30 | Prof. Job Boekhoven on A Simple Mechanism Which Could Have Been Decisive for the Development of Life |
| February 6 | Dr. Laura Sánchez on Mountains in Motion |
| May 2 | Dr. Markus Hölzel on Crystal Structures of Fluorine Revisited by Neutron Diffraction |
| May 8 | Prof. Majid Zamani on Towards Certifiable Autonomy |
| May 15 | Prof. Thorsten Bach on De-Racemization – The Vanished Mirror Image |
| May 22 | Dr. Kai Zosseder on the Importance to Unlock the Shallow Geothermal Potential for the Transition to a Climate-Friendly Heating and Cooling of Buildings |
| May 29 | Dr. Thierry Lasserre on First Direct Measurement of the Neutrino Mass with the KATRIN Experiment |
| June 5 | Prof. Christoph Hugenschmidt on A Tricky Experiment: Simultaneous Storage of Positrons and Electrons |
| June 19 | PD Dr. Harald Oberhofer on Molecular Lego: How Theory can aide in the Search for New Organic Semiconductors |

June 26 — Prof. Anja Rammig on Rainforest at Risk – AmazonFACE Research Project on the Effects of Climate Change on the Rainforest

July 3 — Prof. Kai Müller on Generation of Non-Classical Light – From Fundamental Physics to Quantum Engineering

July 10 — PD Dr. Simon Jacob on Lost in Translation: The Challenge of Bringing Together Animal and Human Experiments to Explore Cognitive Brain Functions

July 17 — Prof. Frank Pollmann on Stability of Quasiparticles in Quantum Systems: The Cycle of Decay and Rebirth

July 24 — Prof. André Platzer on Cyber Physical System Safety

October 23 — Prof. Kathrin Lang on Targeted Labelling of Proteins with Ubiquitin via an Expanded Genetic Code

October 30 — Prof. Michael Knap on What is the Perfect Quantum Theory?

November 6 — Prof. Eugénia da Conceição-Heldt on Legacies and Innovations in Global Economic Governance: 75$^{th}$ Anniversary of Bretton Woods

November 13 — Gabriele Semino on Inside the Hyperloop Vision: From a Student Competition to a Full-Scale System

November 20 — Prof. Laura Fabbietti on A Temperature of 800 Millions Degrees in the Cosmic Kitchen

November 27 — Andreas Dunkel on New High-Throughput Tools for Volatile Metabolite Quantitation in Food Analysis and Nutrition Science

December 4 — Prof. Thomas Brück on Towards a Climate Effective Bioeconomy – Biotechnology Centered Processes for the Conversion of $CO_2$ and Chemically Complex Biomass to Sustainable Chemical and Material Entities

December 11 — Dr. Gunther Korschinek on Stardust in the Antarctic Snow – Iron-60 Discovery in the Antarctic Provides Information on the Environment of the Solar System

January 25

Speakers' Series on "New Frontiers in Battery Science and Technology" 2019: **Thermal and Structural Stabilities of LixCoO2 Cathode for Li Secondary Battery Studied by a Temperature Programmed Reduction and High Performance Cathode Materials for Lithium-Sulfur Batteries**
Speaker: Prof. Sung-Soo Kim (Chungnam National University / Nazarbayev University) and Prof. Zhumabay Bakenov (Nazarbayev University)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

February 18

**Visit of the President of The Republic of Armenia Dr. Armen Sarkissian**
Speakers: Dr. Armen Sarkissian, Prof. Wolfgang A. Herrmann (TUM President), Prof. Ernst Rank (TUM-IAS Director), Prof. Daniel Cremers | Carl von Linde Senior Fellow, Prof. Stephan Paul (Department of Physics, TUM), Prof. Stefan Schönert (Department of Physics, TUM)


March 18–19

Munich Battery Discussions 2019: **Improvement of Li-ion Batteries through Electrolyte Development: from Liquid to Solid-State Electrolytes**
Organization: Prof. Hubert Gasteiger (Department of Chemistry, TUM), Dr. Filippo Maglia | Rudolf Diesel Industry Fellow, Dr. Peter Lamp | Alumnus Rudolf Diesel Industry Fellow, Dr. Odysseas Paschos (BMW Group)

March 25–26

**Bi-Annual Research Meeting of the Institute of Applied Mechanics (ICAM)**
Organization: Prof. Bert Roozen | TUM-IAS Visiting Fellow

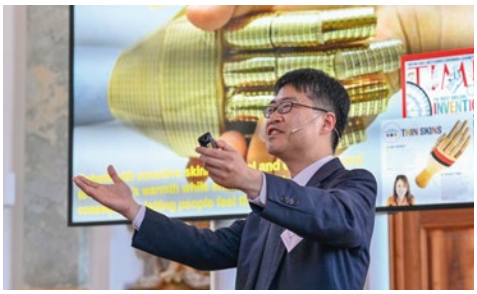
April 1

Talk **Challenges and Recent Developments in Analytical and Numerical Tools for Acoustic-Flow Coupling and Propagation**
Speaker: Prof. Michaël Bauerheim (ISAE-Supaéro)
Organization: Focus Group Data-driven Dynamical Systems Analysis in Fluid Mechanics

May 10 Speakers' Series on "New Frontiers in Battery Science and Technology" 2019:
**Determination of Parameters for Physics-Based Models of Li-Ion Batteries**
Speaker: Dr. Charles Delacourt (Université de Picardie Jules Verne)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

May 15 Inaugural Lecture **Safe, High-Performance Real-Time Computing for Cyber-Physical Systems**
Speaker: Prof. Marco Caccamo | Alexander von Humboldt Professor

May 23–24 **TUM-IAS General Assembly 2019**


June 4 Talk **Laser Doppler Vibrometry Measurement Techniques in Building Acoustics: A step Towards an Improved Reproducibility at Low Frequencies?**
Speaker: Prof. Bert Roozen | TUM-IAS Visiting Fellow

June 6 Festive Lecture "Single-Particle Cyro-EM: Visualization of Biological Molecules in their Native States" by **Nobel Prize Winner and TUM-Alumnus** Prof. Joachim Frank in the Course of his Award of the TUM Distinguished Affiliated Professorship
Organization: TUM Department of Chemistry and TUM-IAS

June 7 Tutorial **Structural Intensity**
Speaker: Prof. Bert Roozen | TUM-IAS Visiting Fellow

June 25 — Workshop **Neuro@TUM**
Organization: Prof. Thomas Misgeld | Alumnus Hans Fischer Tenure Track Fellow, Prof. Jakob Macke (Professorship for Computational Neuroengineering, TUM), Prof. Ilona Grunwald Kadow (Professorship of Neuronal Control of Metabolism, TUM)

July 8–11 — **Meeting of the international subgroup of the 3rd UBIAS Intercontinental Academia (ICA)** on Laws: Rigidity and Dynamics

July 15–16 — **Munich Workshop on Coding and Cryptography 2019**
Organization: Prof. Antonia Wachter-Zeh | Rudolf Mößbauer Tenure Track Professor, Prof. Camilla Hollanti | Hans Fischer Fellow, Prof. Eitan Yaakobi | Hans Fischer Fellow

July 15 — Talk On **Mitigating Congestion in High Performance Networks**
Speaker: Prof. Abhinav Bhatele | TUM-IAS Visiting Fellow

July 19 — Speakers' Series on "New Frontiers in Battery Science and Technology" 2019:
**Beyond Dendrites, Cycling Li-Metal Across Garnet at High Current Densities**
Speaker: Prof. Eric D. Wachsman (University of Maryland)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

July 22 — **TUM-IAS Summer Faculty Day 2019**



July 26 — Speakers' Series on "New Frontiers in Battery Science and Technology" 2019:
**Computational Discovery of Materials for Energy Conversion and Storage from Transport Properties of Ions, Electrons and Phonons**
Speaker: Prof. Boris Kozinsky (Harvard University)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

August 13 — Talk **Designing More Effective Remote Presence Systems for Human Connection and Exploration**
Speaker: Prof. Leila Takayama | Hans Fischer Fellow

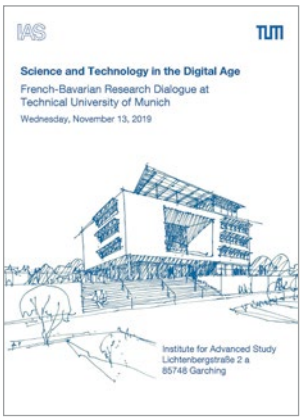
September 6 — Speakers' Series on „New Frontiers in Battery Science and Technology" 2019:
**From Graphene to Graphene-Enabled Batteries for EV Application: A 17-Year Journey**
Speaker: Prof. Bor Z. Jang (Global Graphene Group)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

October 22
Talk **Reversible and Irreversible Covalent Probes: From Serendipity to Clinical Trials**
Speaker: Prof. Jack Taunton | TUM-IAS Visiting Fellow

October 28–29
**Focal Period Workshop on Hot Carrier Dynamics in Advanced Concept Solar Cells**
Organization: PD Dr. Gregor Koblmüller (Walter Schottky Institute, TUM), Prof. Jonathan J. Finley (Walter Schottky Institute, TUM), Prof. Stephen Goodnick | Alumnus Hans Fischer Senior Fellow

November 8
Speakers' Series on "New Frontiers in Battery Science and Technology" 2019: **Development of High-Capacity, Manganese-Rich, Lithium-Ion Cells**
Speaker: Dr. Jason R. Croy (Argonne National Laboratory)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

November 13
**French-Bavarian Research Dialogue at TUM: Science and Technology in the Digital Age**
Organization: TUM and TUM-IAS




December 13
Speakers' Series on "New Frontiers in Battery Science and Technology" 2019: **From Atomistic Models to High-Precision Charge Counting: Reading Tales Told at Tabs and How to Convert Them Into Pounds**
Speaker: Prof. Harry Hoster (Lancaster University)
Organization: Dr. Filippo Maglia | Rudolf Diesel Industry Fellow

December 17–18
International Workshop on **Built Environment Digital Twinning**
Organization: Dr. Ioannis Brilakis | Hans Fischer Senior Fellow, Prof. André Borrmann (Chair of Computational Modeling and Simulation, TUM)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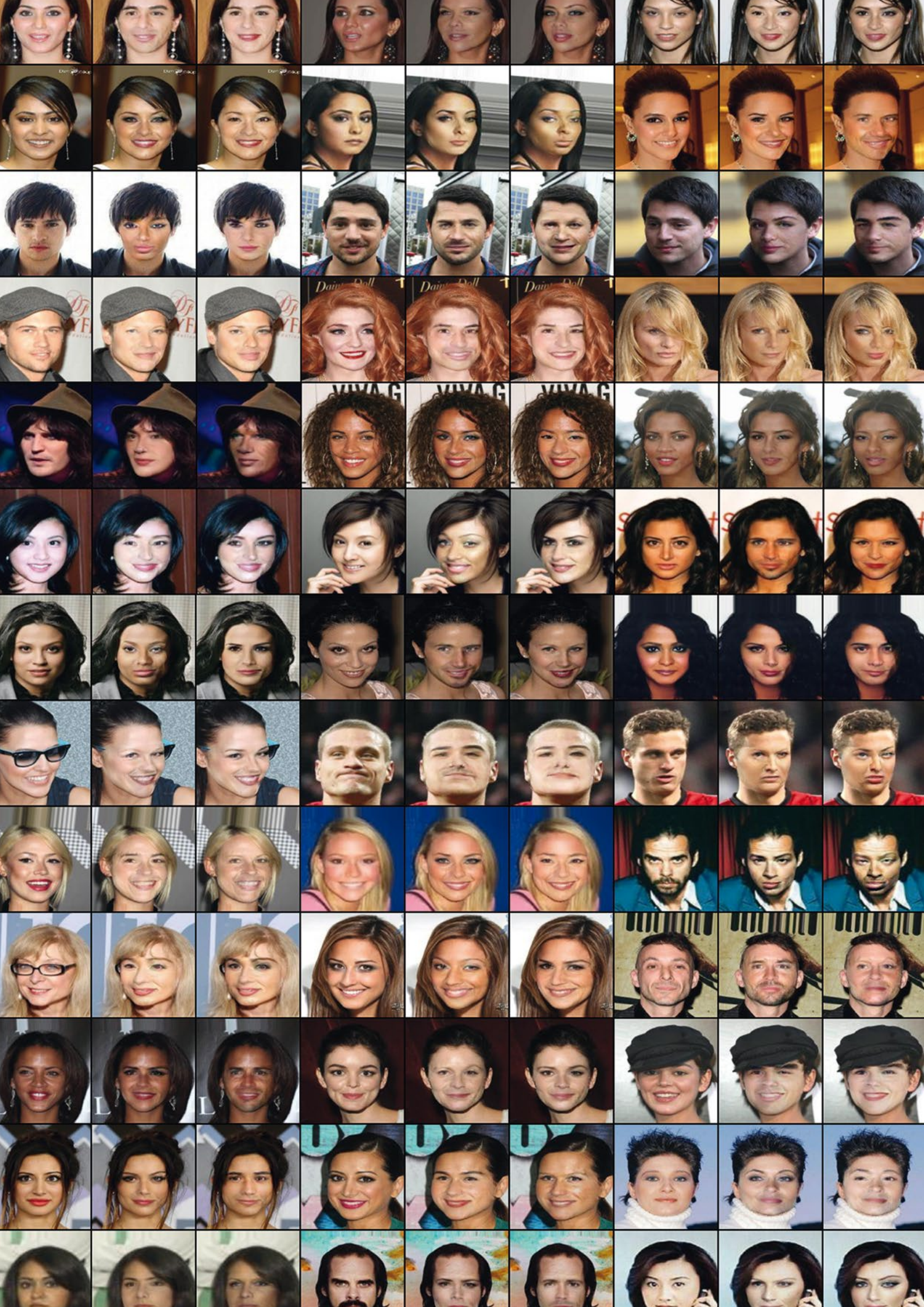
# In Focus

Computer Vision and Machine Learning
Visual Computing
Dynamic Vision and Learning



# Computer Vision and Machine Learning
# Visual Computing
# Dynamic Vision and Learning



At the increasingly open border between research enabling computers to see and advances in teaching them to learn, things are hopping. Interdisciplinary research is progressing rapidly, with wide-ranging implications for technology, business, and society. And a lot of the action is taking place right here.

*As Rudolf Mößbauer Tenure Track Professors, Laura Leal-Taixé (Dynamic Vision and Learning Group) and Matthias Nießner (Visual Computing Lab) were both recruited through a TUM-IAS program designed to establish novel and often interdisciplinary fields at TUM. Daniel Cremers heads the Chair of Computer Vision and Artificial Intelligence in the TUM Informatics Department and currently is a TUM-IAS Carl von Linde Senior Fellow. Nießner is the host of the TUM-IAS Focus Group on Visual Computing, with Hans Fischer Senior Fellow Leonidas Guibas of Stanford University and Hans Fischer Fellow Angel X. Chang of Simon Fraser University. Cremers hosts the Focus Group on Computer Vision and Machine Learning, in collaboration with Rudolf Diesel Industry Fellow Michael Bronstein, whose current affiliations are with Imperial College London and Twitter, which acquired his startup Fabula AI in 2019.*

*In March 2020, the TUM-IAS conducted interviews with these six researchers about their trailblazing work and the framework for collaborative exploration that the Institute offers them. Their answers have been edited for clarity and length.*

Daniel Cremers

Michael Bronstein

» ... the core question revolves around how to expand the success of machine learning and so-called deep networks to other application domains beyond standard images.«

Q: Clearly, all six of you have a lot in common in terms of research interests. What are the most important common threads, and what kinds of differences in topics or emphases distinguish one group from the other?

Cremers: For me, the core question revolves around how to expand the success of machine learning and so-called deep networks to other application domains beyond standard images. One of the core ingredients that Laura and I and Michael in particular are working on is so-called graph neural networks. One of the most important enabling advances in the last couple of years, which has enabled many things not just in vision but well beyond computer vision, is the advent of so-called deep neural networks. They were actually developed for vision, back in 2012, to address one of the biggest quests in computer vision, a quest that one of our colleagues set out to solve – it's a quest called the ImageNet Challenge. One of my friends and colleagues at Stanford, Fei Fei Li, compiled with her students a data set of millions of images, everyday-type photographs, where every photograph is classified as being an image of an airplane, an image of a car, or a cat, or some other object. The challenge was to devise a machine that tells us what's in each image. And to summarize a long story, with the advent of deep networks, we were able not only to reach human-level performance, but even to outperform the average human on this challenge.

This was a big breakthrough, and I don't think it's really been acknowledged much in the public. When people hear about artificial intelligence, they generally think about chess-playing computers. And the truth is, for a machine to play chess, that's not a challenge. Humans on the other hand did not evolve to play chess, but they did evolve to recognize objects and images. To beat the human on a task that humans are arguably designed to solve was a much more significant breakthrough. And from computer vision, these deep networks have since swept into virtually all areas of science and data analysis. The question is how to go beyond standard image analysis. That means for example how to deploy it for dynamic data, as Laura is doing with videos.

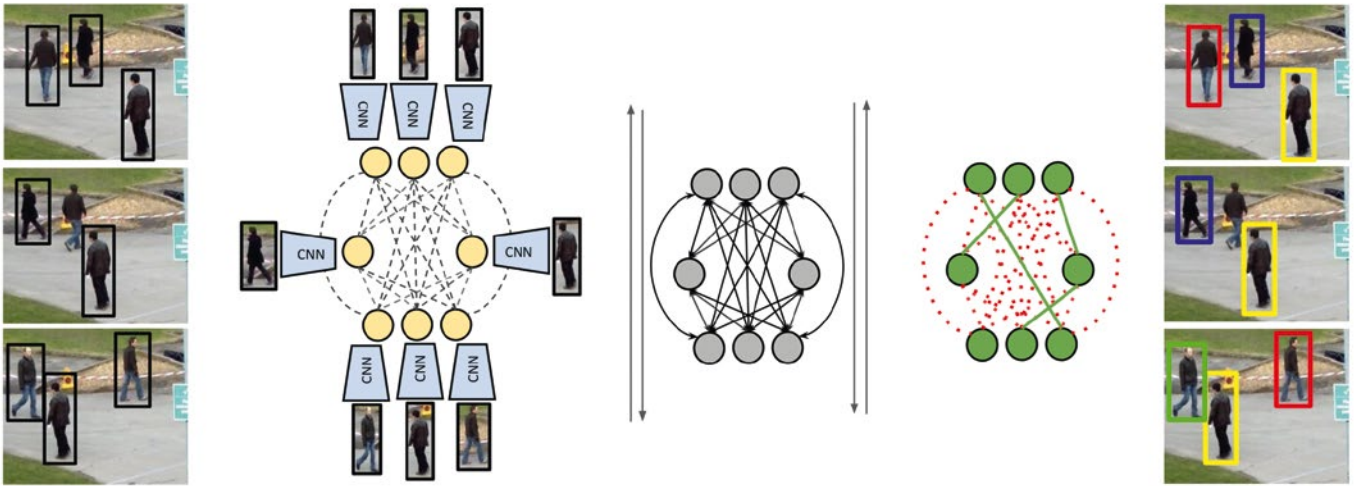
Laura Leal-Taixé

Matthias Nießner

Leonidas Guibas

Angel X. Chang

Leal-Taixé: The interest of our group is dynamic vision and learning. The key word there is dynamic. We are interested not only in analyzing images, but in actually analyzing videos. A very strong component is analyzing motion in a scene. In particular, we look a lot at human motion. For example, for an autonomous car, you want to know where are the pedestrians around the car, where are they going to go in, let's say, the next ten seconds. So there's a lot of trajectory prediction and tracking. We want to allow the robots or autonomous cars to have a sense of what is around them and a sense of what is moving around them and how it is moving. We focus on humans because their motion is very interesting. It's hard to predict. The motion of a car is constrained by the lanes, for example, and the rigidity of the car itself, while the motion of a pedestrian is quite random sometimes. It's hard to predict where pedestrians want to go, and they might suddenly change where they want to go and turn around. All of these things make the problem very interesting from a scientific point of view, because we're interested in exploiting not only the motion of each person individually, but also the relationship of motion between the pedestrians, for example, how they avoid each other when they cross paths, as well as the motion of pedestrians with respect to cars. So when you reach a crossing, you typically stop a little bit before crossing, you look around, and these are interactions that can be modeled with such a neural network.




a) Input

b) Graph Construction + Feature Encoding

c) Neural Message Passing

d) Edge Classification

e) Output

Michael Bronstein (left) with the team of Fabula AI at Twitter office in London, Photo: Stacey Conti.

Cremers: The so-called graph neural networks operate not just on Euclidean data – images are typically Euclidean, that is, they have planar structures – but also on graph structures that are non-Euclidean.

Q: Does this help to explain how it could be that your research touches on applications like protein interactions, food design, fake news, and particle physics as well as enabling computers to better understand, and also better synthesize, moving pictures?

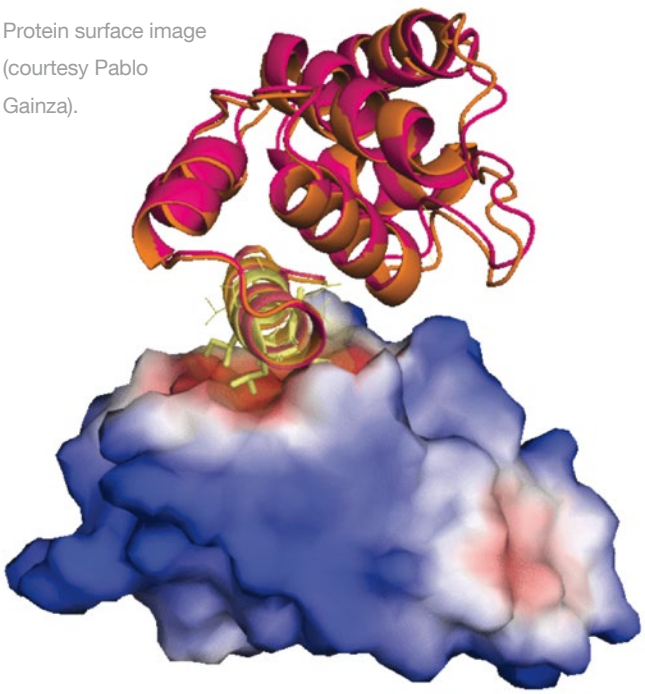
Bronstein: What they have in common is this new class of machine learning methods that we call geometric deep learning. Graph neural networks, or graphic representation learning, is a particular example. Basically these methods try to extend deep neural networks to non-Euclidean structured data: graphs, manifolds, point clouds. We want to exploit the geometric structure of the data in a mathematically principled way. We try to build deep neural networks that allow us to learn on data that has these underlying structures, of a graph or a manifold or a point cloud.

In all the examples you mention, we have data that lives on a graph, and the graph is part of the data. In the case of fake news, we have a social network and a propagation graph representing how news spreads in time. In the case of foods, we have a graph that represents protein-protein interactions. There are about 20,000 proteins in our body; their binding to each other is responsible for multiple biochemical processes. Simplistically speaking, sometimes these processes break down and we get sick. We then take a drug, which is designed to bind to one or multiple proteins and fix these broken processes. We can represent the effect of a drug as a signal on the protein-protein interaction graph and use graph neural networks for "drug repositioning" – finding molecules that can act, for example, as oncological drugs.

Let's say, we take examples of drugs that are approved for use against certain types of cancer, and train a classifier that predicts oncological "drug-likeness" from their protein binding signals. We can then use this classifier to screen other molecules. Take for example food: Some fruits and vegetables contain compounds that belong to the same chemical classes as some chemotherapeutic drugs. By using our drug-likeness classifier, we can identify foods rich with molecules that are similar to oncological drugs, though in much lower concentrations. We call them "hyperfoods." Unsurprisingly, all the boring foods like cabbage or celery or green tea are hyperfoods.

The thing about these methods is that it's completely data-driven. So if tomorrow you want to find, for example, potential drug-like candidates that allow you to beat a particular kind of cancer, or potential antiviral drugs to fight the new coronavirus, we could apply the same process.

Protein surface image (courtesy Pablo Gainza).




TEDx Talk by Michael Bronstein in Lugano, 2019.

Q: To what extent are the neural networks you're talking about implemented in software, and to what extent in hardware?

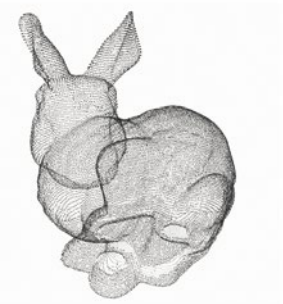
Cremers: Initially they're in software. Typically the hardware you need to run them is so-called GPUs. Laura and I spend a lot of time discussing how much more GPU time we need to buy for our team to continue working. We're spending a significant amount of funding on that kind of hardware. There are efforts to develop hardware implementations of deep networks, different ones that are, say, more power-efficient. But this is not really our expertise. We are more on the algorithmic and software side.

Q: Matthias, Leo, and Angel, how would you describe the research topics, approaches, and potential applications that best define your Focus Group?

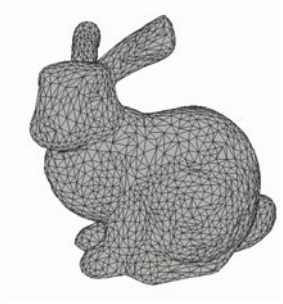
Nießner: We've been working on bilateral projects for a very long time actually, at least five or six years now. This is how various topics are emerging. One commonality is the underlying 3D understanding of things. From a geometric perspective, or from a language perspective with Angel. My specific angle to it is more the visualization part. I want to recreate photorealistic images. Eventually I would like to create holograms of 3D worlds and make sure we use all the content available in virtual environments. To synthesize photorealistic humans, faces, and environments, that's already being done, and by better understanding the environment you can get better synthesis. With Leo we're asking: Can we first figure out the object itself, do we know where objects are, and can we get the geometries of these objects? And then, can we use this information to synthesize better results? All of these areas come together.

From a methodology standpoint, all of our efforts are anchored in 3D learning techniques and 3D computer vision, with a lot of current progress in neural networks focused specifically on 3D data. We all argue that the world is not 2D, right? If you want to understand what things do in a 3D environment, you want to directly learn in 3D. There are good examples for that. A human has two eyes to see things in stereo. We have depth perception, we learn spatial correlations, we learn how to interact in 3D. We know how to describe and to touch things in 3D. And then we also know how to visualize things and imagine things in 3D.

Guibas: Three-dimensional understanding poses many challenges when it comes to machine learning, because 3D data tends to be different. Two-dimensional data is regular pixel grids, all with the same format. But in 3D there are many different representations that have existed for decades and serve different communities – point clouds or meshes, for example – and all of them tend to be irregular. A lot of the traditional machine learning techniques, especially convolutional networks, require regularity to be able to share coefficients and other optimizations. So if you have this irregular data, you have to do things differently. Part of our work has been to address this problem, how to represent 3D and how to process it even though it is not regular.



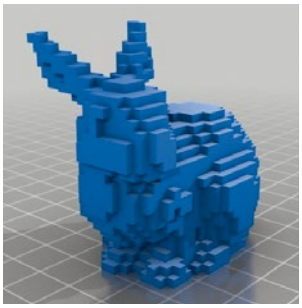
Point-Cloud



Surface-Mesh

Chang: I come from a natural language processing background, so what I'm interested in is how people talk about 3D things, using language. And so what can be very, very interesting is the connection between language and 3D representations. Recently there have been lots of methods where you can basically, using neural networks, take language and then take images and put them into a shared representation. And then through that we can connect language and other modalities. So with Dave Chen, a doctoral candidate in Matthias's team, we are working on being able to localize objects in 3D – where someone might say, for instance, "the chair that is in the corner of the room," and then be able to actually identify, in a 3D bounding box, what the person is referring to.

Guibas: With Matthias, I share many interests in computer vision, and in fact inspired by Angel I have also started dabbling a bit in language in relation to geometry. My own background is much more in geometric algorithms and geometry processing, the more classical field before the advent of deep learning. So I'm dealing with both the design of geometric algorithms and also suitable representations for 3D geometry, including how to take noisy data and try to improve it in various ways. We do research in classic areas like image processing, where one has noisy images and tries to get rid of the noise, and also in geometry processing where one has noise and tries to improve the geometry. But together we can try to do something that didn't exist before, such as in texture processing, being able to take images that are living on a manifold, images living on meshes, and capture them better and understand them better. That's one interesting direction we're pursuing in collaboration with Matthias.



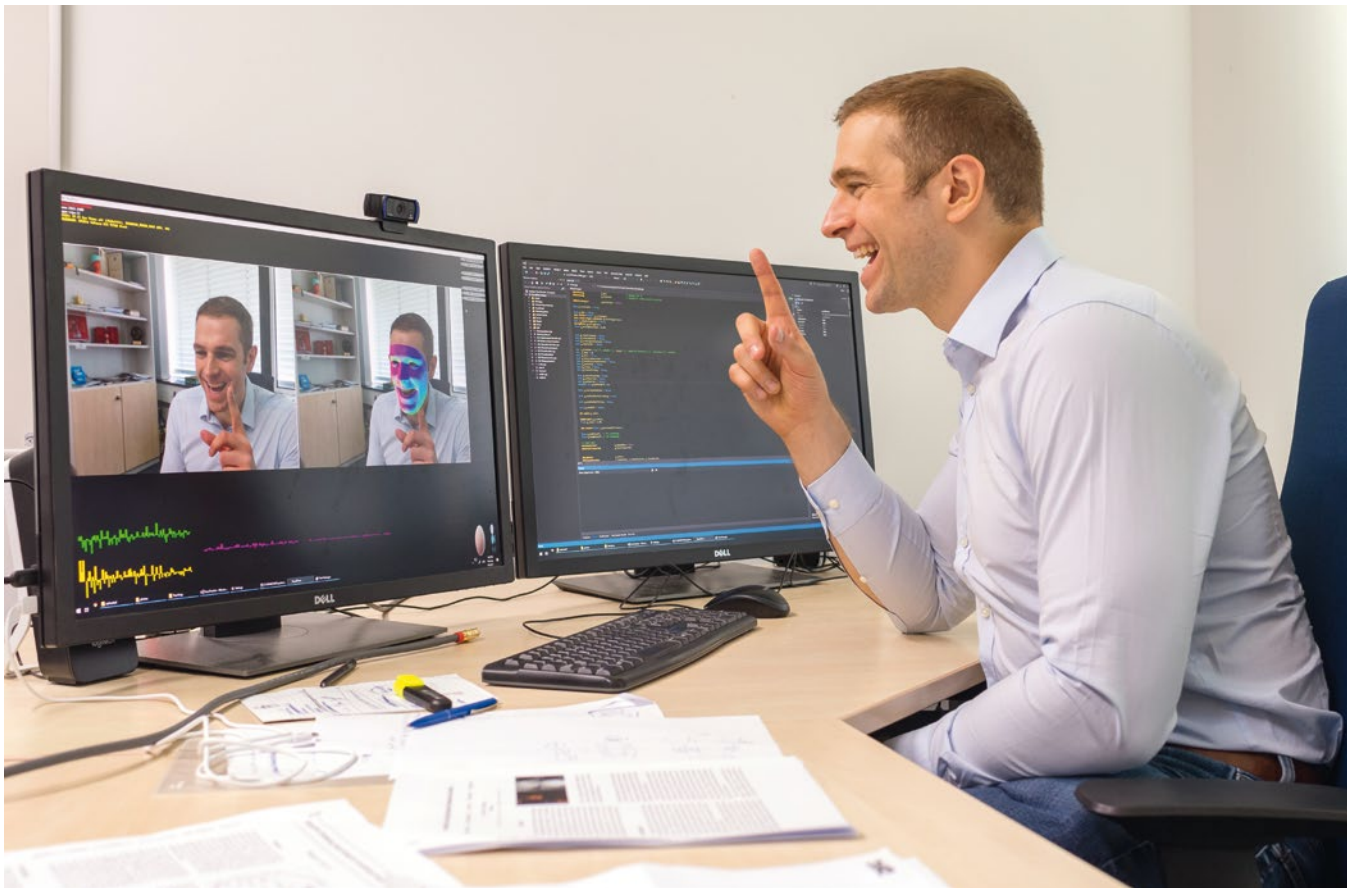
Volumetric

Multi-View Images

On my side, I have a bit more emphasis on the content creation side, that is, being able to not just capture some object that's out there in the world, but to have interesting tools for creating new geometry, new objects essentially.

Q: Would you call that 3D synthesis?

Guibas: Synthesis, indeed. And in fact these come together in another collaboration with Matthias where the goal is to replace extant scanned geometry with a CAD model that has been adapted to the scan, so that you can have a clean model that represents an object in the world. We've started a project that focuses on understanding scenes, with the purpose of acting on them. Not just what is there, but what could be there, how things could be different, how can I change them, so that we make it possible for an effect to happen in space. How do I close the door? How do I open the drawer? How do I move my laptop from this table to that counter? The focus on understanding not just what is but what could be is a central part of this effort.

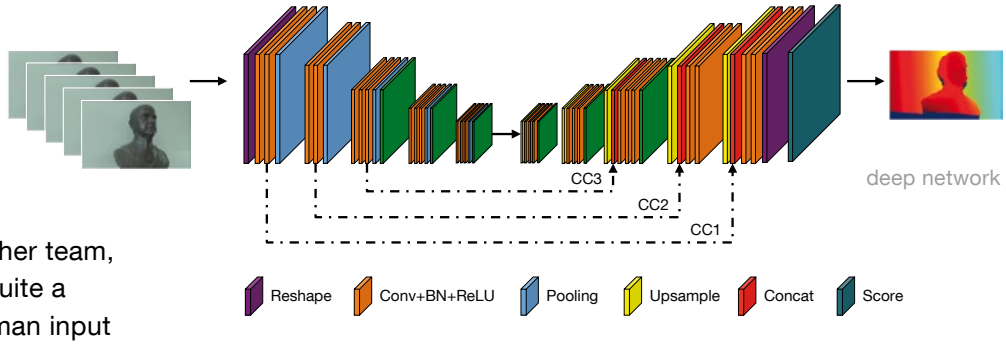


So there are two specific themes of research we could highlight. One would be trying to replace dirty, noisy scanned objects with clean-cut models. Another is to be able to acquire high-quality textures of objects and to be able to use that also to understand the scene.

Q: What are the hurdles to achieving those two things?

Nießner: You're never going to get perfect information. A camera has noise, and you only see things from the current perspective. Humans are pretty good at recognizing things. Computers are pretty bad at recognizing things if they're not the same. Just comparing two numbers is a very difficult problem. Two integer numbers, it's very easy, 5 equals 5, right? But if you have two floating point numbers, like 5.00001 and 5.00002, they're two different numbers, and the computer makes only a binary decision there. And this expands to the whole machine learning field essentially. You have to learn features that make these comparisons easier. This counts for the recognition task, but it also counts for the task of making things look good. If I do a reconstruction, I want to have textures on top of it, and I want to make it appealing, and these things are very difficult for computers to do.

Guibas: Think about this problem of trying to replace a noisy scanned object with a CAD model. There are many, many, many objects in the real world. We don't have a CAD model of everything. You will never find the perfect CAD model. So then the question becomes, how do you adapt the CAD model to the actual data? This is quite tricky, because this adaptation has to be aware of the semantics of the object. Maybe there's a sedan parked on the side of the street. I have a similar sedan, but it's a little too short. I can't simply stretch it, because then the wheels will become ovals. I want to make the body longer, but the wheels should stay round. I have to understand the semantics of what's there. And I can only learn that when I understand many, many models together in a joint structure. There are many subtle problems in extracting this "wisdom of the collection."




Nießner: This brings up another important theme: How do we teach machines these things that Leo just described? With Angel and her team, we have been working for quite a while on how to use the human input to teach the machine to think. How do we know that the sedan is this way, and another way, it's the same car. We do it indoors, we do it for furniture, tables and chairs and things like that. But eventually we have to annotate data, label data, and devise a user interface to do this very efficiently. Do we do this with images and 3D space and so on? How do we get the information from the humans to the machines, and the other way around? There are also projects between Angel and Leo, where they are for example adding the natural language descriptions.

Q: What are some of the strongest links between the groups?

Nießner: Laura and I are pretty much the two people organizing the curriculum in deep learning at TUM right now. Also, we started at more or less the same time, as professors, and our groups are relatively closely connected. Of course there are different topics. Laura is doing a lot of research on localization, video, tracking, and things like that. Daniel has a lot of shared interests with Leo on the geometry processing side. Everybody has a few specialties, but I would say locally we are all very connected. We are all part of an artificial intelligence and vision cluster, as well as a computer vision cluster.

Cremers: To give you another perspective on how important deep networks are becoming, when Laura started teaching the first classes on deep networks here at TUM, the class was a hundred or so people. At this point, after just a few semesters, she has more than a thousand students in her classes on deep networks, master's level classes. We don't actually know where this is heading, but it shows you, even the students sense this need for deep networks that the world has, and Laura is at the center of it all.

Q: This kind of success can be a bit of a burden.

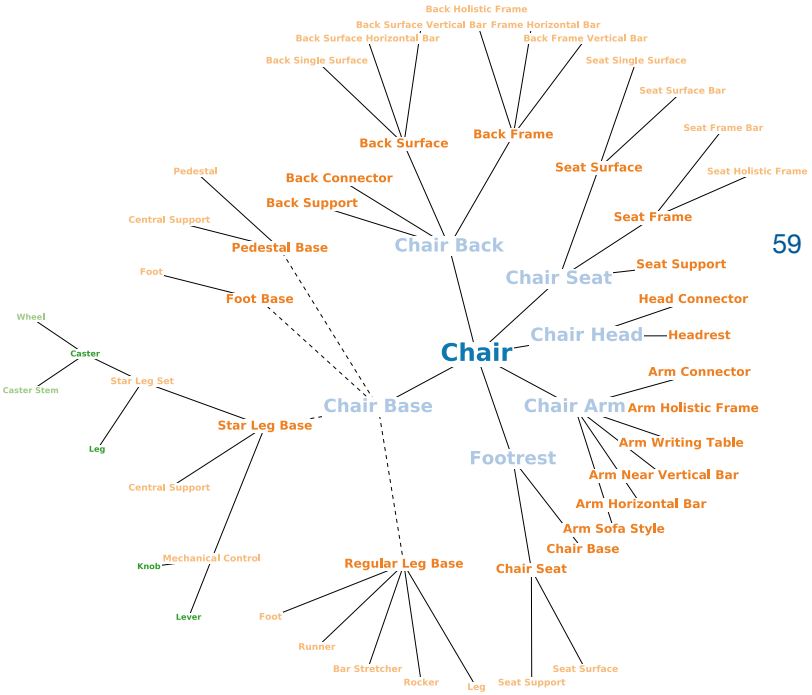
Leal-Taixé: It's not easy. It's an issue, how to balance research and teaching.

Q: I don't suppose you could employ an AI program to take over some of your duties.

Leal-Taixé: That's not a bad idea.

Guibas: I have had many connections with Michael over the years, even before our association with the TUM-IAS. For example, in 2011 we published a paper called "Shape Google" about shape search, how to find similar shapes. And last year we had a collaboration on how to build robust nets against adversarial attacks, using several kinds of graph convolutions. So our associations and interactions form a connected graph, in multiple ways and with many edges.

Bronstein: I spent some time in Leo's group when I was at Stanford after my PhD, more than ten years ago now, and have collaborated with him and his students, many of whom are faculty members in their turn now. Our most recent collaboration was on using graph neural networks to make convolutional neural networks – the type of deep learning that is used in self-driving cars – more robust to adversarial attacks. It is known, for example, that making a few changes to the traffic signs can confuse the computer vision system that recognizes these signs. I think the actual threat this poses may be a bit exaggerated, but it does showcase potential vulnerabilities of convolutional neural networks, a particularly popular type of deep learning used in computer vision. Last year we published a finding that we can regularize convolutional neural networks with graph-based approaches and make them significantly more robust to these kinds of attacks.




Chair neighborhood

Q: Michael and Matthias, you both have received a lot of attention – from high-profile news coverage to Twitter's acquisition of the startup Fabula AI – regarding the detection of "fakes" of one kind or another in social media. But your targets and approaches seem completely different. What's the best way to clarify this?

Nießner: Creating synthetic imagery has been a topic for decades. In computer graphics, creating realistic – photorealistic – imagery from synthetic content is a thing that people have been doing for a long time. Nothing new. It's just gotten easier. And a lot of what people refer to as "deep fakes" is just face-swapping, where you can take some face and copy that to a different face. What people don't realize is that most of the time in fact you're actually getting a hybrid between two people; for example you're getting a mixture between Trump and Putin out of it. So I ask why do they think this is a problem. And they're telling me, well, you're making Trump and Putin "be" each other. And I say no no, you're creating a person, it's somebody who doesn't exist. That person cannot jeopardize democracy, because he doesn't exist. It's not a person who can do any harm. The reality is that the deep fake is not really a problem at this point. Most of it is actually pornography or other sketchy areas, not fake news.

Still, you want to provide tools on the detection side, to reliably identify whether this is a real person or a fake. We have a major project, FaceForensics – currently the leading project in the field – that not only covers deep fakes but also a larger variety of facial manipulations, that for the most part can reliably detect these changes and edits. At the moment detection is much easier than generation. If you know the method, you only need to know that a few pixels are wrong, and then you can detect it. You need to know what you're looking for. You need to know the methods, but then it's easy.

Q: And Michael, do I understand correctly that you are detecting fake news entirely without regard to the content? You train neural networks to look at its propagation characteristics?

Bronstein: That's a special thing about the technology we have developed at Fabula. We have shown that graph propagation features contain important information that allows us to classify whether a piece of news spreading on the social network is fake or not fake. In many cases you really cannot use content, especially when it is language-dependent. We build deep neural networks that allow us to learn on data that has these underlying geometric structures. In the case of graphs, we can apply deep learning to social networks. On Twitter or Facebook, you post something and people interact with this content; they like it, they view it, they repeat or repost it, and then you get a kind of cascade. And by looking at the way in which this information spreads, we have been able to train a classifier – a graph neural network – that allows us to predict with high accuracy, with just a few hours of propagation of a piece of content, whether it was true or fake. That was the technology that we developed into the startup Fabula AI, which was acquired by Twitter last year.

Q: Of all the various ways your research might have an impact on society, what other areas do you think it's most important to highlight?

Leal-Taixé: From my side, I think that if you want to have a society where robots are interacting with people, whether it's robots running around in your home or autonomous cars, these robots need to have a really strong perception. And this is essentially what we are working for. So in the end, giving such a human type of perception to robots is, I think, super challenging, but at the same time at the core of robotic intelligence, and very much a need we can address.

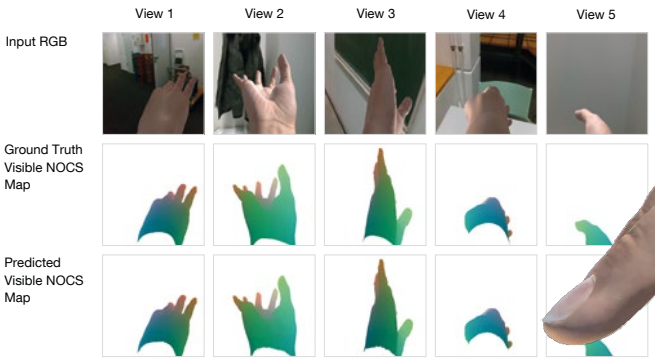
» I think that if you want to have a society where robots are interacting with people, whether it's robots running around in your home or autonomous cars, these robots need to have a really strong perception. «

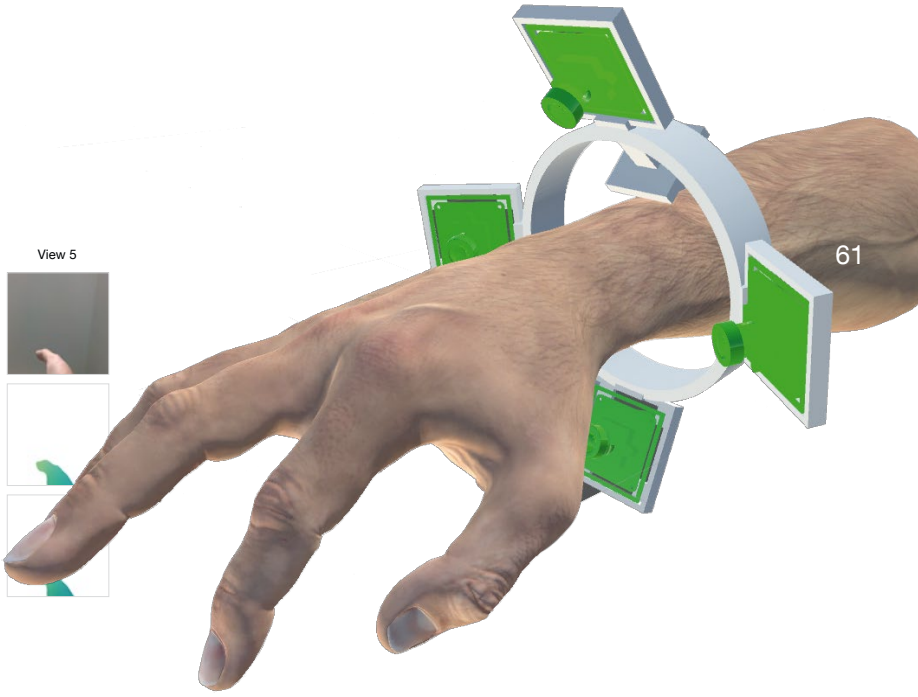
Guibas: There are several different directions in which the work can have an impact. Understanding the 3D environment can be useful not just for robots, like self-driving cars or home robots, but it can be useful to humans, to offer assistance to humans. Maybe there's an elderly person who has difficulty carrying out some task. If a system can understand the environment, understand what the person is doing, and infer the intent, it can offer assistance. And that can mean either providing information or creating visual content that fits that person's environment and makes it clear how they should proceed to complete the task. That's one direction. Providing instruction, education, and assistance, and creating these virtual actions that help people. Another direction is entertainment. Once you can start to freely pull content from the real world into the virtual and from the virtual back to the real, then you can create new experiences for people on top of the real world, or you can create new virtual experiences that use their own objects, their own world. I think both are interesting.

Chang: It's very important to understand that you need to come to it from the point of view of 3D, in the sense that there are these spatial relations that we use all the time: like top and bottom. Even if we're saying the stock market now is "tanking" or "cratering," this also has a geometric interpretation. A lot of these metaphors that we use are related, so I feel that fundamentally for us to have a deeper understanding from the natural language processing side, it's necessary for us to understand how it relates to the real world and to the geometry of things.

And if we can give a machine – whether it's a robot or just something in the cloud – a better understanding of the physical world that we exist in and how we talk about it, then it is better equipped to meet some real-world need. We may not be so far away from being able to tell a robot, "Bring me the chair from the living room," or "Get me my coffee." Or, once we have this space where we are virtually interacting with each other, if I think of something I need that's not currently in the room, I can ask for it. Or if you want, maybe a virtual assistant or agent can predict what we're going to need before we ever ask for it, just by listening to our conversation.

Nießner: I agree that robotics is very much a consumer of the research that we're doing, self-driving cars that can get you from A to B. But I think the ultimate goal will be virtual environments, so you don't have to go from A to B any more. Right now everything is shut down because of the coronavirus, and there are limitations on how we can communicate. A longer-term question is how do we work in the future, how do we socially interact in the future, how do we communicate in the future. And this goes from entertainment to workspaces alike. There will be language barriers. How can we translate languages automatically? How can we integrate natural language processing into it? And the video can be adapted toward the specific target, whether that means telemedicine or repairing a machine. You may not have all the expertise where you need it, but you can remotely communicate. Having this combination of the real world and a virtual world requires, first, a fundamental understanding of



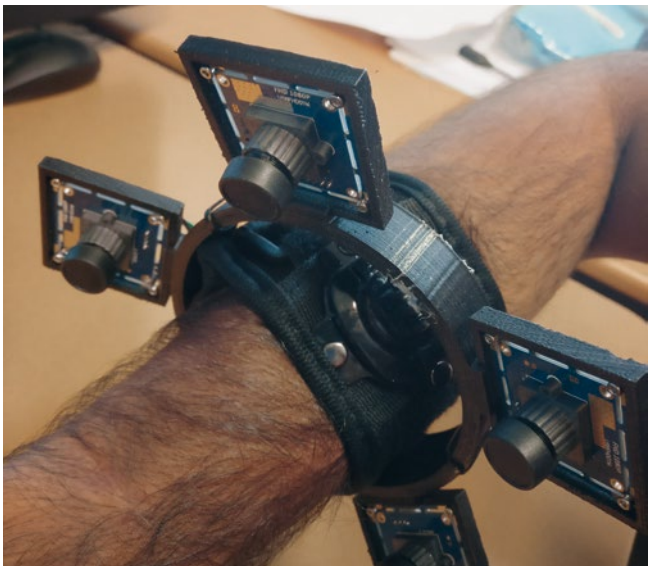
the real world; and the second thing you want is to be able to connect people in different parts of the world in virtual environments – a combined, mixed reality.

Cremers: One way what we develop becomes really of use to society, and gets used, is through technology transfer, creating startups and bringing things into the market. I've been involved personally in a number of startups, most recently one called Artisense, where we are developing technologies for self-driving cars, autonomous cars, and driver assistance. These are technologies where we leverage cameras to do 3D perception. For me, Michael Bronstein is a great inspiration. He just keeps creating one startup after the other, and he addresses lots of open challenges in society. It seems like he's almost driven to solve important problems for humanity, from fake news detection to predicting protein structure and function, or even trying to identify cures for Covid-19 by using intelligent algorithms. So it's not only that he has these ideas, but he actually brings them to life and makes them happen. This is one way to make sure that what we do actually affects and helps humanity.

You can solve lots of societally relevant problems with this power of the deep networks. In this context, we are in the process of setting up a big institute called the Munich Data Science Institute, and one of the ambitions we have is to bring the success of machine learning, and in particular deep networks, to all areas of data analysis: physics, chemistry, materials sciences, earth observation. There are so many areas that will profit enormously from this kind of transfer of knowledge.

Q: How would you describe the role the TUM-IAS plays in facilitating and enhancing your collaborative research?

Nießner: First, you basically want to get people together who have some shared interests but also add different expertise. And in our case that's exactly what's happening. Angel is a very good example. At TUM right now, we don't have any natural language processing expertise, so without her, we couldn't do research in that area. Same thing goes for Leo's expertise. He's probably the top expert in 3D geometry around the whole globe. Without the TUM-IAS, we would not be able to do these kinds of collaborations. The second part is help with the funding. It enables us to co-advise doctoral candidates.



Guibas: There are a lot of really excellent people at TUM, and it's always a pleasure to visit and spend time and interact with them. And as Matthias said, I think a lot of the real action happens with the PhD candidates we co-advise and engage with in joint projects. Ultimately this builds more permanent bonds, at a more fundamental level.

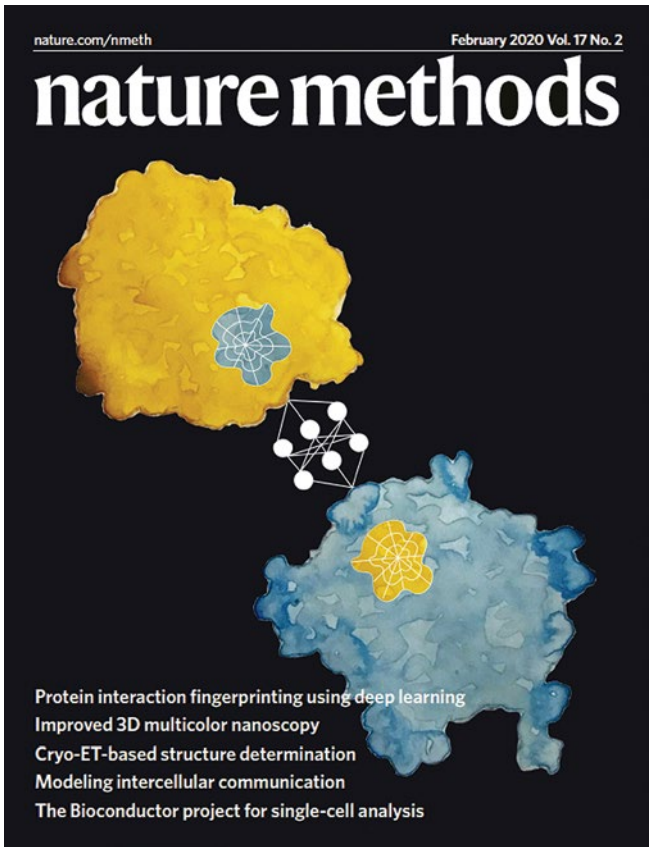
Chang: I just want to agree that it's a wonderful opportunity. I've also worked with Matthias's and Leo's PhD candidates quite a bit. And the funding for travel, which we hope will eventually be possible again, gives students as well as professors a chance to spend significant time at their collaborators' home institution.

Leal-Taixé: I would add that, as a scientific hub, the TUM-IAS provides an interesting network. I've met many tenure track professors like myself who work in other fields and actually get super excited when I tell them what we can do with neural networks, because they are not really aware of these techniques. And now we have even started collaborations with their students to bring our knowledge to their problems. They can potentially be solved using deep learning, it's just that they don't know it. So it's exciting to work on these very different topics.

Q: For example?

Leal-Taixé: One is in astrophysics. It has to do with gravitational lensing. Another project is concerned with mapping brain signals to images – essentially trying to predict the behavior of neurons when you show a subject a very specific object or a very specific person. So apparently there are these conceptual neurons – for example, there could be a neuron that is dedicated to firing when a picture of Maradona appears on the screen. We want to help them find out how these neurons are formed.

Cremers: The great thing about the TUM-IAS is that it is a platform that brings together talented people who

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share common interests and offers a forum to exchange ideas, to discuss, to do workshops together, to collaborate together. The TUM-IAS provides support for organizing workshops, for bringing top people from all over the world to Munich. A perfect example was the TUM-IAS Workshop on Machine Learning for 3D Understanding in the summer of 2018.

Bronstein: Leo was one of the organizers of the workshop, together with me and Daniel, and Lourdes Agapito from University College London, who is also the co-founder of the startup company Synthesia together with Matthias. It's a small community.

Everyone knows each other. We're connected in many ways. We wanted to break from our usual circle, by bringing together not only people from geometry, machine learning, computer vision, and graphics, but also from other communities like genetics and protein science. This is not something you would usually see in a machine learning or computer vision conference.

For example, we invited three protein experts, one from Harvard doing protein folding and two from EPFL doing protein engineering. They publish their work in biological journals and normally do not intersect with our community. One direct result from this meeting was our paper on designing synthetic proteins.

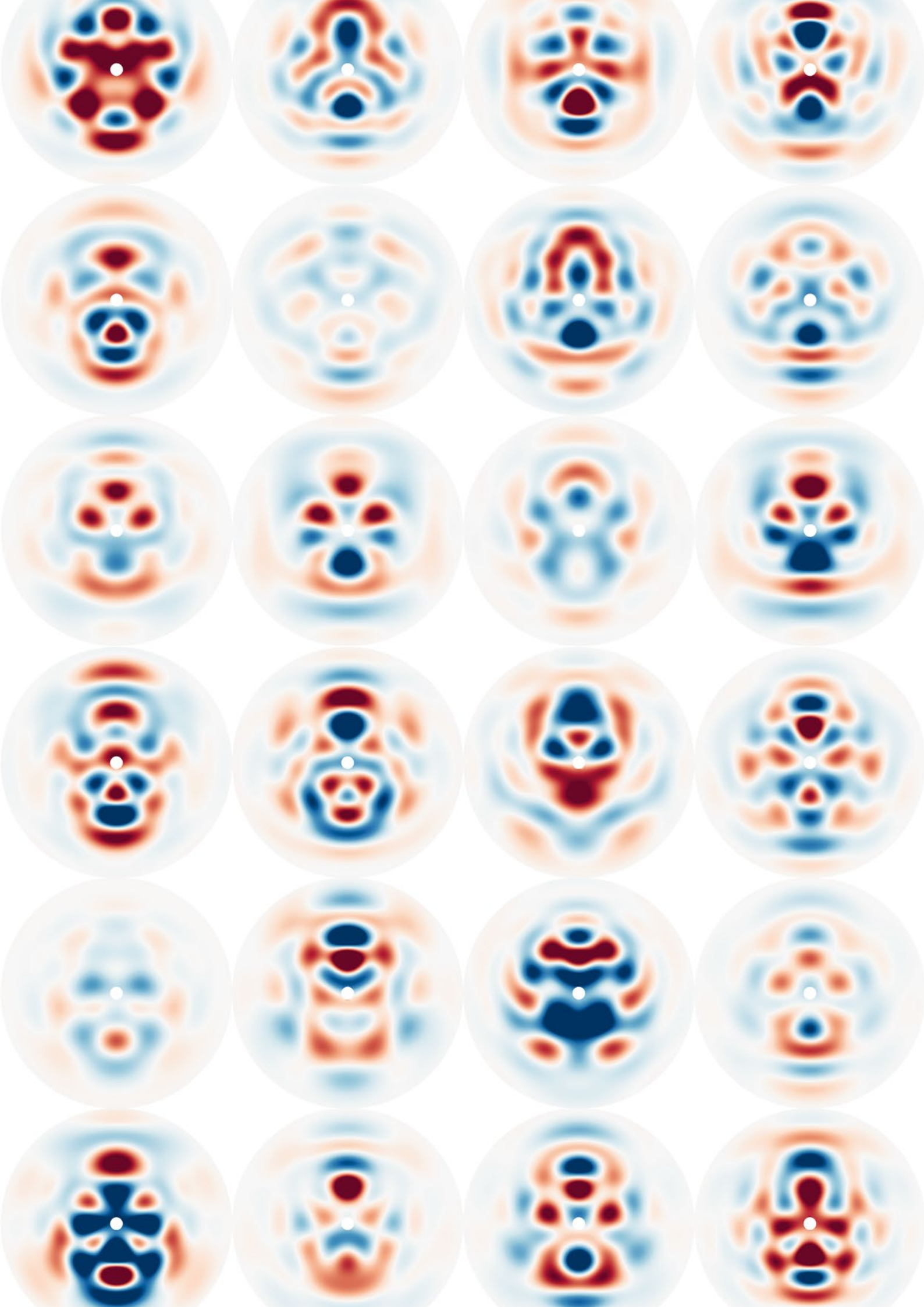
The problems in protein science are very geometric. You can think of protein molecules as surfaces that have to fit together like pieces of a 3D puzzle. It is somewhat more complicated than simple geometric complementarity, because there are electrostatic forces and chemical phenomena involved. There are multiple classical problems in protein science that can be addressed, or can be improved, when you think of them in geometric terms. One is protein folding: how a long one-dimensional chain of amino acids can fold into a complex 3D structure. Another is protein binding, basically how these proteins stick together. Understanding how proteins interact is fundamental to a lot of biological processes in every form of life that we currently know, and also crucial for the design of future drugs.

So as a result of this collaboration, we had a paper that appeared in February 2020 on the cover of *Nature Methods*, on the use of geometric deep learning to gain insight into protein interactions. It is the first paper in such a high-profile journal that I am aware of to have "geometric deep learning" in its title.

Q: And that can be traced straight back to the conference you held at the TUM-IAS?

Bronstein: That is correct.

Scientific Reports

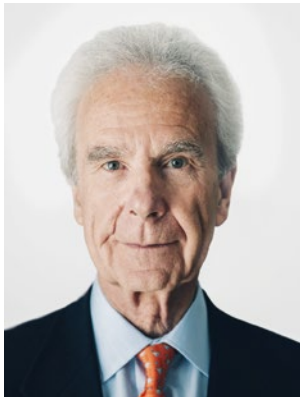


# Scientific Reports

# Focus Group **Computational Transport Oncophysics**

Prof. Bernhard Schrefler (University of Padova) | Hans Fischer Senior Fellow funded by TÜV Süd Foundation
Johannes Kremheller (TUM) | Doctoral Candidate

Scientific Reports



Bernhard Schrefler

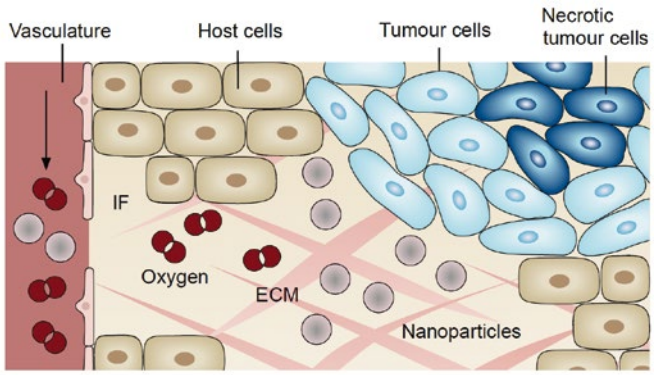
Host
Prof. Wolfgang Wall
Computational Mechanics, TUM

## Toward *in silico* prediction of tumor growth and cancer treatment

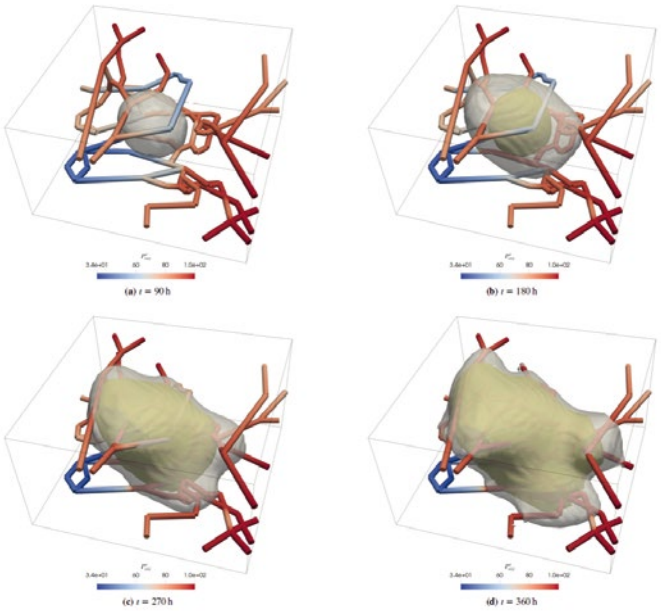
Capturing the complexity of cancer through mathematical models requires cutting-edge numerical algorithms. In the Focus Group Computational Transport Oncophysics, we have considerably advanced these methods and combined them into a holistic finite element framework developed at the Institute for Computational Mechanics. Building on one of the most sophisticated tumor growth models to date, developed by Bernhard Schrefler and his group [1], we have enhanced its applicability as a predictive tool for more clinically relevant scenarios. While the previous model only described the first avascular stage of tumor growth, we can now also incorporate the second vascular stage including angiogenesis (the formation of new blood vessels from the pre-existing vasculature). The so-called angiogenic switch from avascular to vascular growth is crucial for the tumor to become harmful. Hence, a sophisticated cancer model able to provide clinically relevant data has to take angiogenesis and vascular tumor growth into account.

Therefore, we have established a novel computational approach to facilitate the modeling of vascular tumor growth [2,3]. The pre-existing vasculature is taken into account as a one-dimensional inclusion and embedded into the three-dimensional tissue through a suitable coupling method, which allows for non-matching finite element meshes in 1D and 3D domains. The neovasculature, which is formed during angiogenesis, is represented in a homogenized way as a phase in our multiphase porous medium system. This splitting of models is motivated by the highly complex morphology, physiology, and flow patterns in the neovasculature, which are challenging and computationally expensive to resolve with a discrete, one-dimensional angiogenesis and blood flow model. The novel approach allows us to investigate blood vessel networks of arbitrary complexity as occurring *in vivo* (see also figure 2). Furthermore, our method enables us to predict blood flow and species transport in large tumor blood vessel networks of more than 100,000 individual blood vessel segments [4] obtained from *ex vivo* imaging. Sophisticated *in vivo* imaging techniques currently do not allow resolution of the structure and morphology of the smallest vessels, i.e., the capillary bed. This is where our hybrid embedded/homogenized treatment of the vasculature [3] could provide valuable insight. We can include the larger vessels, which can be obtained from imaging, as 1D inclusions and treat the capillary bed in a homogenized way as an additional pore space besides the interstitial fluid.

A further application of our model is the evaluation and prediction of different drug delivery strategies. Here, we have focused on novel approaches using nanoparticle-mediated drug delivery, which is based on the idea of a more specific targeting of malignant cells. However, the particles have to be transported across several scales and biological barriers to finally reach the tumor as described by the concept of transport oncophysics. Recently, we have extended our framework to also include nanoparticle transport [5]. This novel model permits the examination of the interplay between the size of vessel-wall pores, the permeability of the blood-vessel endothelium, and the lymphatic drainage on the delivery of particles of different sizes. Solid tumors develop a non-perfused core and increased interstitial pressure.




1 | Components of the multiphase model: The extracellular matrix (ECM) as the solid phase; the three fluid phases healthy cells (HC), tumor cells (TC) and interstitial fluid (IF); the neovasculature as independent porous network; necrotic tumor cells (NTC), oxygen, and nanoparticles as species transported in the different phases.



2 | Three-dimensional growth of a tumor along a pre-existing blood vessel network (outline is visualized in grey, necrotic core is visualized in olive green). The tumor grows primarily along pre-existing blood vessels due to large nutrient availability there; the inner core becomes necrotic due to blood vessel compression and impaired nutrient transport.

Our model confirms that those two typical features of solid tumors limit nanoparticle delivery by hindering sufficient penetration into the entire tumor volume. We can conclude that nanoparticles are able to reach the tumor core if (or even "only if") transport in the interstitial fluid is diffusion-dominated.

Ultimately, the goal of mathematical tumor models is to provide decisive information about patient-specific tumor evolution, response to a specific treatment, or even more personalized treatment strategies. Computational tumor models in combination with clinical image analysis and data processing should aim at more personalized treatment strategies in order to improve the therapeutic outcome and to limit side-effects. Our approach is not based purely on "big data" or "artificial intelligence" but on the underlying physical mechanisms. We believe that only the integration of mechanism-based computational models with statistical data can predict the patient-specific evolution of tumors and the efficacy of treatment strategies. Our vascular multiphase tumor growth model is physics-based and thus can provide crucial insight into mechanisms that cannot be conclusively investigated either *in vivo* or *in vitro*.

We are currently working on establishing an interdisciplinary collaboration bringing together experts from chemistry, biology and oncology with mathematicians, physicists, and computer scientists to further validate our *in silico* predictions with suitable experimental and clinical data. During the TUM-IAS Focal Period on Advanced Computational Modeling for Tumor Growth Prediction (2018), we and three partner Focus Groups were able to facilitate valuable and lasting contacts among clinicians and oncologists from TUM and experts in cancer modeling from all over the world. This interdisciplinary network will allow us to refine the model and bring it toward clinical applicability.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Computer Vision and Machine Learning**

Prof. Michael Bronstein (Imperial College / University of Lugano / Intel / Twitter)
Rudolf Diesel Industry Fellow
Prof. Daniel Cremers (TUM) | Carl von Linde Senior Fellow

Scientific Reports

Michael Bronstein

Daniel Cremers

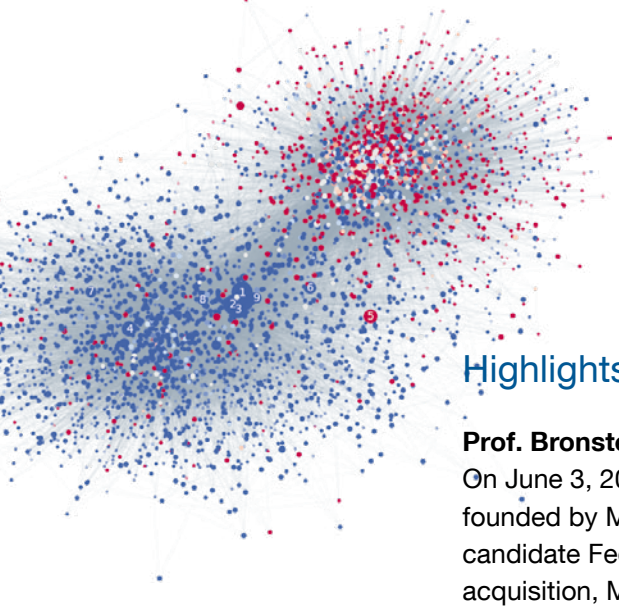
Host
Prof. Daniel Cremers
Computer Vision and Artificial Intelligence, TUM

The activities of our Focus Group are primarily centered on the interplay between geometry, machine learning, and computer vision. Analysis of geometric objects has been a topic of computer vision and pattern recognition since the inception of the field. Classical computer vision problems of “shape-from-X” aim at recovering the geometric structure of a 3D object from multiple images (shape from stereo) or different illumination conditions (photometric stereo). In recent years, the interest in 3D data has increased dramatically, fueled in part by the commercial availability of affordable and compact 3D sensors. Such sensors are nowadays found in a broad range of applications, from drones and augmented reality to self-driving cars.

Members of the group have both academic and industrial experience in these applications. Michael Bronstein was until 2019 a principal engineer at Intel responsible for the development of RealSense range-sensing technology, and since 2019 he is the head of Graph Learning Research at Twitter. Daniel Cremers is the founder and Chief Scientific Officer at the autonomous driving startup Artisense.

Of particular interest to our Focus Group is the development of next-generation machine learning methods capable of dealing with geometric data. Deep learning, a particularly successful machine learning paradigm based on differentiable programming, has had a revolutionary impact on computer vision in the past decade. Deep learning technologies are estimated to have added billions in business value, created new markets, and transformed entire industrial segments. Most of today’s successful deep learning methods, such as convolutional neural networks (CNNs), rely on classical signal processing models that limit their applicability to data with underlying Euclidean grid-like structure, e.g., images or acoustic signals. Yet many applications deal with non-Euclidean (graph- or manifold-structured) data such as social networks in computational sociology, molecular graphs in chemistry, interactomes in system biology, and 3D point clouds in computer vision and graphics. Until recently, the lack of deep learning models capable of correctly dealing with non-Euclidean data has been a major obstacle in these fields.

One of our research directions is trying to bridge the gap between geometric and deep learning by generalizing neural architectures and the underpinning mathematical models to non-Euclidean domains. The term “geometric deep learning”, coined by Prof. Bronstein, is now widely used as an umbrella term for graph- and manifold-based neural network architectures. In the past few years, the community has shown increased interest in the field. Graph neural networks have now become a standard tool in the machine learning toolset, widely used in a broad range of applications with successful results. We believe the rapid movement of these methods from a niche interest to the spotlight of research are in part thanks to our contributions and the activities of our Focus Group.



# Highlights of 2019

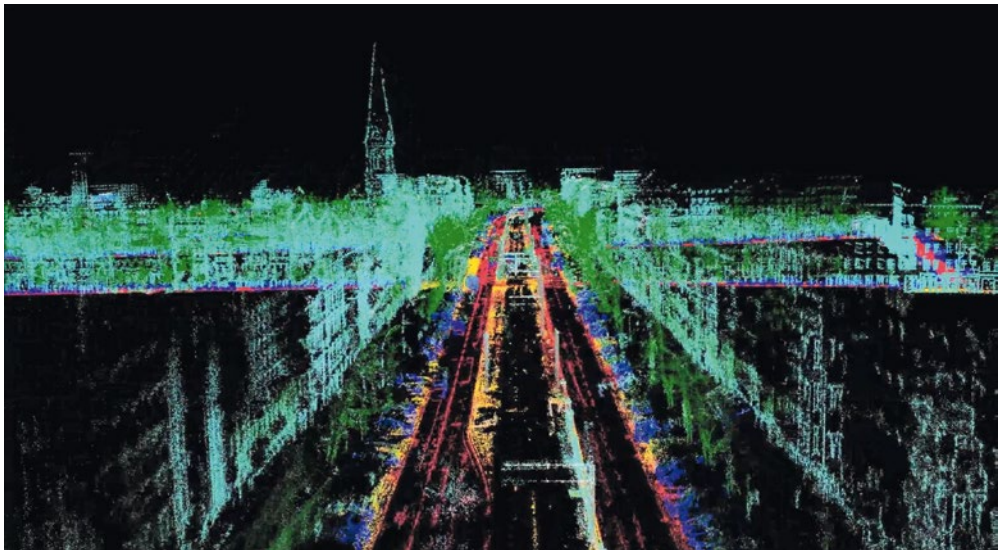


**Prof. Bronstein's startup company Fabula AI acquired by Twitter**
On June 3, 2019, Twitter announced the acquisition of Fabula AI, a company founded by Michael Bronstein, who served as its chief scientist, while doctoral candidate Federico Monti served as chief technical officer. As a result of the acquisition, Michael Bronstein joined Twitter as its new head of Graph Learning Research. Parag Agrawal, CTO at Twitter, announcing the details of the acquisition, said: "Graph deep learning is a novel method for applying powerful ML techniques to network-structured data. The result is the ability to analyze very large and complex datasets describing relations and interactions, and to extract signals in ways that traditional ML techniques are not capable of doing. This strategic investment in graph deep learning research, technology and talent will be a key driver as we work to help people feel safe on Twitter and help them see relevant information."


1 | Prof. Bronstein (left) with the team of Fabula AI at the Twitter office in London.

Fabula AI was founded in 2018 and built upon Michael Bronstein's research on geometric deep learning. The company focused on the problem of detecting misinformation (colloquially known as "fake news") on social networks by learning the respective specific spreading patterns. This technology was rather unique compared to traditional content-based approaches, in that it allowed a content-agnostic analysis based on the way information propagates on the social graph. The company reported the capability of accurate detection of "fake news" on Twitter in a paper presented at the ICLR 2019 Workshop on Representation Learning on Graphs.

**Hyperfoods TEDx Talk**
In September 2019, Michael Bronstein delivered a TEDx talk in Lugano based on his recent work on applying graph neural networks to find biomolecular compounds in food with oncological drug-like properties. This approach relies on protein-to-protein interaction networks. The research highlighted several common food ingredients rich with such compounds, such as cabbage, celery, and green tea, and represents the first step toward data-driven design of personalized nutrition that could help prevent and even cure diseases such as cancer.



3 | Semantic reconstruction of Berlin computed with the camera-based 3D perception technologies of Artisense

As co-founder and Chief Scientific Officer of the company Artisense, Prof. Cremers supports technology transfer and the development of camera-based 3D perception for autonomous systems and self-driving cars: Figure 3 shows semantic 3D reconstructions of Berlin generated in real-time from low-cost camera-based sensor systems installed in cars. And most recently, Artisense has pioneered deep-learning enhanced algorithms for visual localization and mapping that exhibit unprecedented precision. With these advances, Artisense is establishing cameras as the lead sensor for 3D perception and scene understanding in autonomous systems and self-driving cars.

**Nature Methods cover paper**

Michael Bronstein's work on the use of geometric deep learning for protein design has appeared on the cover of the February 2020 issue of the journal Nature Methods. Protein-based drugs are becoming some of the most important therapies of the 21st century. The typical mechanism of action of these drugs is a strong protein-protein interaction (PPI) between surfaces with complementary geometry and chemistry. Over the past three decades, large amounts of structural data on PPIs has been collected, creating opportunities for differentiable learning on the surface geometry and chemical properties of natural PPIs. Since the surface of these proteins has a non-Euclidean structure, it is a natural fit for geometric deep learning. In particular, the paper showed computationally designed binders for PD-L1 proteins, a common target used for cancer immunotherapy drugs. This work is a collaboration with the EPFL Protein Design and Immunoengineering lab, headed by Bruno Correia, who was a visitor in summer 2018 and participated in the TUM-IAS Workshop on Machine Learning for 3D Understanding.

*Publications by this Focus Group can also be found in the section Publications of this report.*

## Activities in 2019

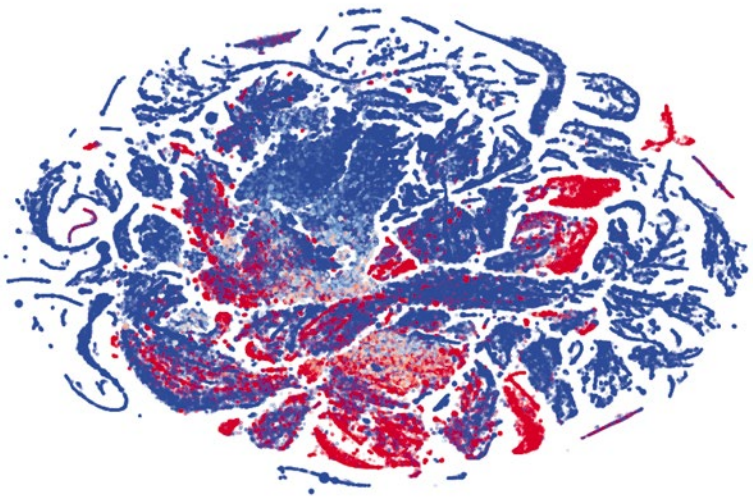
**ELLIS Program on Geometric Deep Learning and first Workshop at DALI** (San Sebastian, Spain)
Michael Bronstein, recently elected Fellow of ELLIS, is co-chair (together with Max Welling) of the new program on Geometric Deep Learning. The program kicked off with the first workshop on the topic at DALI conference in Spain.

**New research competence in the Munch area**
Over the last year, Daniel Cremers engaged in several activities to build up research competence in machine learning and data science in the Munich area. Together with Thomas Seidl and Bernd Bischl from LMU, he coordinates the Munich Center for Machine Learning (MCML), one of four national competence centers in the field of machine learning. Together with Massimo Fornasier (TUM Mathematics), he is building up the Munich Data Science Institute (MDSI) which will bring together experts on machine learning and data science and explore a variety of societally relevant application areas. Together with Massimo Fornasier and Fabian Theis (TUM Mathematics & Helmholtz), he founded and coordinates ELLIS Munich, the Munich-based hub of the European Machine Learning network ELLIS.

**Geometry Meets Deep Learning Workshop at ICCV** (Seoul, South Korea)
Organized by Michael Bronstein and Emanuele Rodolà (La Sapienza), a former postdoctoral fellow at TUM, the workshop focused on the use of geometric deep learning models in computer vision applications. The line of keynote speakers, among others, featured two TUM-IAS Fellows, Matthias Nießner and Daniel Cremers.

**New ERC Advanced grant awarded to Professor Cremers**
In 2020, Daniel Cremers was awarded the ERC Advanced Grant SIMULACRON. Its principal focus is the development of algorithms for inferring physical simulations of deformable objects from video observations. Whereas traditionally 3D computer vision is constrained to recovering the 3D shape of objects from cameras, the aim is therefore to go beyond the reconstruction of geometric structure and actually infer the underlying physics. This should create a more complete understanding of the observed phenomena while requiring less camera observations. Moreover, it should enable us to extrapolate an observed action into the future (using the inferred simulation), allowing us to predict what will happen next. Following a Starting Grant, a Consolidator Grant and two Proof of Concept Grants, SIMULACRON is Daniel Cremers' fifth grant from the European Research Council.

**Graph Representation Learning Workshop at NeurIPS** (Vancouver, Canada)
Organized by Michael Bronstein together with colleagues from Stanford, MIT, Google, DeepMind, MILA, and ICLA, this was one of the most popular workshops at NeurIPS with attendance near 1500 participants. The workshop focused on the most recent advances and challenges in geometric deep learning on graphs, and it featured prominent experts from industry and academia as keynote speakers: Peter Battaglia (DeepMind), Jure Leskovec (Stanford/Pinterest), and Marinka Zitnik (Harvard).



4 | T-SNE embedding of the vertex-wise features produced by our neural network at the last convolutional layer representing all the users in our study, color-coded according to their credibility (blue = reliable, red = unreliable). Clusters of users with different credibility clearly emerge, indicative that the neural network learns features useful for fake news detection.

# Focus Group **Data-driven Dynamical Systems Analysis in Fluid Mechanics**

Dr. Luca Magri (University of Cambridge) | Hans Fischer Fellow
Dr. Nguyen Anh Khoa Doan (TUM) | Postdoctoral Researcher

Scientific Reports

Luca Magri

Host
Prof. Wolfgang Polifke
Thermo-Fluid Dynamics, TUM

## Physics-constrained data-driven methods for unsteady fluids

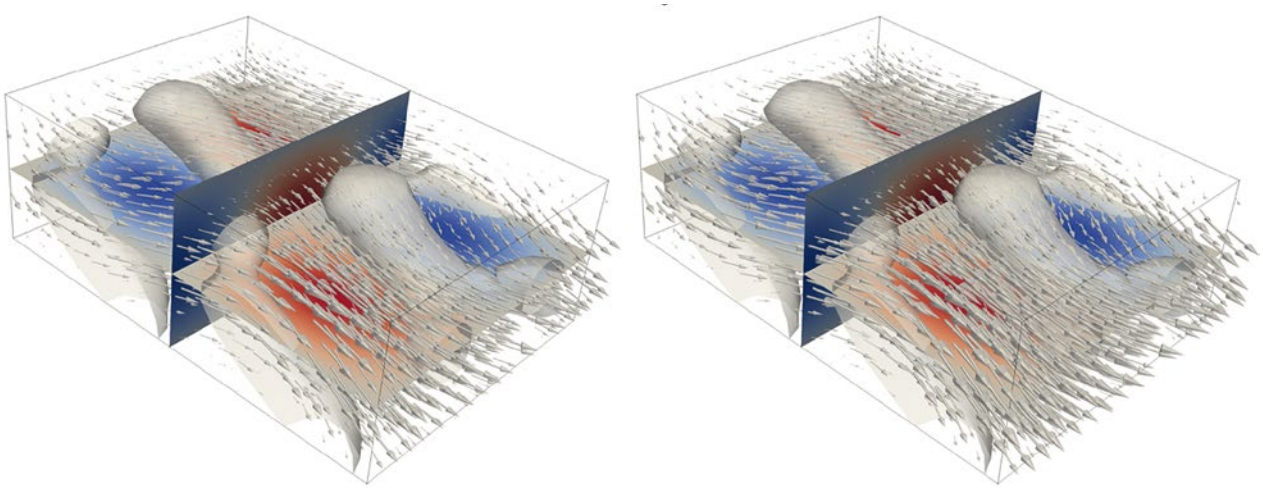
At least one hundred trillion bytes of data have been created in the world while you were reading this sentence. The traditional triad of the scientific method (theory, experimentation, and simulation) has added big data now. Central to big data science are artificial intelligence and machine learning, which are automated ways of transforming information into empirical knowledge. Whereas empirical knowledge is crucial to many practical applications, such as facial recognition, empirical models do not necessarily fulfill physical principles, for example, conservation laws.

The overarching aim of the research carried out by L. Magri (Hans Fischer Fellow) and Dr. N. A. K. Doan (TUM-IAS postdoctoral fellow) is twofold. The first objective is to develop mathematical and computational methods to combine physical principles with artificial intelligence and machine learning into a consistent approach: physics-constrained data-driven methods. The second objective is to apply the methods to fluid mechanics, which underpins many industries and helps society address such issues such as climate science, energy consumption, and air transportation.

The methods we are developing make qualitative computational models quantitatively accurate, so they can be used to optimize the design of green aircraft engines, predict the occurrence of extreme events, and reconstruct high-resolution physics from low-resolution experimental measurements.

We tackle two big open questions: (1) “Do machine learning algorithms scale to engineering configurations?” and (2) “Can we extrapolate the learned knowledge in time and space?” In particular, we are interested in flows that are unsteady, unpredictable, and uncertain across a range of spatiotemporal scales. We investigate flows characterized by multi-physics and multi-scale interactions, which lead to the occurrence of sudden and violent changes. These changes are called extreme events, such as sudden ignition spots and turbulent bursts. We have been awarded additional funding for computational time on supercomputers by the UK Engineering and Physical Sciences Research Council Research Council and the Partnership for Advanced Computing in Europe, which have funded the projects “Data-driven prediction of rare and extreme events in turbulent reacting flows” and “Physics-Informed Neural Network for Turbulent Flows”, respectively. These projects aim at high-fidelity simulation of turbulent flows on CPUs for the development of physics-constrained data-driven methods on GPUs.

First, we have developed a physics-constrained data-driven algorithm that synergistically combines information from both physical knowledge and small data. This approach, which we call the physics-informed echo state network, has successfully

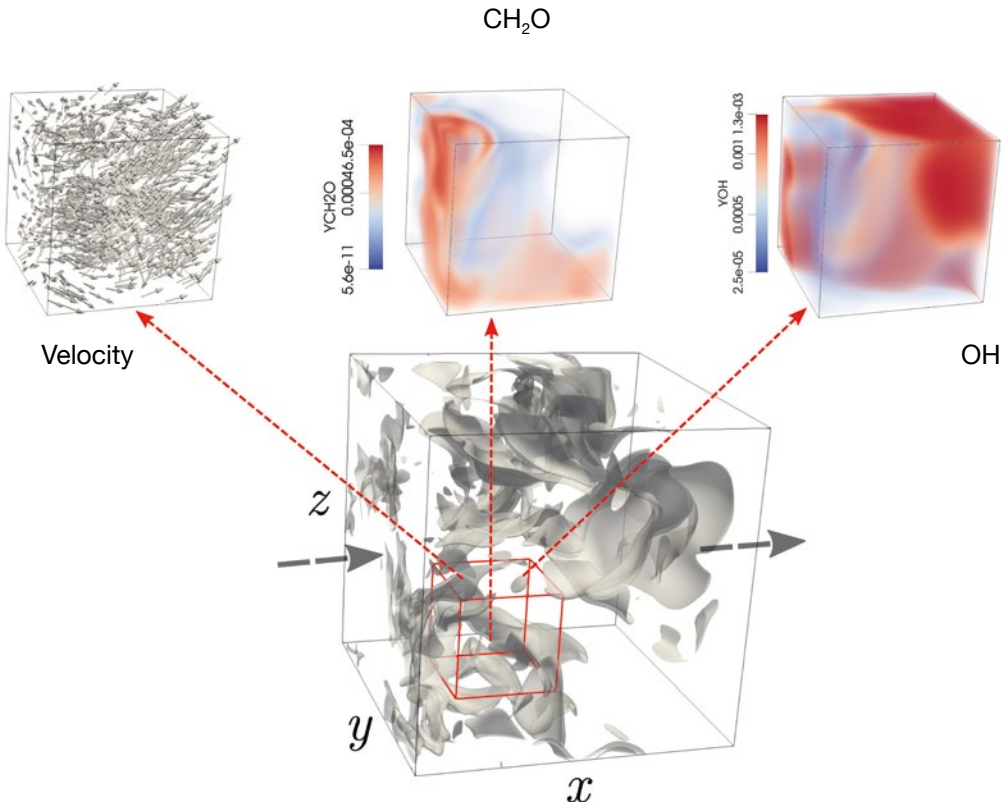


1 | This turbulent flow exhibits sudden changes (extreme events) when the vortices break down. The extreme events occur in time in an exceedingly unpredictable way (left figure). The physics-informed echo state network (right figure) approach can time-accurately predict the extreme events and the evolution of the flow [2], [3] by combining physical knowledge with data. The arrows represent the velocity field, the grey surfaces highlight regions of high vorticity) and the cuts represent the downstream (horizontal cut) and transverse (vertical cut) velocity magnitude.

been applied to a chaotic system. We have shown that this approach can accurately predict the time evolution of erratic dynamics beyond the time horizon that is normally predictable [1]. As shown in Figure 1, this method has enabled the real-time prediction of extreme events in a turbulent shear flow. This prediction is exceedingly difficult to achieve with purely data-driven methods [2], [3].

Second, we have generated high-quality datasets with direct numerical simulations to develop Bayesian data-assimilation techniques. We have shown that under-resolved simulations can accurately predict the occurrence and evolution of ignition spots in turbulent reacting flows (Figure 2) by combining numerical simulations of the flow physics [4] with higher quality data [5]. This opens new possibilities for the time- and space-accurate prediction of turbulent flows by combining cheap simulations with high-fidelity data. These tools have recently interlaced reduced-order models with data from large-scale numerical simulations and experiments for on-the-fly adaptive modeling [6]–[15]. To carry out data assimilation research, L. Magri received funding from the USA (NSF) for a four-week visit at the Stanford University Center for Turbulence Research.

Scientific Reports
Data-driven Dynamical Systems Analysis in Fluid Mechanics




2 | Bayesian data assimilation enables the spatiotemporal prediction of seemingly random ignition spots in a turbulent reacting flow direct numerical simulation [5].

Third, we are currently generating high-quality datasets to scale up physics-informed echo state networks to high-dimensional systems. In particular, we are developing methods to learn the dynamics of unmeasured quantities (i.e., hidden states) from an incomplete set of data [16].

We have taught part of the developed computational methods to postgraduate students, engineers, and senior researchers during a winter school at KTH Royal Institute of Technology in Stockholm [17].

The Focus Group as a whole (including Prof. Thomas F. Sattelmayer and Dr. Mirko Bothien) is organizing an international conference in thermoacoustics: SoTiC 2020 - Symposium on Thermoacoustics in Combustion: Industry meets Academia [18] with invited speakers who are world leaders in gas turbine and rocket motor industry and research.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Data-driven Dynamical Systems Analysis in Fluid Mechanics**

Dr. Mirko Bothien (Ansaldo Energia) | Rudolf Diesel Industry Fellow

Scientific Reports

Mirko Bothien

Host
Prof. Thomas Sattelmayer
Thermodynamics, TUM

## Toward decarbonized power generation using hydrogen in gas turbines

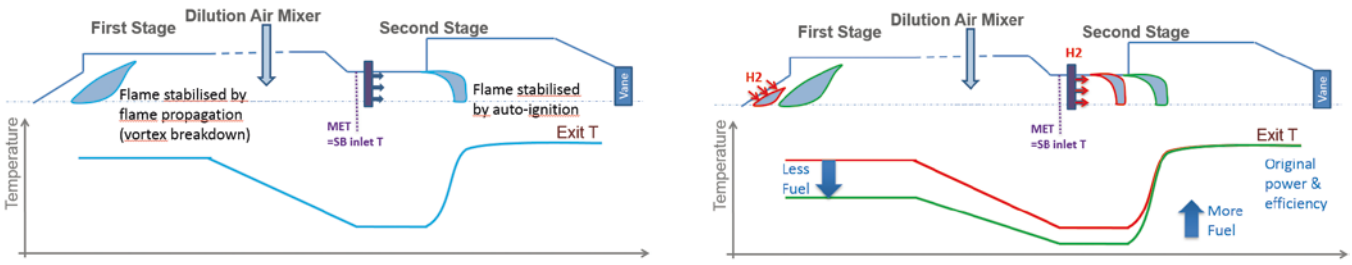
**Introduction**

Climate change is one of today's most important environmental and social concerns. In order to achieve the Paris Agreement's goals, decarbonization of the power generation sector is essential. This will result in a fast-increasing share of variable renewable power, which has to be balanced by technologies that allow for dispatchable power generation able to flexibly respond to a varying load demand and renewables production. Gas turbines, especially in so-called Power-to-X-to-Power schemes, are predestined to take over this role.

Compared to natural gas, the main challenge of hydrogen combustion is its increased reactivity, which results in a decrease in engine performance for conventional premix combustion systems. Gas turbines equipped with the unique sequential combustion technology can overcome this drawback, allowing the utilization of the full range of hydrogen in a low NOx premix system [1,2]. Although very promising results have been achieved and much higher hydrogen contents can be used compared to traditional gas turbine combustors, research is required to understand the impact that hydrogen has on combustion dynamics. We intend to make important contributions to unravel, and subsequently gain the ability to predict, the combustion dynamics of auto-ignition flames in general and specifically with respect to hydrogen.

## Sequential combustion

Ansaldo Energia's GT36 H-class gas turbine utilizes an advanced sequential combustion system with significant advantages in terms of low emissions and fuel flexibility. It is composed of two complementary combustion stages in series, overcoming the limits of traditional premix combustion systems by tuning the temperature between the first stage and the second (mixer exit temperature, or MET). Figure 1 (left) shows the schematic of flame positioning for operation with natural gas. MET is maintained at a relatively high level, ensuring maximum turndown performance. In figure 1 (right), the upstream shift of the flame usually caused by introduction of hydrogen (red) is avoided by means of MET reduction (green). A shift of fuel from the first stage to the second compensates for the higher hydrogen reactivity on both stages, maintaining the flame position at the desired location. This allows for the turbine inlet temperature to be maintained at full H class level.




1 | Schematic of sequential combustion with flame positions for natural gas (left) and hydrogen (right).

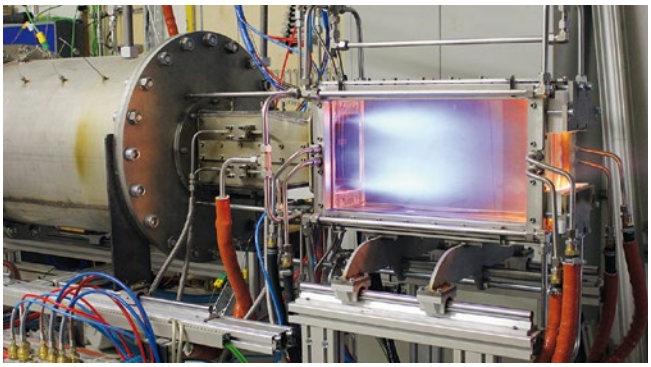
## Research objectives and status

Two main research objectives are targeted:

**1. Modeling of high-frequency combustion instabilities of auto-ignition flames**
Before the full potential of two-stage lean reheat combustion for further reduction of pollutant emissions can be exploited, suitable strategies for avoiding high-frequency (HF) combustion instabilities must be developed. In this context, the challenge for basic research is to identify the mechanisms leading to loss of stability and to close the current gap in modeling of HF instabilities by providing the missing models on acoustic flame feedback and effective stability analysis methods. Our research aims at providing data from a novel test facility of unique acoustic design, which has been particularly designed for HF instability research of (partially) auto-ignition-stabilized flames [3]. This platform has been successfully commissioned and is operational, ready for use in the proposed project (see figure 2).

**2. Build a physics-based stability model for hydrogen reheat flames to enable large-scale power generation in Power-to-H2-to-Power schemes**
A combination of analytical, numerical, and experimental investigations will be used to obtain data-driven insight into the physics of hydrogen auto-ignition flames. Based on this, suitable models will be derived enabling a description of their dynamic behavior in the early development stages of future gas turbines [4]. The unique test facility at TUM will be used to systematically investigate the dynamical features that will provide the basis for deriving a low-order model.

In a first step, funding for these two objectives had to be secured. Two proposals have been submitted to the German Science Foundation (DFG) and the Research Council of Norway (RCN), respectively. Both proposals have been granted and funding for two doctoral candidates could thus be secured. Currently, for the first (DFG) project, the existing rig at the Chair for Thermodynamics is being adapted to allow for the planned experimental investigation. The second project is part of a consortium together with NTNU Trondheim, Sintef Energy, Ansaldo Energia, and Equinor. The doctoral candidate at TUM starts in January 2020.



2 | Reheat test rig at the Chair for Thermodynamics, TUM.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Data Mining and Analytics**

Prof. Stephan Günnemann (TUM) | Rudolf Mößbauer Tenure Track Professor
Marin Bilos, Aleksandar Bojchevski, Bertrand Charpentier, Maria Kaiser, Johannes Klicpera, Anna Kopetzki, Aleksei Kuvshinov, Armin Moin, Oleksandr Shchur, Daniel Zügner (TUM) | Doctoral Candidates

Scientific Reports

Stephan Günnemann

Host
Data Analytics and Machine Learning, TUM

## Can you trust your machine learning model?

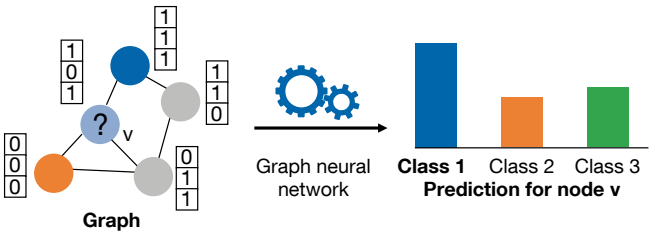
The Focus Group Data Mining and Analytics studies principles for robust and trustworthy machine learning. Specifically, we are interested in learning principles for non-independent data such as graphs and temporal data.

As the number of machine learning models deployed in the real world grows, questions regarding their robustness become increasingly important. Are the models' predictions reliable or do they change if the underlying data gets slightly perturbed? In particular, for safety-critical and scientific use cases, it is essential to assess the models' vulnerability to *worst-case* perturbations – ensuring that we can trust the machine learning model even in the worst case.

## Robustness of graph neural networks

In this regard, our group specifically focuses on graph neural networks. Indeed, graph neural networks (GNNs) have emerged as the *de facto* standard for many learning tasks, significantly improving performance over the previous state of the art. They are used for various high-impact applications across many domains, such as molecular property prediction [1], protein interface prediction, fraud detection, and breast cancer classification. And indeed, as we have shown in our work [2], GNNs are highly non-robust with respect to deliberate perturbations on both the graph structure and the node attributes, making their outcomes highly unreliable. Likewise, in a follow-up study, we generalized these results to unsupervised node embeddings [3].

Motivated by these insights, our group developed the first principles for provable robustness of GNNs: Given a certain space of perturbations, the goal is to provide a guarantee that no perturbation exists that will change the prediction. That is, in this case one can trust the prediction. As it turns out, providing such so-called "robustness certificates" is extremely challenging due to the discreteness of the graph structure, the non-linearity of the neural network, and interactions taking place in the graph neural network. Despite these challenges, in our work [4] we provided the first robustness certificate for perturbations to the nodes' attributes, while in [5] we proposed the first certificate for graph structure perturbation. Thus, for the first time we can give guarantees about a GNN's behavior. Likewise, both works show how one can improve the robustness of the GNNs by adapting an enhanced training procedure. Overall, these works significantly extend the applicability of GNNs, paving the way for their use in scientific and critical application domains where reliable predictions are essential.



## Uncertainty in ML models for temporal data



In a second line of research, we tackled the aspect of uncertainty. Quantifying uncertainty in neural network predictions is a key issue in making machine learning reliable. In many sensitive domains, including robotics, financial, and medical areas, giving autonomy to AI systems is highly dependent on the trust we can assign to them. In addition, being capable of informing humans, AI systems have to be aware about their predictions' uncertainty, allowing them to adapt to new situations and refrain from taking decisions in unknown or unsafe conditions.

In [6], we proposed the first method that incorporates uncertainty when predicting a sequence of discrete events that occur irregularly over time. This is a common data type generated naturally in our everyday interactions with the environment. Examples include messages in social networks, medical histories of patients in healthcare, and integrated information from multiple sensors in complex systems such as cars. We present two new architectures, modeling the evolution of the distribution on the probability simplex. In both cases, we make it possible to express rich temporal evolution of the distribution parameters, and we naturally capture uncertainty. In the experiments, state of the art models based on point processes are clearly outperformed for event and time prediction as well as for anomaly detection. Particularly noteworthy is that our methods give uncertainty estimates for free.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Dynamic Vision and Learning**

Prof. Laura Leal-Taixé (TUM) | Rudolf Mößbauer Tenure Track Professor

Scientific Reports

Laura Leal-Taixé

Host
Dynamic Vision and Learning, TUM

## Probing vision, studying learning

Our Focus Group is working on key problems in computer vision and machine learning. The main goal of the current team of eight researchers is to perform dynamic scene understanding, i.e., to allow robots to see and understand the world around them from visual (video) input. The team works with cutting-edge deep learning tools and combines them with classic computer vision knowledge such as 3D geometry and graph theory.

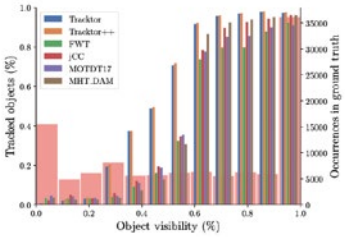
## Relevance and impact

Understanding the world through the eye of a camera means identifying all elements of a scene, both dynamic as well as static ones, and further tracking them in time in order to predict their motion in the future. This is key for applications such as autonomous driving or mobile robots that will be expected to navigate in crowded environments. Toward this end, we work on basic problems such as multiple same-class object tracking [1] and push the capability of algorithms to function in extremely crowded environments [2,3,4]. We are also interested in exploiting similarities between objects – in appearance as well as motion – in order to better understand their characteristics [5].

Finally, we embed the computer vision understanding of the 3D geometry in order to improve camera localization with neural networks [6,7]. Our research should enhance the capability of technical systems to understand the physical world around us, both static and dynamic, which is a key element in robotic intelligence.

## Future plans

Within the *socialMaps* project, which won the team 1.65 million euros in the form of a Sofja Kovalevskaja Award from the Humboldt Foundation, the goal is to extend dynamic scene understanding to crowded environments, so that our algorithms are able to analyze and understand the complex interactions found in cities. This should allow for *social and dynamic information* to be incorporated into current maps to improve the flow of information to the users.




1 | We illustrate the ratio of tracked objects with respect to their visibility evaluated on the Faster R-CNN public detections. The results clearly demonstrate that none of the more sophisticated methods can achieve performance superior to our approach. This is especially noticeable for highly occluded boxes. The transparent red bars indicate the ground truth distribution of visibilities. Image: twbnw, from paper [1]


2 | Retrieval results on a set of images from several public datasets using our Group Loss. The green square indicates that the retrieved image is from the same class as the query image, while the red box indicates that the retrieved image is from a different class. Taking advantage of object similarities in the optimization process dramatically improves results. Image: retrieval, from paper [5].


3 | Video super resolution results of our method TecoGAN compared to three competing methods (first three rows). The last row shows the ground truth results. Note that our method achieves a greater level of detail in the reconstructed scenes. Image: super-resolution, from paper [10]

*Publications by this Focus Group can also be found in the section Publications of this report.*

Additional material and a list of publications are available our website: https://dvl.in.tum.de

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# Focus Group **Neuromorphic Computing**

Prof. Hai (Helen) Li (Duke University) | Hans Fischer Fellow
Shuhang Zhang (TUM) | Doctoral Candidate

Scientific Reports

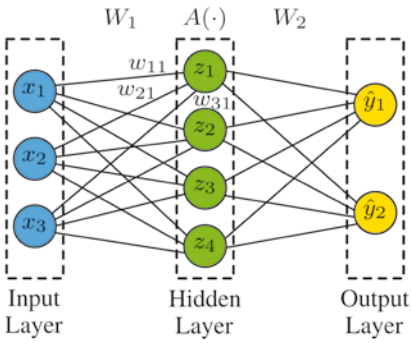
Helen Li

Host
Prof. Ulf Schlichtmann
Electronic Design Automation, TUM

## A high-performance neuron design for neuromorphic computing

Neuromorphic computing aims to utilize very-large-scale integration (VLSI) systems to mimic biological architectures, thus achieving cognitive functionalities and self-learning abilities. The key aspects of neuromorphic computing are understanding the topology of biological neural systems and converting them into comprehensive models.

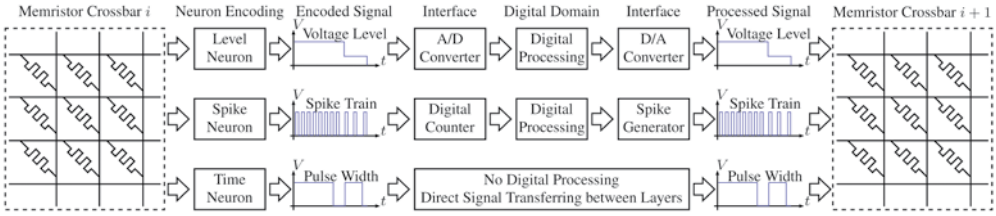
In the past decades, the software implementation of neuromorphic computing has drawn great attention from researchers due to remarkable breakthroughs in various fields, such as pattern recognition and natural language processing, widely using artificial neural networks. Figure 1 shows the basic structure of a neural network, which consists of an input layer, a hidden layer, and an output layer. The nodes represent neurons, and connections represent the relations between neurons in different layers. In a neural network, the output of a neuron is a function of the inputs and the connection weights. However, the traditional computing architecture (Von Neumann architecture) cannot support high-performance neural networks efficiently, because of the processing time mismatch between CPU and memory. This phenomenon is also known as the Memory Wall. Power consumption, which is limited by conventional CMOS technology, is another critical problem in addition to computing latency. Therefore, to improve the performance of neuromorphic computing, the hardware should also be carefully reshaped.




1 | Software implementation of neuromorphic computing.

With traditional CMOS technology, it is hard to overcome these problems. But the invention of memristor technology gives us the opportunity to fundamentally change the computing platform, because memristors can be used as both processing and memory units. In addition, the scalability and power-efficiency of memristors make them a promising candidate for high computing density and efficiency.

The memristor-based implementation of artificial neural networks can be reshaped with memristor crossbars as synapses and specific-designed circuits as neurons. Figure 2 shows the structure, where memristors sit on the crosspoints of horizontal




2 | Hardware implementation of neuromorphic computing with three different encoding mechanisms.

wordlines and vertical bitlines, representing the synapses between neurons. By programming these memristors (synapses) to different conductances, they represent different neuron connections in biological systems. The neuron circuits receive activations delivered by these memristors and generate information transferred to the next layer. Therefore, by combining memristors and traditional CMOS technologies, we can implement neural networks at the hardware level and achieve better performance. Published results show that memristor-based neuromorphic computing can achieve 240 times speedup and 94 times better power efficiency over traditional implementations.

In neuromorphic computing, neuron circuit design is very important as it significantly affects the computing efficiency. In traditional neuron designs, the neurons receive the activation from memristors and then generate voltage levels or spikes to the following neurons, as shown in Figure 2. In traditional designs, the transferring latency is too high and requires additional processing units, such as analog/digital converters and digital/analog converters for level-based designs, and counter and spike generators for spike-based designs, leading to extra area requirements and power demands. Moreover, traditional neuron designs break the consistency in a neural network and require the presence of digital processing, which violates the concept of biological neural networks. Therefore, we propose a novel neuron design called the Time Neuron, which receives activation and encodes it into a variable-length pulse instead of voltage levels or spikes. The pulse can then be transferred to the following neurons directly. This neuron design demonstrates a new encoding mechanism with which the computing latency of a neural network can be reduced significantly – more than 100 times. In the meantime, the area and power consumption can be reduced by up to 75% and 25%, respectively.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Visual Computing**

Prof. Matthias Nießner (TUM) | Rudolf Mößbauer Tenure Track Professor
Prof. Leonidas Guibas (Stanford University) | Hans Fischer Senior Fellow
Prof. Angel X. Chang (Simon Fraser University) | Hans Fischer Fellow
Armen Avetisyan, Manuel Dahnert, Ji Hou, Andreas Rößler, Dave Zhenyu Chen (TUM)
Doctoral Candidates



Matthias Nießner

Leonidas Guibas

Angel X. Chang

Host
Visual Computing, TUM

The Visual Computing Focus Group is a collaboration of research enthusiasts pushing the state of the art at the intersection of computer vision, graphics, and machine learning. Our research mission is to obtain high-quality digital models of the real world, which include detailed geometry, surface texture, and material in both static and dynamic environments. In our research, we heavily exploit the capabilities of RGB-D and range sensing devices that are now widely available. However, we ultimately aim to achieve both 3D and 4D recordings from monocular sensors – essentially, we want to record holograms with a simple webcam or mobile phone. We further employ our reconstructed models for specific use cases, such as video editing, immersive AR/VR, semantic scene understanding, and many others. Aside from traditional convex and non-convex optimization techniques, we see great potential in modern artificial intelligence, mainly deep learning, in order to achieve these goals.

The relevance of this research ranges across several areas of research and technology that are affected by 3D digitization and semantic scene understanding. These include applications in entertainment, communication, medicine, and autonomous robotics. The primary goal, however, is to replace videos and images with the interactive but photo-realistic 3D content of the future – i.e., holograms, which we believe will have an impact on a wide range of industries.

The practical research impact of the group can be seen by its massive media presence, including several TV appearances in documentaries and news (*Pro7 Galileo*, *ZDF Morgenmagazin*, *RTL Nachrichten*, etc.) as well as coverage in prominent news outlets (*Wall Street Journal*, *New York Times*, *Der Spiegel*, etc.).

## Highlights of 2019

- *New York Times* from 24th November 2019: Internet Companies Prepare to Fight the ‘Deepfake’ Future [1]
- Nießner / Thies / Rößler visiting Chancellor Angela Merkel and her cabinet in Berlin (Meseberg) as part of the Digital Summit (discussing AI, synthetic media, and media forensics) [2]

Looking ahead, the digitization and understanding of real-world 3D environments is still a wide-open research field. First of all, we will continue our current developments on neural networks specifically tailored to the 3D case, in order to process and analyze 3D geometry, associated RGB images, and alternative data input. One critical component is known as generative networks; these are required to generate clean 3D geometry for realistic 3D capture and photorealistic re-rendering. While the community has seen a lot of progress in the last years along these lines, there are still significant challenges and existing research opportunities on the path toward 3D holographic capture.

*Additional material can be found on this website: https://niessnerlab.org/publications.html*

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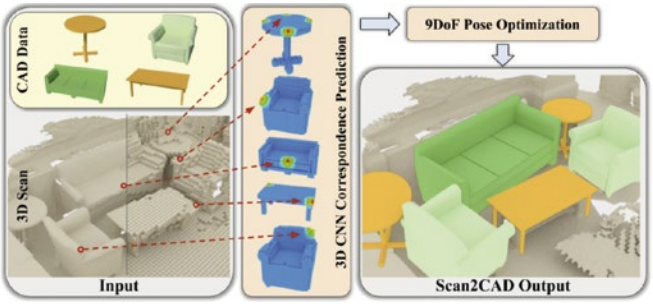
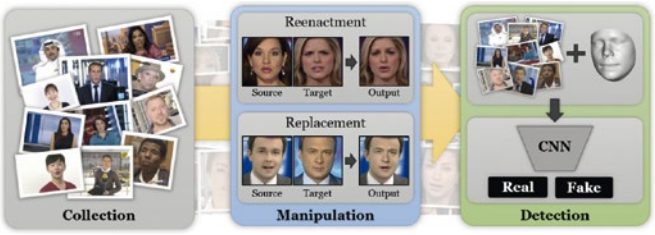
*Publications by this Focus Group can also be found in the section Publications of this report.*

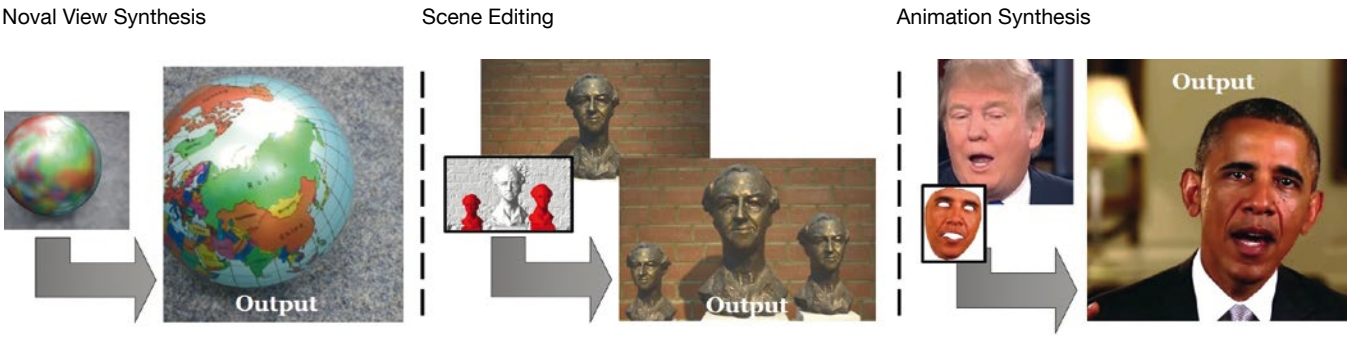
1 | Prof. Nießner, Dr. Thies, and M.Sc. Andreas Rößler presenting and discussing the research of the Focus Group Visual Computing to the federal German government (in photo: Chancellor Merkel and Vice-Chancellor Olaf Scholz) in Meseberg, near Berlin; Digitalgipfel 2019




2 | Scan2CAD takes as input an RGB-D scan and a set of 3D CAD models (left). We then propose a novel 3D CNNapproach to predict heatmap correspondences between the scan and the CAD models (middle). From these predictions, we formulate an energy minimization to find optimal 9 DoF object poses for CAD model alignment to the scan (right).




3 | FaceForensic is a database of facial forgeries that enables researchers to train deep-learning-based approaches in a supervised fashion. The database contains manipulations created with three state-of-the-art methods:, Face2Face, FaceSwap, and DeepFakes.




4 | The modern computer graphics pipeline can synthesize images at remarkable visual quality; however, it requires well defined, high-quality 3D content as input. In this work, we explore the use of imperfect 3D content, for instance, obtained from photometric reconstructions with noisy and incomplete surface geometry, while still aiming to produce photo-realistic (re)renderings. To address this challenging problem, we introduce Deferred Neural Rendering, a new paradigm for image synthesis that combines the traditional graphics pipeline with learnable components. Specifically, we propose Neural Textures, which are learned feature maps that are trained as part of the scene capture process. Similar to traditional textures, neural textures are stored as maps on top of 3D mesh proxies; however, the high-dimensional feature maps contain significantly more information, which can be interpreted by our new deferred neural rendering pipeline.

# Focus Group **Image-based Biomedical Modeling**

Prof. Bjoern Menze (TUM) | Rudolf Mößbauer Tenure Track Professor

Scientific Reports

Bjoern Menze

Host
Image-based Biomedical Modeling, TUM

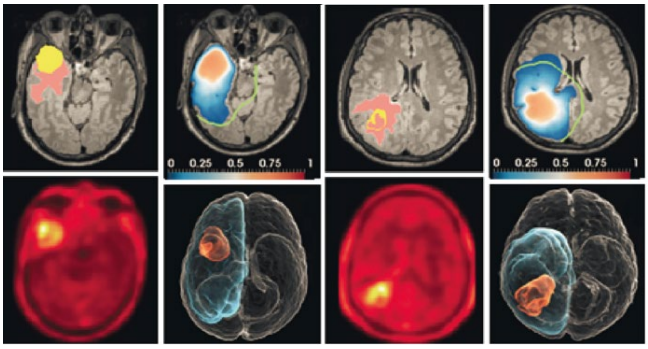
The Focus Group Image-based Biomedical Modeling develops computational algorithms that analyze biomedical images using statistical, physiological, and biophysical models. The work strives toward transforming the descriptive interpretation of biomedical images into a model-driven analysis that infers properties of the underlying physiological and patho-physiological processes by using models from biophysics and computational physiology. A related effort is the application of such models to big clinical databases in order to learn about correlations between model features and disease patterns at a population scale. In this, the main focus is on applications in clinical neuroimaging and the personalized modeling of tumor growth.

## Modeling tumor growth and optimizing radiation treatment

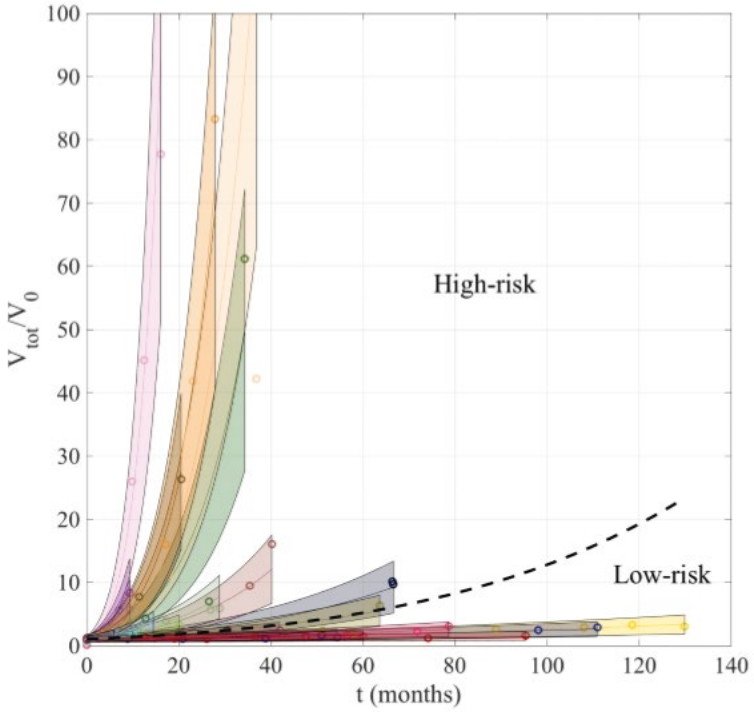
A major line of research in the Focus Group is the modeling of processes underlying images acquired in common diseases of the brain. This includes the analysis of images acquired in glioma and stroke patients, for example, and the development of algorithms for the analysis of brain lesions. The main sources of information are multimodal and multiparametric clinical image data featuring magnetic resonance, positron-emission tomography, and computer tomography scans. In the past year, we proposed a new approach to infer spatial distributions of tumor cells in brain tumor patients [1]. We are using formal mathematical models of tumor growth that we adapt to multimodal images of a patient in a principled probabilistic framework. We propose to use the resulting tumor cell distribution maps for optimizing radiation treatment in a personalized and patient-specific manner.

## Modeling lesion growth and dissemination in tumor diagnostics

Another project was modeling tumor growth at a global scale: not at the organ level with a single lesion, as for the glioma case, but describing the evolution of all tumor metastases and the global tumor "load" of a patient [2]. We present a mathematical model for the relations in the growth of initially detected lesions and the tumor dissemination process, i.e., the development of new lesions, both of which contribute to the development of the tumor ‘load’. As for the glioma project, a principled Bayesian model allows us to infer model parameters, and their uncertainties, at levels ranging from the individual patient to the population. We leverage this descriptive disease progression model into model-aware biomarkers for personalized risk assessment. As a use case, we study multiple myeloma, a disseminating plasma cell cancer, in which proper diagnostics is essential to differentiate frequent precursor states without end-organ damage from the rapidly developing disease requiring therapy.




1 | Two patient examples for the local modeling of tumor growth. We are using information from magnetic resonance (top left) and positron tomography (bottom left) images to infer tumor cell distributions (top right) in 3D (bottom right) that can be used for informing decisions in radiation treatment [1].




2 | Evolution of the global tumor volume in patients with multiple myeloma and related precursor disease. Relying on parameters in our descriptive tumor growth model, we can find critical markers that distinguish high-risk from low-risk patients [2].

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Microfluidic Design Automation (MDA)**

Prof. Krishnendu Chakrabarty (Duke University) | Hans Fischer Senior Fellow
Prof. Tsung-Yi Ho (National Tsing Hua University) | Alumnus Hans Fischer Fellow
Chunfeng Liu, Yasamin Moradi | Doctoral Candidates

Scientific Reports

Krishnendu Chakrabarty

Tsung-Yi Ho

Host
Prof. Ulf Schlichtmann
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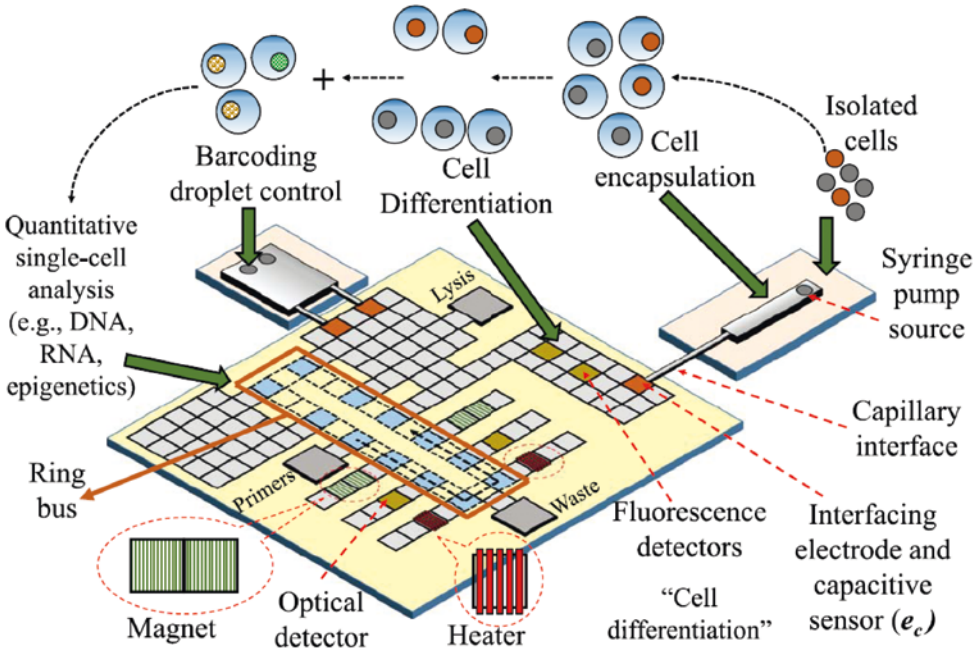
## Systematic design automation for hybrid microfluidic platforms and applications

Microfluidic biochips have been revolutionizing the traditional biochemical experiment flow with their high execution efficiency and miniaturized fluid manipulation [1, 2]. In such chips, operations such as mixing and detection are executed in devices of micrometer size. Fluid samples are transported through microchannels or micropaths between devices to carry out bioassay protocols. All these functions are performed at the nanoliter level and controlled by microcontrollers without human intervention. The efficiency and reliability of such miniaturized and automated chips endow them with a great potential. Accordingly, genomic bioassay protocols, such as nucleic-acid isolation, DNA purification, and DNA sequencing, have been demonstrated with biochips successfully, and they have thus attracted a lot of commercial attention, such as from Illumina and Agilent.

The objective of the Focus Group Microfluidic Design Automation (MDA) has been developing an automatic design flow for microfluidic biochips. This flow is able to make the full capability and potential of microfluidic biochips available to scientists and engineers in the biochemical community and industry. Reciprocally, the feedback from the biochemical community and industry can also stimulate further improvements of microfluidic architectures and design flow.

Specifically, several major topics have been explored in the current period of the Focus Group MDA. From the application view, single-cell analysis has been investigated closely to develop an efficient microfluidic platform. This bioassay has a tremendous significance in advancing the understanding of various diseases, such as cancer. In this analysis procedure, thousands of heterogeneous cells are analyzed individually in order to understand the cell population. To accelerate this procedure, we have introduced new techniques to classify cells efficiently and conduct biochemical experiments on multiple cell types concurrently. Nondeterministic cell-type identification, system integration, and design automation are also addressed in this context, leading to a hybrid microfluidic platform as shown in Figure 1 as well as an associated design-automation and optimization framework, referred to as co-synthesis (CoSyn) [3].

From the design view of microfluidic platforms, we have investigated the control logic of flow-based microfluidic biochips. Instead of assigning an independent pressure source to every microvalve, we have developed an automatic synthesis approach for control logic that is able to switch multiple control channels simultaneously. Consequently, the control efficiency of biochips can be improved significantly to reduce the area and cost of the whole platform. Moreover, we have proposed the first fault-aware design in control logic by introducing backup control paths to maintain the correct function even when manufacturing defects occur.




1 | Hybrid platform for single-cell analysis with a flow-based biochip for cell encapsulation and droplet generation, a digital biochip for quantitative analysis, and a reconfigurable valve-based fabric for barcoding [3].

Before a microfluidic biochip is deployed to execute biochemical assays, the components in the chip need to be tested to guarantee correct output results. In a complex biochip, the number of possible transportation and execution paths becomes very large, so that an efficient test strategy is mandatory. To address this challenge, we have introduced efficient test patterns based on the concepts of test paths and cuts. These patterns together can cover multiple faults in both flow and control layers. We have also introduced the concepts of test trees and multiple cuts to deal with faults in flow-based biochips with multiple ports. The proposed test method can be applied to generate test patterns for traditional flow-based biochips with predefined architectures, as well as for fully reconfigurable chips such as valve arrays.

The research of the Focus Group MDA covers the major design and test phases of microfluidic platforms. With the results of this research, a systematic design automation solution to bridge biochemical applications with microfluidic biochips of ever-increasing integration is already emerging on the horizon. New concepts such as efficient control mechanisms, fault-tolerant design, secured applications, and microfluidic platforms have arisen from this exploration. These innovative approaches not only benefit the designers of microfluidic biochips, but also open up new prospects for designers of biochemical assays by highlighting the tremendous potential of state-of-the-art biochips, thus enabling new joint research advances in both communities.

*Publications by this Focus Group can also be found in the section Publications of this report.*

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[2] J. Melin and S. Quake, "Microfluidic Large-Scale Integration: The Evolution of Design Rules for Biological Automation", Annual Review of Biophysics and Biomolecular Structure, vol. 36, no. 1, pp. 213–231, 2007.

[3] M. Ibrahim, K. Chakrabarty, and U. Schlichtmann, "Synthesis of a Cyberphysical Hybrid Microfluidic Platform for Single-Cell Analysis", IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, vol. 38, no. 7, pp. 1237–1250, 2019.

# Focus Group **Subcellular Dynamics in Neurons**

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Host
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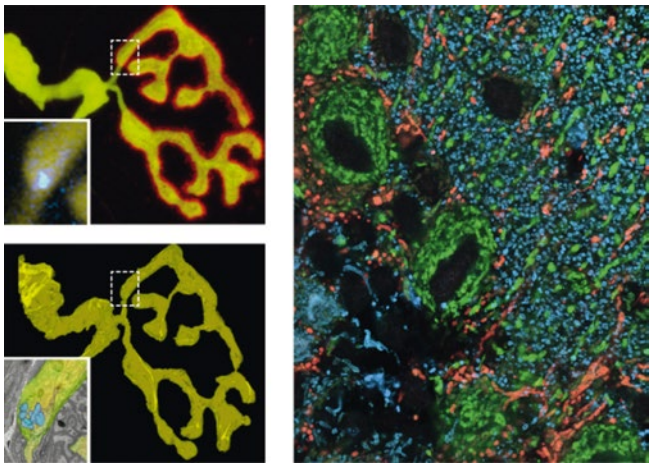
## *In varietate concordia* - Organelles and their varied life in cells

*Organelles do many things in many cells:* Cells have distinct functional compartments, called organelles ("small organs") – just as our bodies have organs. However, in contrast to the original principle by which these organelles were described as the predominant seat of a specific cellular function (e.g., mitochondria as the "power houses" of cells), it is now clear that practically all organelles harbor multiple functions. These involve "efferent" actions, where organelles contribute specific metabolites or processes to cells, as well as "afferent" tasks, where organelles act as signaling hubs that integrate multiple cellular signals to adapt organellar behavior. This picture is further complicated by the fact that cells themselves can be highly specialized, and the various roles of organelles need to adapt to these specializations. For instance, in the mammalian central nervous system alone, the number of different cell types is now estimated to be as high as one thousand! So, how are organelles adjusted to life in a vast and extended cell, such as a motor neuron, which can possess a one-meter-long cellular process? In contrast, what about the small and compact cells that nourish and hold together neurons, the glial ("glue") cells?

Over the past years, the TUM-IAS Focus Group Subcellular Dynamics in Neurons has addressed such questions for mitochondria, a ubiquitous and central organelle in metabolism, which is also the target of numerous neurological disease processes. For this, we have used a two-pronged approach: One team is working on the mitochondrial "life cycle" in one of the nervous system's largest and most complex cells, the motor neuron. The other focuses on the question of how the organelle itself differs between cell types of the cerebellum, a particularly well characterized part of the nervous system.

## Both teams achieved major results in 2019:

In the first line of work (*Team Transport*), we have discovered a new organelle degradation site in the synapses of motor neurons (i.e., the site where a nerve cell innervates a muscle fiber; *Marahori et al., in preparation*). This discovery explains the conundrum of how an extended cell, which needs to deliver many hundreds of new organelles every day, can keep this complex system of organelle delivery in long-term equilibrium. It turns out, to a large degree mitochondrial disposal is a one-way delivery – so instead of landfill or centralized recycling, the sustainability of mitochondrial turn-over in neurons appears to depend on many small "compost heaps" in the neuron's periphery, where the leftovers of centrally delivered "produce" are decomposed. As the process of mitochondrial degradation is disturbed in several neurodegenerative diseases, such as Parkinson's disease, it will be our future aim to study this new synaptic degradative site in models of neurological diseases.



1 | Left: Correlated light (top) and electron (bottom) microscopy of a neuromuscular synapse (axon in yellow, postsynaptic membrane red), inset showing localized degradative compartment (cyan). Right: Mitochondrial diversity in the cerebellum, revealed by cell type-specific markers for mitochondria in types of neurons (green, cyan) and one type of glial cell (red).

In the second line of work (*Team Contact Sites*), we have completed a major piece of work (*Fecher, Trovò et al., 2019*), which results in a new and systematic approach to studying mitochondrial diversity. By generating a new mouse line and a tailored purification approach, we can now "tag" mitochondria in any cell type we chose, and then isolate cell type-specific mitochondria to determine their molecular composition and functional capacities. Through this approach, we discovered that between the three major cell types in the cerebellum alone, up to 20% of all mitochondrial proteins are present in substantially different amounts (Figure 1). On this basis, we will now be able to study how mitochondrial diversity contributes to the unresolved question of why general defects in ubiquitous organelles can result in highly specific neurological symptoms that are causes by specific cell types.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Coding for Communications and Data Storage (COD)**

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Prof. Camilla Hollanti (Aalto University) | Hans Fischer Fellow
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Scientific Reports

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## Coding for distributed data storage and private information retrieval

Our Focus Group works on coding and cyptography and their application to security, communications, and data storage. One important research direction addresses distributed data storage and privacy.

In recent years, the development of web services and social media content has generated an astronomical quantity of digital data. This led to the construction of huge data centers spread over different locations (illustrated in Figure 1). Each of these data centers consists of a network of storage disks or servers where the data is distributed among the servers. However, given the massive number of storage servers, server failures happen on a daily basis. Therefore, it is necessary to store redundant data alongside the initial data via a storage code in order to prevent loss of the data in case of server failures.

With the increase in usage of distributed services such as cloud storage and peer-to-peer networks, the importance of user privacy is constantly on the rise. Recently, private information retrieval (PIR) in the context of coded storage has gained a lot of interest. With PIR, a user is able to download a desired file from a database or distributed storage system (DSS) without revealing the identity of the file to the servers (see Figure 2). In order to efficiently provide this feature from the multitude of different DSSs, recent research has considered several different models, such as, e.g., DSSs employing erasure codes and / or offering streaming content. To approach these problems systematically, it is paramount to understand the fundamental trade-offs between the security offered and the amount of data that can be retrieved, which is referred to as the PIR capacity of the DSS.

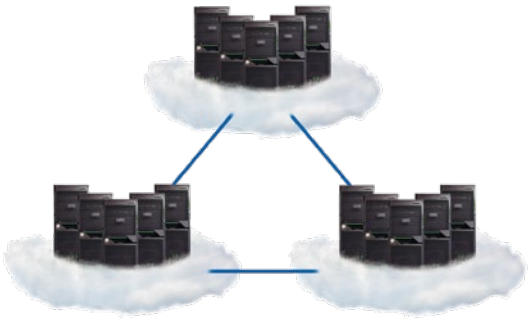
In [1], we first have proven the capacity for DSSs that are protected against failures of servers by erasure codes for the use case where the user is only supposed to learn exactly what he desired, which is referred to as symmetric private information retrieval (SPIR). Further, we considered a stronger security model, where subsets of the servers of a certain size are allowed to cooperate / collude without harming user privacy. We have also proven the capacity for a family of schemes relevant for practical applications, called strongly linear PIR schemes, thereby showing that the so-called star product scheme proposed by Freij-Hollanti et al. is optimal under some practical restrictions.

In [2], the star product scheme has been adopted, with appropriate modifications, to the case of private (e.g., video) streaming. It is assumed that the files to be streamed are stored in a distributed manner over several servers by an erasure code, and that the download is carried out in a manner suitable for streaming applications. The recently proposed star product scheme has been adapted for this special case, and various properties were analyzed for two channel models related to straggling and unreliable servers, both in the baseline case and with colluding servers.

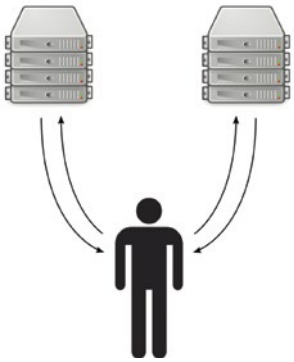
The achieved PIR rates for the given models were derived and, for the cases where the capacity is known, the first model was shown to be asymptotically optimal, when the numbers of files are large. The second scheme introduced in this work was shown to be the PIR-equivalent of a well known class of codes well suited for streaming applications. For the unreliable server model, it is shown to outperform the trivial scheme of downloading stripes of the desired file separately without memory.

In [3], we have focused on how to optimally repair a certain number of failed servers by contacting the least amount of other servers. We have derived the trade-off between the redundancy and the failure tolerance of a storage system when the number of repair servers changes according to the number of failed servers. Then, we have analyzed the repair property of a class of storage code, and we have shown that this class yields a complete optimization of the number of repair servers according to the number of failed servers. Moreover, this class achieves the best trade-off between redundancy and failure tolerance with this repair property.

In ongoing research, we are working on increasing the practicality of PIR by changing the security model from perfect security to security models based on computational hardness; that is, we protect the user against an attacker with limited computational power. This is a highly practical assumption, as computational power is never infinite in practice, and almost all modern cryptography relies on it. Further, it has recently been shown that PIR schemes operating on quantum computers have a capacity larger than the capacity of systems operating on classical computers. We are investigating the combination of such schemes with modern DSSs protected by erasure codes in order to increase their versatility and offer better trade-offs between system parameters.



1 | Distributed data storage: Cloud data is stored on multiple distributed servers.



2 | Private Information Retrieval (PIR): The user wants to download a file without revealing its identity to the server.

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[3] M. Grezet and C. Hollanti, “The Complete Hierarchical Locality of the Punctured Simplex Code”, 2019 IEEE International Symposium on Information Theory (ISIT), 2019.


*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Artificial Electronic Skin**

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Dr. Mohsen Kaboli (TUM) | Postdoctoral Researcher

Scientific Reports

Takao Someya

Host
Prof. Gordon Cheng
Cognitive Systems, TUM

## Technological advances for a better quality of life

Our Focus Group aims at the realization of a novel paradigm that could lead to important advances in robotics and help to enhance the quality of life. This research pursues the creation of an artificial electronic skin that imitates the properties of human skin using innovative fabrication techniques of printed electronics. The essential element of the “artificial electronic skin” concept is a network of fully printed unit-cells comprising printed sensors and specific integrated circuitry designed to mimic the human skin’s sense of touch. A large number of sensor cells will be connected to a cell network that determines touch information across large areas and transmits it in a manner comparable to the human nervous system.

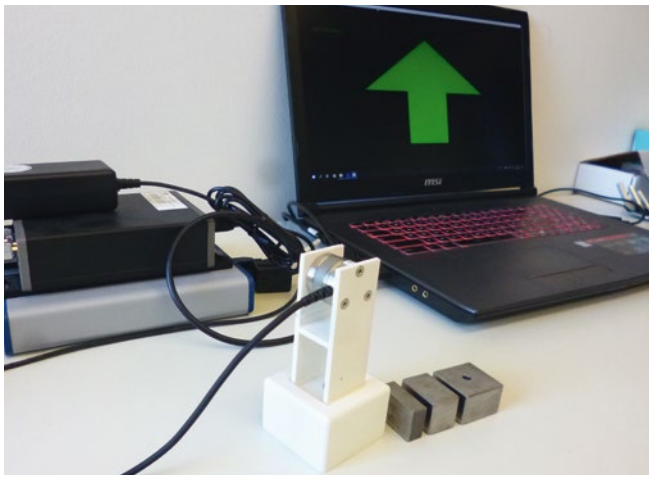
One or more cells can be connected to a processing system to interpret the sensor information and support other perception channels, for example in a humanoid robot. A similar architecture may be applied on prostheses as well as for health and fitness monitoring. Printed electronics technology offers inherent advantages to the development of an artificial skin: Mechanically flexible and even stretchable materials of large size can be utilized as a substrate for recently developed inks of electronic materials. These possess interesting properties, such high conductivity, high dielectric permittivity, and tunable work functions. One of the main challenges will be the integration of these sensors on large-scale areas while fulfilling mechanical requirements such as stretchability and flexibility similar to that of human skin.

The impact of artificial electronic skin is potentially enormous, as it could be applicable across multiple domains in building safer robots, improving healthcare monitoring, bringing a new dimension to entertainment, and enabling wearable technologies that enhance people's lives.

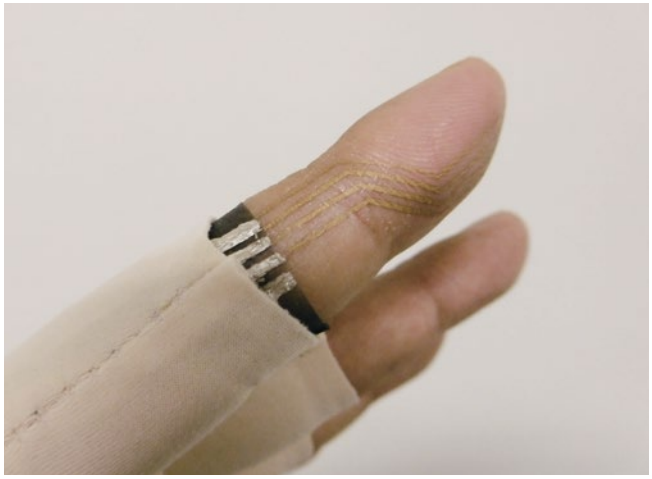
## Technical challenges

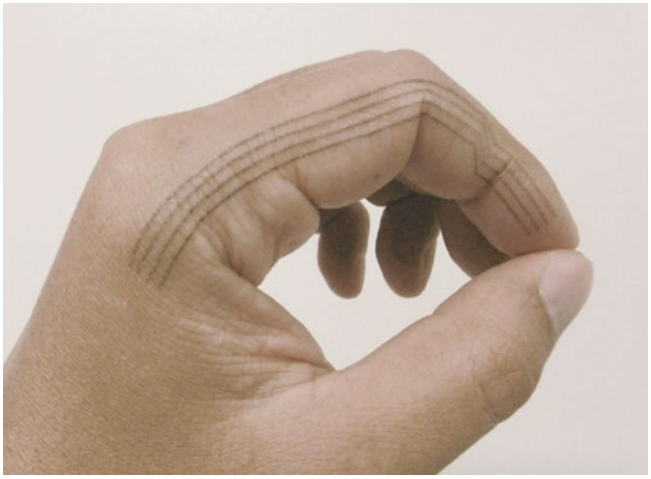
Over the past year, we investigated how to optimize the bendability and stretchability of connections between artificial skin cells such that we can integrate stretch sensors into the connection to monitor the distance between skin cells. Measuring the distance between skin cells is essential to enable automatic 3D surface reconstruction for skin patches, which provide the location of each skin cell.

The original aim was to integrate the sensor, data communication links, and power supply lines in one substrate. After many tests, we have concluded that stretchable substrates with the required properties are not the best solution to the problem, when we consider the current limitations of the technology. On the basis of these findings, we have altered the whole structure. We developed a new concept, where we only implement the stretch sensor on stretchable material and combine this sensor with the technology currently used for connecting skin cells at the Chair for Cognitive Systems.



1 | Experimental setup for the object manipulation task for the human participants. Object is printed with a 3D printer and force transducer (Nano 25, ATI) mounted in the middle of the object. Subject will pick up the object with 4 different weights and hold for 5 seconds. The grip force is measured with 1kHz sampling, and compared for different materials applied on the subject's finger tips in order to investigate the effect.





2 | Ultrathin nanomesh sensor directly applied on the finger of a human participant. These sensors are designed to measure a biological information (pressure, temperature, strain, etc).

We have been developing and testing our new implementation of this structure of the electronic sensor. We arranged our flexible sensors with electronic circuits along the stretchable material that we were using for connecting skin cells. This stretchable material plays a role in both data communication and power supply. We have been testing the prototype and are currently satisfied with the result. Due to the multidisciplinary features of artificial electronic skin, it is important to enhance collaboration among researchers in different research fields. Our research has been strengthened by a new collaboration with another research group at TUM. Prof. David Franklin, who leads the Neuromuscular Diagnostics group in the Sport and Health Sciences department, is a leading scientist in the field of human cognition and interaction. He shared an interest in the artificial sensory input system we have been developing. After several meetings, we developed a collaboration plan to apply ultrathin nanomesh sensors directly on human skin and examine their effect during object manipulation tasks. We have already tested this scheme and have preliminary results. We anticipate a joint publication in 2020.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Embedded Systems and Internet of Things**

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Scientific Reports

Sebastian Steinhorst

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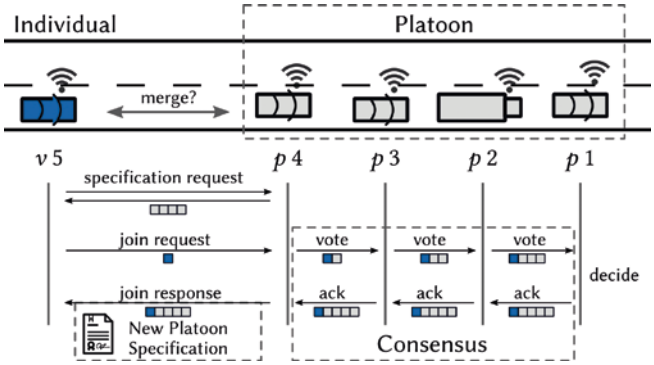
## Toward an internet of collaborating autonomous systems

Within the emerging area of the Internet of Things (IoT), communication capabilities enable the collaboration of autonomous system components. Our research centers on the question of how to make such system architectures resilient, efficient, safe, and secure. Within this line of research, we consider the automotive domain as an interesting application area. Autonomous vehicle platoons, for example, are energy-efficient and increase the road throughput by allowing vehicles to drive with a reduced inter-vehicle distance.

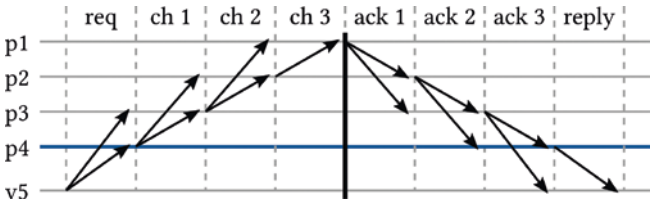
In this context, we have proposed a distributed platoon management scheme, where platoon operations such as join or merge are decided by consensus over a vehicular ad hoc network (VANET). Since conventional consensus protocols are not suitable for cyber-physical systems (CPS) such as platoons, we have introduced Chained Unanimous Byzantine Agreement (CUBA) [1], a new validated and verifiable consensus protocol especially tailored to platoons, which considers their special communication topology. In contrast to majority-based consensus protocols, CUBA requires all vehicles to agree on the same decision and requires this decision to be verified by all vehicles, as shown in Figure 1.

To ensure that all vehicles will receive the ⟨Ack⟩-message of a successful consensus round, each vehicle must be able to send messages to the next two vehicles in each direction. This message exchange of the protocol is illustrated in Figure 2. CUBA focuses on failure detection and guarantees to terminate within a fixed time window. As another aspect in the automotive domain, we are investigating how to efficiently achieve a fail-operational design of autonomous automotive systems. In the absence of a driver who can maintain control of the car in a critical failure scenario, automotive systems have to be fail-operational by design, using hardware or software redundancy.

We have developed a methodology to design fail-operational automotive software using agent-based graceful degradation. In contrast to existing solutions, our agent-based approach finds task mappings at run-time and ensures the fail-operational behavior of tasks in the system using passive software redundancy. By shutting down non-critical applications, resources can be freed at run-time to restart safety-critical applications after the failure of an electronic control unit (ECU). Additionally, the dynamic nature of the agent-based system allows reconfiguration of the system by restoring the lost redundancy. With this work, accepted for publication in 2020, we have shown that a run-time fail-operational approach that does not add any costly redundant hardware resources is possible.




1 | Our idea of a consensus-based join maneuver. An individual vehicle requests to join an existing platoon. The join request is forwarded to each platoon vehicle, which will vote on the request. If all vehicles agree, the new vehicle is accepted and the new specification is sent to all vehicles.




2 | Message flow of a join-request. Vehicle $v_5$ sends the request to the platoon vehicles $p_4$ and $p_3$. $p_4$ will start a consensus round, and when $p_1$ receives a valid chain of accepting votes, it decides for the new platoon and sends an ⟨Ack⟩ back to $v_5$.

Our third contribution in the automotive domain focuses on holistic cybersecurity solutions for the Internet of Vehicles (IoV). Here, we are contributing to the EU-funded H2020 “nIoVe” project [2] by providing research solutions for decentralized identity management, shared threat repositories, and attack response strategies.

Industrial automation is another area where system autonomy is on the rise. With our new BMBF-funded cooperation project ReMiX, which started in 2019, we are applying our expertise in IoT system architecture decentralization to improve the resilience of mixed-criticality industrial measurement and control systems.

Our activity in the industrial IoT context is further extended with our involvement in the standardization activities in the World Wide Web Consortium (W3C), which aims to tackle the interoperability problem arising from an ever-increasing diversity of devices in industrial environments, as well as smart homes and cities. In addition to our contributions to the Thing Description standard [3], we are also working with the Eclipse Foundation on the Thingweb project and operating our own WoTify platform [4].

## References

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[2] https://niove.eu/.

[3] https://w3c.github.io/wot-thing-description/.

[4] https://wotify.org/.

*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Environmental Sensing and Modeling**

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Dr. Shrutilipi Bhattacharjee (TUM) | Postdoctoral Researcher
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Scientific Reports

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## Measuring greenhouse gas (GHG) emission in cities

The majority of anthropogenic greenhouse gas (GHG) emissions originate from cities. Therefore, monitoring emissions in cities is essential to fight climate change. In Germany and many other countries worldwide, emission reduction goals are evaluated by using software that is based on a bottom-up calculation method instead of measuring the real emissions, because of the difficulty of measuring the emissions of a big area source. That's why we have developed the differential column measurement approach [1]. Thereby ground-based FTIR (Fourier-transform infrared) spectrometry is used to determine the column-averaged concentrations of $CO_2$, CO, and $CH_4$ upwind and downwind of a city. The difference between those two concentrations is then proportional to the city's emissions.

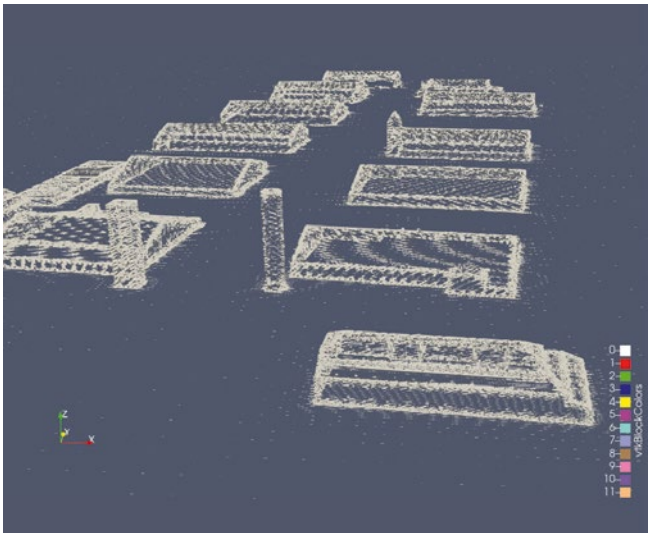
## Launch of our greenhouse gas network

In summer 2019, we launched our greenhouse gas network, which is unique in the world, to determine the city emissions of Munich. The network consists of five fully automated and highly precise FTIR monitoring systems using the sun as a light source [2, 3]. It allows us to measure $CO_2$, $CH_4$, CO, and $NO_2$ column concentrations throughout the year. From now on, we will assess the Munich emissions for the first time not only by calculations (the government's standard procedure) but also by measurements. The network will run fully automated in the coming years to measure greenhouse gas concentrations all year long. The five systems are distributed in and around Munich. They are located at our university building in the city center, Oberschleißheim, Gräfelfing, Feldkirchen, and Taufkirchen (see Figure 1). The network is funded by the German Research Foundation (DFG).

## Measuring emissions of the Oktoberfest

In addition to operating our stationary network, we conducted a measurement campaign in September and October to determine the emissions of the Oktoberfest again, as in 2018. In 2019 the goal was to look more closely into the source attribution. For that reason, we used both a portable gas measurement system in a backpack and additional air sampling bags to examine the isotopic composition of exhaust gas. In contrast to 2018, we were allowed to enter the festival with our instrument to investigate the emission hotspots thoroughly. The measurements were carried out both during and after the time of the festival to compare the differences in emission strength and distribution. Furthermore, a sophisticated CFD (computational fluid dynamics) simulation was developed to determine the emission number of the festival in an improved way (see Figure 2). We reported the results of our Oktoberfest campaigns published as a highlight article in Atmospheric Chemistry and Physics [4], The study is also featured by Science [5] and Nature as a research highlight [6].


1 | Setup of the fully automated urban greenhouse gas network in Munich.



2 | CAD mesh model of Oktoberfest for CFD simulation.

## Urban modeling of greenhouse gases

As measurements cannot cover the complete urban area, a suitable modeling framework is needed to quantify all the urban emission sources. To predict column-averaged abundances of $CO_2$,and $CH_4$ ($XCO_2$ and $XCH_4$), we are using the Weather Research and Forecasting (WRF) model coupled with GHG modules (WRF-GHG) developed for mesoscale atmospheric GHG transport. To assess the precision of WRF-GHG and provide insights on how to detect and understand sources of GHGs within urban areas, we used WRF-GHG in a case study in Berlin at a high spatial resolution of 1 $km^2$. There, we compared the model results with the results of a measurement campaign. The findings of this study show that WRF-GHG is suitable for precise GHG transport analysis in urban areas when it is combined with differential column measurements [7].

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[5] K. Kupferschmidt, “Hold my beer. Munich’s Oktoberfest beats Boston for methane emissions”, Scienes Magazine, 25th October 2019, doi:10.1126/science.aaz9918.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Modeling Spatial Mobility**

Prof. Rolf Moeckel (TUM) | Rudolf Mößbauer Tenure Track Professor
Prof. Kelly J. Clifton (Portland University) | Hans Fischer Senior Fellow
Dr. Ana Tsui Moreno Chou, Dr. Carlos Llorca Garcia (TUM) | Postdoctoral Researchers
Nico Kühnel, Cat Silva, Qin Zhang (TUM) | Doctoral Candidates



Rolf Moeckel

Kelly J. Clifton

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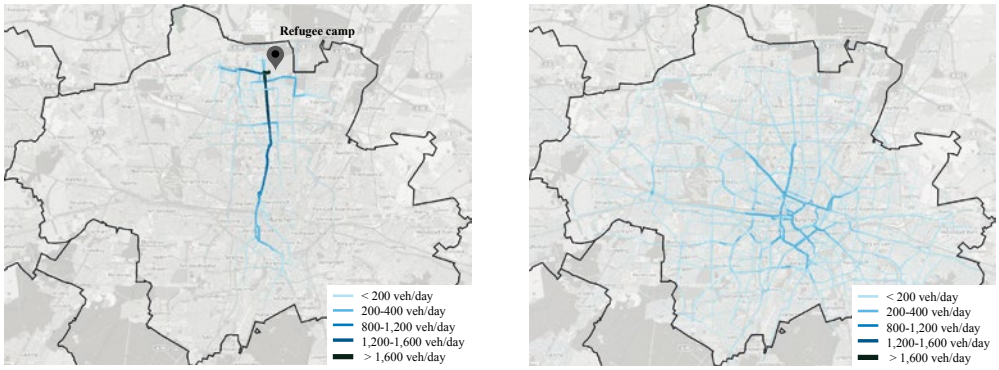
Mobility, TUM

## Transport modeling and travel behavior research

The Focus Group Modeling Spatial Mobility (MSM) conducts research on integrated land use/transport modeling and travel behavior. This includes the development of land use, transport, and related models, such as environmental impact and health models. This also includes the spatial analysis of travel behavior and location choice of households and firms. The interaction between land use and transport is of particular interest.

An integrated land use/transport modeling suite has been implemented for the Munich Metropolitan Area. The base year is 2011, and the model simulates land use and travel behavior through 2050. The study area consists of 444 municipalities with a population of 4.5 million. The study area has been delineated on the basis of commuter flows. The size of the study area was chosen because of long commute distances found in the area, driven in part by rather high cost of living in Munich.

Figure 1 shows the difference in travel demand of 15,000 refugees depending on whether they are concentrated in one (imaginary) refugee camp or proportionately across town.




1 | Travel generated by an (imagined) refugee camp in Northern Munich with 15,000 refugees (left) and by 15,000 refugees who have been distributed proportionately across town

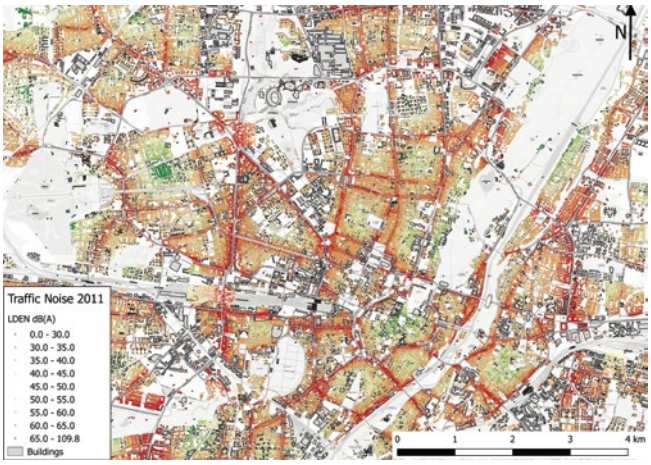
The modeling suite consists of the land use model SILO, the travel demand model MITO, and the assignment model MATSim. The former two were developed from scratch by this research group, and the latter was developed at ETH Zurich and TU Berlin. All three models are built as agent-based models that simulate individual households and persons.

The entire modeling suite is currently implemented for Munich, Cape Town, South Africa, and the Kagawa Region in Japan. By using various study areas in very different social and economic concepts, the transferability of these models is stress-tested, and the scenario sensitivities for different environments are analyzed.

In cooperation with Prof. Kelly Clifton of Portland State University, we further integrated the existing modeling suite with the pedestrian model MoPeD. MoPeD in turn has been improved to overcome several limitations of the previous version. First, the new MoPeD model is developed in Java. This change made the model efficient and operational for the entire region with a runtime of a few minutes. Trip generation models for non-home-based trip purposes were improved. We constructed a new measurement of the pedestrian environment that reflects pedestrian accessibility and simplifies characteristics of the built environment. The new MoPeD model has been reestimated to evaluate walk and non-walk transport demand in the Munich region. MoPeD also was integrated with the SILO/MITO/MATSim modeling suite described above, which improved the representation of walking behavior in this model. Transport-related policies that affect pedestrian travel demand were investigated for the Munich region.

To complement person travel demand, a freight model was built in cooperation with the chair of Logistics and Supply Chain Management in the TUM School of Management (Prof. Stefan Minner). A national database of freight flows is disaggregated to a finer spatial resolution using input-output coefficients. Flows traveling by truck are converted to vehicles and assigned to the network. Using mathematical optimization algorithms, the optimal locations of “micro-depots” for cargo bikes was selected. Thereby, the model makes it possible to trace individual parcels from global shipment to national transport to urban distribution centers to micro-depots to the final recipient.

Environmental issues are an important factor for household relocation. A combination of rent prices scraped from the web and simulated traffic volumes showed a 6 percent rent discount for dwellings that are exposed to traffic noise of more than 55 dB(A). For dwellings with more than 65 dB(A), the rent discount was almost 10 percent. This sensitivity has been added to the SILO/MITO/MATSim modeling suite.




2 | Simulated noise caused by traffic in Munich

Model results show that wealthy households are able to afford less noisy housing locations, whereas low-income households often can only afford dwellings that are exposed to higher noise levels. This setup allows the comparison of who is generating traffic noise and who is suffering from noise. Policies can be developed that target noise generators and benefit households exposed to noise.

All models developed by this research group are open source under the GNU license and provided at https://github.com/msmobility free of charge. Interested users are welcome to download, use, and further develop these models. As far as legally possible, data to run these models are shared as well.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Pollutants and Sustainability Governance**

Prof. Noelle Eckley Selin (Massachusetts Institute of Technology) | Hans Fischer Senior Fellow
Prof. Henrik Selin (Boston University) | Hans Fischer Senior Fellow
Fiona Kinniburgh (TUM) | Doctoral Candidate

Scientific Reports

Noelle Eckley Selin

Henrik Selin

Host
Prof. Miranda Schreurs
Environment and Climate Policy, TUM

Human societies have fundamentally altered the Earth in ways that have facilitated the development of modern societies but also challenge our ability to protect and improve human well-being over the longer term. One example of this is the intentional and unintentional mobilization of large amounts of material substances into society and the environment. Some of these substances are naturally occurring elements, like mercury and carbon, while other chemicals are manufactured in laboratories. Many substances from both groups have severe negative impacts on human health and the environment, from local to global scales. Our Focus Group develops theories and methods to assess transitions to sustainability, building on social sciences, natural sciences, and engineering, and applies them to richly described empirical cases of selected pollutants. The research aims to draw lessons that inform policy-making and practice with respect to contemporary sustainability challenges. The ultimate objective of the work is to improve theory building about how humans, technology, and the environment interact in the context of institutions and knowledge over time, to help inform sustainability governance.

## Theory and methodological development

The need for additional analytical frameworks, tools, and methods is recognized as a critical challenge in the sustainability science literature. This requires a systems perspective, considering processes and dynamics in the natural environment, human behavior and institutions, and the development of technologies. A key result of our Focus Group is the development and application of a new Human-Technical-Environmental systems framework (the HTE Framework), a structured and comprehensive method for assessing sustainability-relevant issues, particularly those involving pollutants. The HTE Framework is described and applied to empirical examples of mercury pollution using a matrix-based approach in a forthcoming book (Selin and Selin, MIT Press, 2020). Ongoing work evaluates the applicability of the framework to other issues, including air pollution and climate change, and in place-based case studies.

## Empirical cases: Mercury, pesticides, air pollution, and climate change

A major empirical focus has been mercury, which poses substantial health and environmental risks, both locally and through long-range transport. Mercury is emitted from a variety of sources worldwide, including coal burning, industrial processes, and its use in artisanal and small-scale gold mining. More than 110 countries and the European Union are parties to a global treaty, the Minamata Convention on Mercury, that aims to protect human health and the environment from mercury pollution. For pesticides, managing human health risks has historically been the focus of pesticide governance efforts, but mounting evidence of biodiversity loss worldwide is highlighting the chronic impacts these chemicals also have on the environment.

Our work focuses on better understanding the links between these two issues, and the ways in which scientific advice processes are set up to inform policy solutions. With respect to air pollution and climate change, our Focus Group examines how social movements, governments, and interest groups interact in policy change. We also examine the connections between climate change and air pollutants from a systems perspective.

## Workshops, field visits, and other activities

Members of the Focus Group co-organized and participated in two workshops at TUM relevant to our work during 2019. Kinniburgh co-organized an emerging scholars workshop, “Power Sharing or Power Shifts? Examining the role of public-private interactions in global governance.” Schreurs co-organized a Jean Monnet Network on EU-Canada Relations Workshop: “The Social, Territorial, and Political Dimensions of Climate Change: Canada and the European Union,” which was attended by N. Selin and Kinniburgh. Data collection for empirical cases is ongoing through document analysis and interviews. N. and H. Selin carried out interviews and participant observations at the third Conference of Parties to the Minamata Convention on Mercury. Kinniburgh conducted interviews at meetings of 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. Kinniburgh conducted fieldwork and interviews with farmers, pesticide vendors, and policymakers in the Indian states of Kerala and Andhra Pradesh on national implementation challenges for pesticide risk reduction, as well as the potential role of state-level policies for leading a transition to zero-pesticide sustainable farming.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Soil Architecture**

Prof. Johannes Lehmann (Cornell University) | Hans Fischer Senior Fellow
Thiago Massao Inagaki (TUM),
Angela Possinger (Cornell University) | Doctoral Candidates

Scientific Reports

Johannes Lehmann

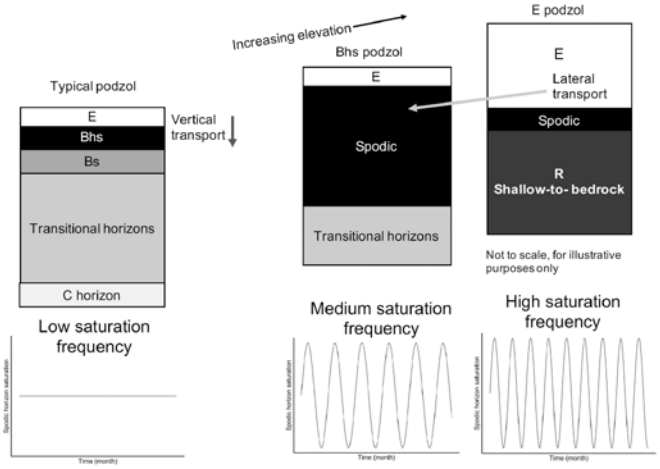
Host
Prof. Ingrid Kögel-Knabner
Soil Science, TUM

Soil organic matter (SOM) plays an important role for food production, water quality and climate, and it functions as a sink for soil organic carbon (SOC). Even small variations in proportions of substances in the soil can lead to significant changes in the emission of greenhouse gases. Therefore, as soils have a recognized capacity for carbon storage, understanding of the mechanisms responsible for SOM stabilization is of high importance. Soil water content is a key variable influencing SOC mineralization, with a well known relationship between soil moisture and microbial respiration. In contrast to the prevailing concept that increased moisture leads to accumulation of SOC due to decreased microbial metabolism, reducing conditions resulting from short-term saturation events in otherwise aerobic soils may drive mineral dissolution and thereby increase mobilization of mineral-associated SOC (Figure 1). We therefore investigated changes in reactive metal and SOC properties and organo-mineral interactions as a function of moisture saturation frequency.

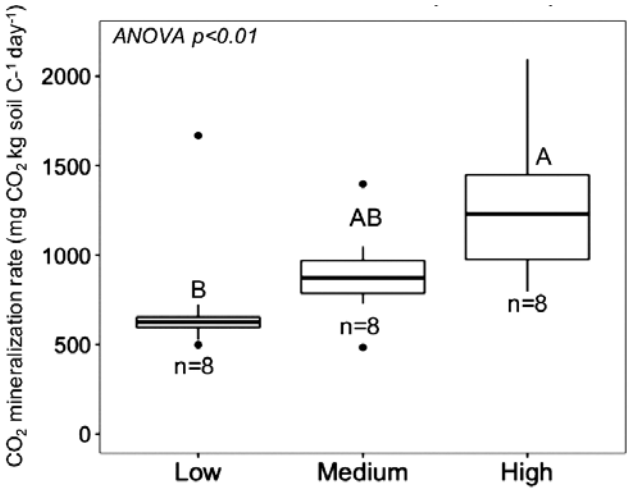
## Moisture effects on soil carbon

We found that organic carbon mineralizability increased with increasing saturation frequency (Figure 2). The concurrent release of dissolved organic carbon was proportional to iron at low saturation frequency, whereas it was proportional to aluminum at high saturation frequency (Figure 3). An increase in both soluble total Fe and $Fe^{2+}$ demonstrated the induction of reducing conditions. At high saturation frequency, the increase in $Fe^{2+}$ with anaerobic conditions was five-fold higher than that at low saturation frequency, suggesting that Fe redox dynamics influence dissolved carbon availability. By pairing imaging and bulk extraction approaches with analysis of organo-mineral bonding, we can use the dataset to infer mechanisms of interaction, in addition to observing changes in organo-mineral spatial association (i.e., co-location) and elemental correlation. The observed shift toward more reduced Fe(II) at higher saturation frequency suggests that the duration of saturation in this system is sufficient to induce reducing conditions; this resulted in not only mobilization and Fe loss, but also shifts to the remaining Fe mineral redox state. These shifts were reflected in increasing Fe(II)-organic complex, decreasing Fe(III)-organic complex, and increasing Fe(II)/Fe(III) mineral content with higher saturation frequency. The observed shift in mineralizability highlights the need to model C stabilization in soils with frequent saturation-draining fluctuations separately from soils with low saturation frequency or persistent saturation.

*Publications by this Focus Group can be found in the section Publications of this report.*



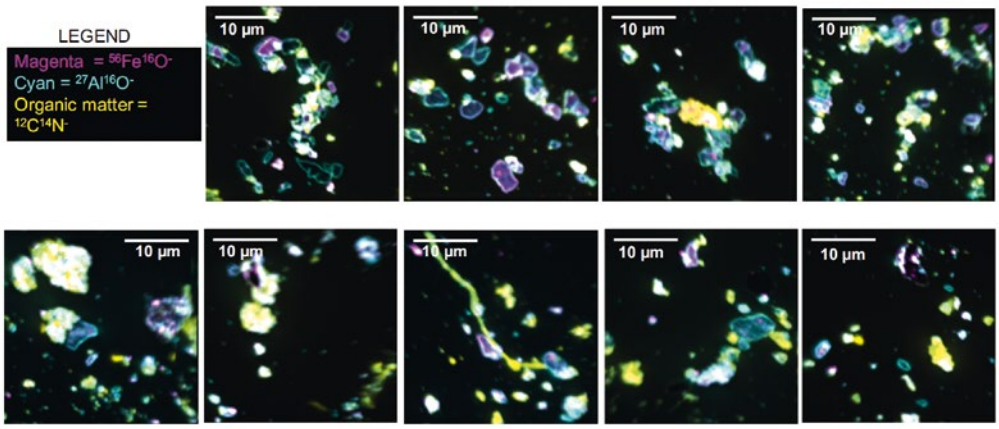

1 | Simplified schematic of moisture variation in soil profiles and transport of carbon.



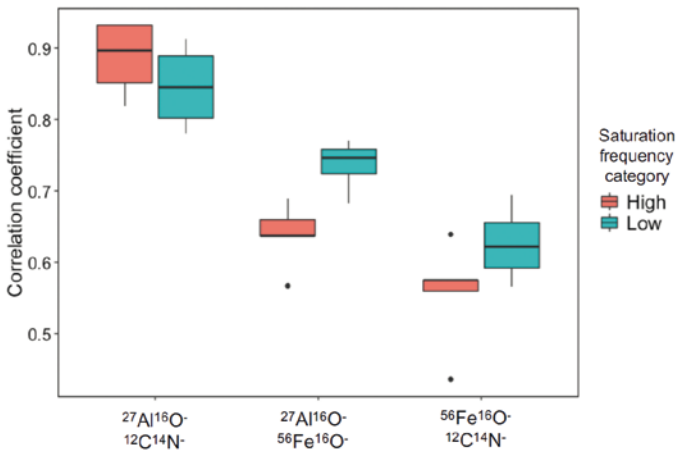

2 | Carbon mineralizability for representative soils from high, medium, and low saturation frequency.

a) Low saturation frequency NanoSIMS elemental maps

b) High saturation frequency NanoSIMS elemental maps




c) Spearman Rank pixel intensity correlation




3 | Elemental maps from nanoscale secondary ion mass spectrometry (NanoSIMS) imaging showing distribution of iron (as $^{56}Fe^{16}O^-$), aluminum ($^{27}Al^{16}O^-$), and organic matter ($^{12}C^{14}N^-$) for low (a) and high (b) saturation frequency categories. c) Element spatial correlations with NanoSIMS elemental maps.

# Focus Group **Biomolecular Design**

Prof. Hendrik Dietz (TUM) | Carl von Linde Senior Fellow

Scientific Reports

Hendrik Dietz

Host
Biomolecular Nanotechnology, TUM

## Programmable self-assembly with nucleic acids: Folding studies, custom sequences, functionalization, and protein-DNA binding

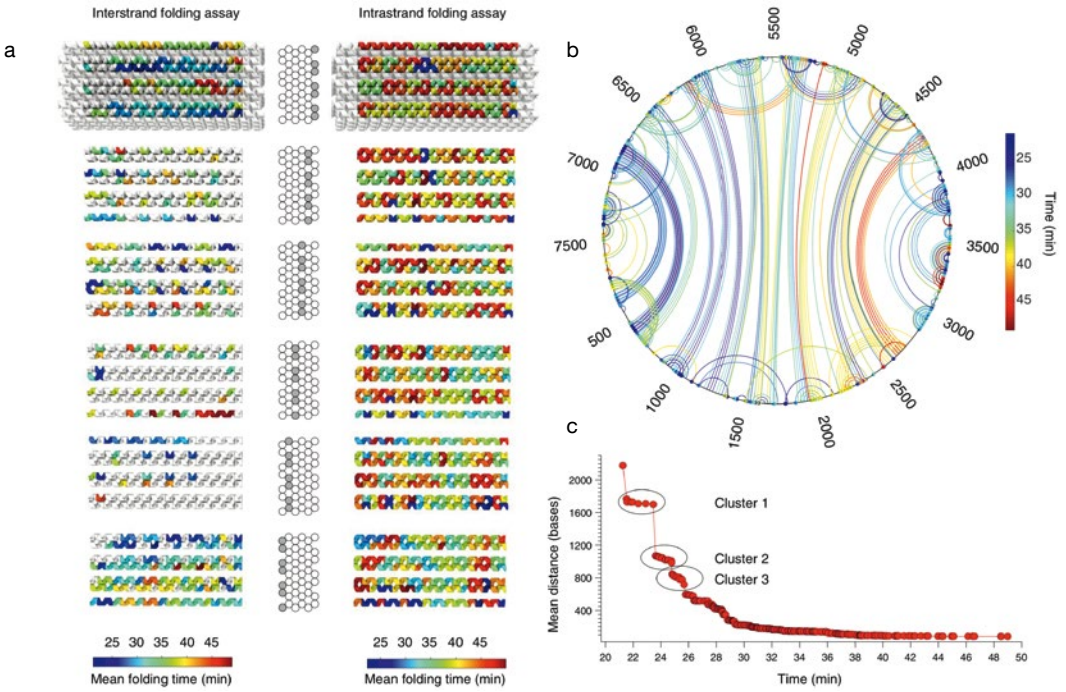
The Focus Group continues to expand our understanding and extend our control of nanoscale construction methods using biological building blocks. Basic exploration is coupled to a vision of providing research and industry with robust, useful technology based on “DNA origami” and related techniques. Selected publications illustrate the range of research we conducted during 2019.

### The sequence of events during folding of a DNA origami [1]

We provide a comprehensive reference dataset of the kinetics of a multilayer DNA origami folding. To this end, we measured the folding kinetics of every staple strand and its two terminal segments during constant-temperature assembly of a multilayer DNA origami object. Our data illuminate the processes occurring during folding of the DNA origami in fine detail, starting with the first nucleating double-helical domains and ending with the fully folded DNA origami object. We found a complex sequence of folding events that cannot be explained with simplistic local design analysis. Our real-time data, although derived from one specific DNA origami object, through its sheer massive detail could provide the crucial input needed to construct and test a quantitatively predictive, general model of DNA origami assembly.

### Custom-size, functional, and durable DNA origami with design-specific scaffolds [2]

DNA origami nano-objects are usually designed around generic single-stranded “scaffolds.” Many properties of the target object are determined by details of those generic scaffold sequences. Here, we enable designers to fully specify the target structure not only in terms of desired 3D shape but also in terms of the sequences used. To this end, we built design tools to construct scaffold sequences *de novo* based on strand diagrams, and we developed scalable production methods for creating design-specific scaffold strands with fully user-defined sequences. We used 17 custom scaffolds having different lengths and sequence properties to study the influence of sequence redundancy and sequence composition on multilayer DNA origami assembly and to realize efficient one-pot assembly of multiscaffold DNA origami objects. Furthermore, as examples for functionalized scaffolds, we created a scaffold that enables direct, covalent cross-linking of DNA origami via UV irradiation, and we built DNAzyme-containing scaffolds that allow post-folding DNA origami domain separation.




1 | From Schneider et al, Science Advances 2019: DNA origami strand routing and folding pathway. a) Layer-by-layer 3D models of the 42-helix bundle, colored according to the experimentally measured mean folding times of the staple strand segments. b) Arcs denote staple strand crossover bridging the terminal staple strand segments to the next-to-terminal segment. Discs indicate the terminal position. Numbers give scaffold strand base indices. Color code indicates the mean folding time of the terminal staple strand segment resolved from the interstrand assay. c) Estimation of the evolution of the average interbase distance on the scaffold over time. Each circle indicates a new compaction event produced by binding of a new staple segment at the mean folding time obtained from the interstrand assay.

## Dissecting FOXP2 oligomerization and DNA binding [3]

Protein–protein and protein–substrate interactions are critical to function and often depend on factors that are difficult to disentangle. Herein, a combined biochemical and biophysical approach, based on electrically switchable DNA biochips and single-molecule mass analysis, was used to characterize the DNA binding and protein oligomerization of the transcription factor, forkhead box protein P2 (FOXP2). FOXP2 contains domains commonly involved in nucleic-acid binding and protein oligomerization, such as a C2H2-zinc finger (ZF), and a leucine zipper (LZ), whose roles in FOXP2 remain largely unknown. We found that the LZ mediates FOXP2 dimerization via coiled-coil formation but also contributes to DNA binding. The ZF contributes to protein dimerization when the LZ coiled-coil is intact, but it is not involved in DNA binding. The forkhead domain (FHD) is the key driver of DNA binding. Our data contributes to understanding the mechanisms behind the transcriptional activity of FOXP2.

### Building machines with DNA molecules [4]

In nature, DNA molecules carry the hereditary information. But DNA has physical and chemical properties that make it attractive for uses beyond heredity. In this Review, we discuss the potential of DNA for creating machines that are both encoded by and built from DNA molecules. We review the main methods of DNA nanostructure assembly, describe recent advances in building increasingly complex molecular structures, and discuss strategies for creating machine-like nanostructures that can be actuated and can move. We highlight opportunities for applications of custom DNA nanostructures as scientific tools to address challenges across biology, chemistry, and engineering.

### Reversible Covalent Stabilization of Stacking Contacts in DNA Assemblies [5]

Stacking bonds formed between two blunt-ended DNA double helices can be used to reversibly stabilize higher-order complexes that are assembled from rigid DNA components. Typically, at low cation concentrations, stacking bonds break and thus higher-order complexes disassemble. Herein, we present a site-specific photochemical mechanism for the reversible covalent stabilization of stacking bonds in DNA assemblies. To this end, we modified one blunt end with the 3-cyanovinylcarbazole (cnvK) moiety and positioned a thymine residue (T) at the other blunt end. In the bound state, the two blunt-ended helices are stacked together, resulting in a co-localization of cnvK and T. Such a configuration induces the formation of a covalent bond across the stacking contact upon irradiation with 365 nm light. This bond can also be cleaved upon irradiation with 310 nm light, allowing repeated formation and cleavage of the same covalent bond on the timescale of seconds. Our system will expand the range of conditions under which stacking-bond-stabilized objects may be utilized.

## References

[1] F. Schneider, N. Möritz and H. Dietz, “The sequence of events during folding of a DNA origami”, Science Advances, vol. 5, no. 5, p. eaaw1412, 2019.

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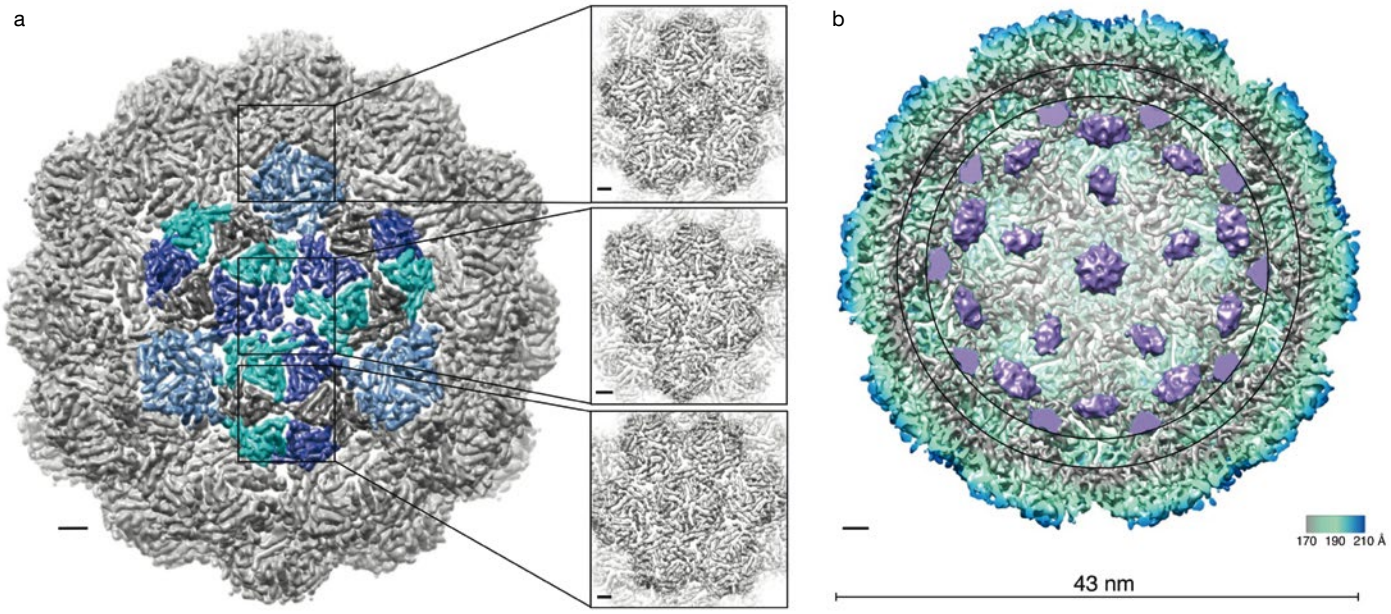
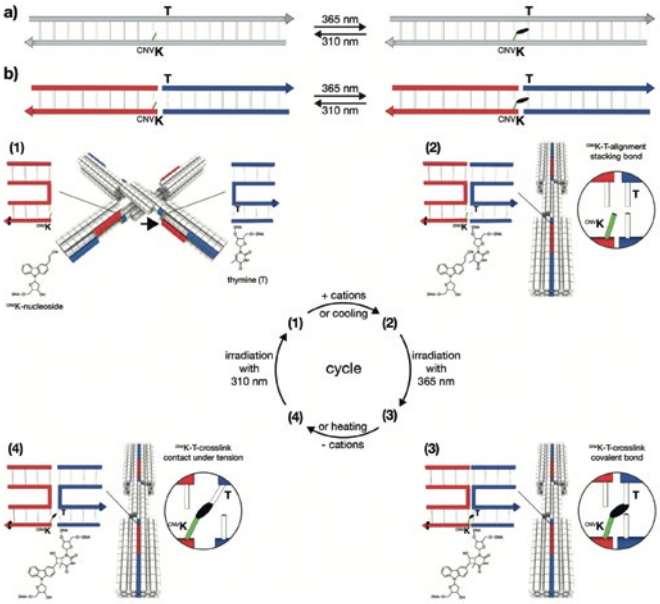
*Publications by this Focus Group can also be found in the section Publications of this report.*




2 | From Sigmund et al, ACS Nano 2019: Cryo-EM reconstruction of encapsulin nanocompartments reveals icosahedral T = 4 symmetry. a) Segmented electron density of QtEnc+QtIMEF purified from mammalian cells. The four different monomer conformations are colored according to their interconnectivity and position. The 5-fold centers are on opposite sides of a 3-fold center with two monomers in between, which indicates a T = 4 icosahedral symmetry of the shell. Boxes show zoomed-in views of the 5-fold, 3-fold, and 2-fold symmetry centers. The resolution of the map is 6 Å; scale bars represent 2 nm. b) Cutaway view through the maximum diameter of QtEnc (~43 nm) showing the shell (radially color-coded) and coexpressed QtIMEF cargo (violet) at different electron densities. A gap of 2.5 nm is apparent between cargo and shell.




3 | From Gerling et al, Angewandte Chemie 2019: Schematic of photo-crosslinking and photo-cleavage of $^{cnv}$K-modified nucleosides across stacking contacts. a) Covalent photo-cross- linking within a continuous DNA double helix. The cyanovinyl group of the $^{cnv}$K-modified nucleobase (light green) can be covalently linked to the thymine residue (T) on the "-1" position (from 5' to 3') of the complementary strand. The black ellipsoid represents the covalent bond. b) Covalent photo-crosslinking within the context of a stacking contact in DNA assemblies. The stacking contact consists of double helical protrusions (red) and double helical recessions (blue) that form discontinuous DNA double helices in the bound state. (1)–(4): Scheme of photo- crosslinking and photo-cleavage using the DNA origami switch object. (1) Open conformation of the switch under low ionic strength. The $^{cnv}$K moiety and T are separated in space. The black arrow indicates the position of the second $^{cnv}$K-modification (Figure S1). (2) Closed conformation of the switch under high ionic strength. The $^{cnv}$K moiety and T are co-localized in space. (3) Formation of the covalent bond between the $^{cnv}$K and T upon 365 nm irradiation. (4) The stacking contact is under tension when decreasing the cation concentration. Cleavage of the $^{cnv}$K–T covalent bond can be triggered upon 310 nm irradiation.

# Focus Group **Cellular Protein Biochemistry**

Prof. Matthias J. Feige (TUM) | Rudolf Mößbauer Tenure Track Professor
Nicolas Blömeke, Joao Coelho, Karen Hildenbrand, Susanne Meier, Yonatan Mideksa, Stephanie Müller (TUM) | Doctoral Candidates



Matthias J. Feige

Host
Cellular Protein Biochemistry, TUM

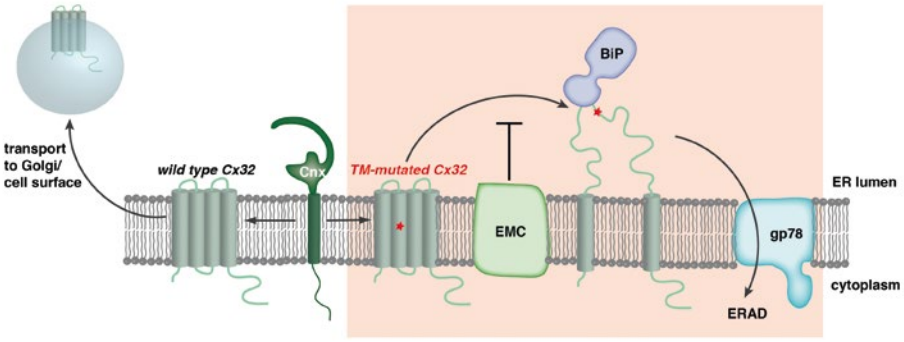
## Developments in the Focus Group for Cellular Protein Biochemistry

In complex organisms, cells need to communicate and interact with each other. This communication is the basis of growth, development, memory formation, and immune defense. Key players in all cellular communication processes are proteins secreted from cells or displayed on the cell surface. Within a mammalian cell, a specialized subcompartment exists that is responsible for the production of these proteins: the endoplasmic reticulum (ER), an extended net-like structure within the interior of the cell. Proteins are not only produced in the ER, but also controlled by it. Only proteins that have acquired their correct biologically active structure are allowed to leave the cell or to be displayed on the cell surface. Faulty proteins are recognized by dedicated molecular quality control machinery and degraded. Insights into protein structure formation and its control in the cell are of immediate medical relevance for human pathologies such as Alzheimer's or Parkinson's disease – but may also inspire new approaches in medicine and biotechnology. In our laboratory for Cellular Protein Biochemistry (CPB lab) we use an interdisciplinary approach ranging from structural biochemistry to mammalian cell biology to understand and ultimately engineer the underlying processes.

Current work in the CPB lab focuses on two major topics. The first is quality control of membrane proteins, where principles are of immediate biomedical relevance yet remain mostly unknown. Failures in membrane protein biogenesis are associated with a large number of neurological disorders. One such example is X-linked Charcot-Marie-Tooth disease, which is caused by mutations in Connexin 32. In our work we were able to show that mutations in Connexin 32 can disturb its proper structure formation and integration into the lipid bilayer [1] (Figure 1). This compromises formation of Connexin 32 gap junctions, nanochannels that allow the transport of small molecules within and between cells and are essential to our nervous system. As a consequence, Schwann cells, which form an insulating layer around nerve cells, die, and signal transmission in the nervous system is compromised. Our insights provide a molecular explanation for certain types of Charcot-Marie-Tooth disease, which may ultimately help in developing new therapeutic approaches.

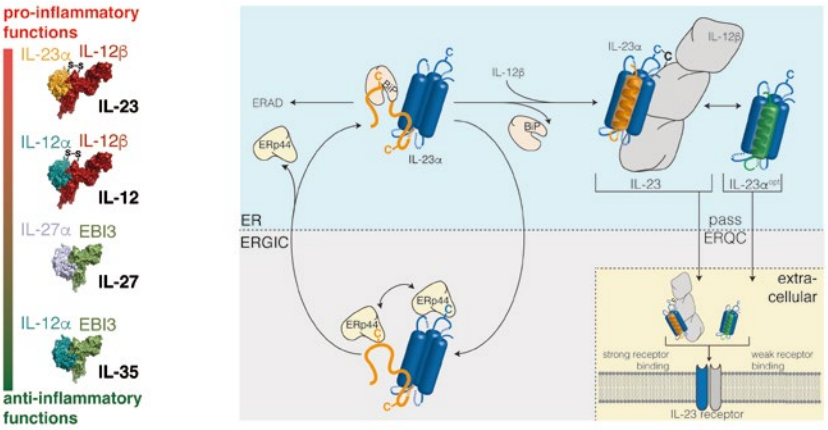
A second research focus in the CPB lab is the biogenesis and engineering of interleukins (ILs), key signaling molecules in our immune system. In humans, more than 40 different ILs exist. Dependent on the individual IL, these mount, sustain, or suppress immune reactions in health and disease. Understanding interleukin biogenesis in the cell in more detail can thus provide an avenue toward rationally tuning immune responses. Our model system is the interleukin 12 (IL-12) family, which comprises four members (IL-12, IL-23, IL-27 and IL-35) that span a broad range of biological functions [2] – from activating immune responses to suppressing immunity (Figure 2a). As such, IL-12 family members are involved in a large number of human diseases including autoimmune disorders, cancer development, and sepsis.

A recent study from our lab has revealed the molecular mechanisms of how cells produce IL-27, an IL-12 family member that is intimately involved in the development of inflammatory diseases. In close collaboration with TUM research groups in




1 | Connexin 32 (Cx32) is normally transported to the cell surface to form gap junctions. If mutated in its transmembrane (TM) regions, membrane integration can be compromised, which is counteracted by the ER membrane protein complex (EMC). Misintegrated TM sequences are recognized by the molecular chaperone BiP, and faulty proteins are ultimately targeted for ER-associated degradation (ERAD) by the ubiquitin E3 ligase gp78. Figure taken from [1].

a




2 | a) Schematic of the IL-12 family. Each family member is an αβ heterodimer and performs distinct roles in regulating immune responses. IL-12 and IL-23 are covalent dimers, connected by a disulfide bond (S-S), whereas IL-27 and IL-35 are non-covalent dimers.
b) The molecular basis of IL-23 biogenesis. IL-23α is retained in the cell by molecular chaperones, that recognize its unfolded first α-helix. Once IL-23α assembles with its partner, IL-12β, it can be secreted and signal via its receptor. *In silico* optimization of IL-23α allows it to pass ER quality control (ERQC) without IL-12β and act as a signaling molecule on its own. Figure in (b) taken from [4].

medicine and physics, we were able to gain detailed insights into how IL-27 acquires its native structure and how cells monitor structure formation of this protein [3]. Using these insights, we engineered a new human interleukin, which we are currently pursuing further as a potential new treatment option for sepsis, one of the deadliest diseases in developed countries without any good causal treatment options. Our patent for this interleukin won recognition with an award, the 2019 Innovation Prize of the Council of German BioRegions. For another family member, IL-23, our studies revealed molecular details of structure formation [4]. This was only possible due to a close collaboration with structural biologists at the TUM/Helmholtz Center, and it allowed us to rationally engineer the folding capacity of IL-23. IL-23 is a strongly pro-inflammatory cytokine involved in autoimmune diseases, and a therapeutic target in the clinics, so that insights into its biogenesis are of high medical interest.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Medicinal and Bioinorganic Chemistry**

Prof. Angela Casini (Cardiff University) | Hans Fischer Senior Fellow
Jens Oberkofler (TUM) | Doctoral Candidate

Scientific Reports

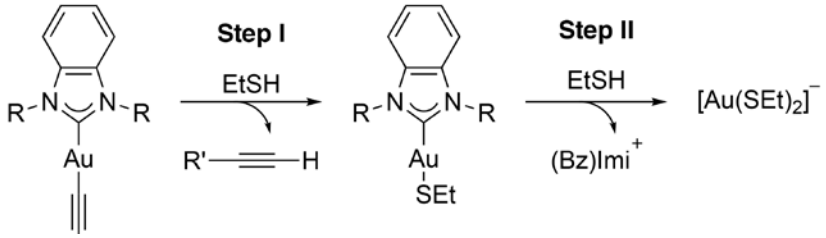
Angela Casini

Host
Prof. Fritz E. Kühn
Molecular Catalysis, TUM

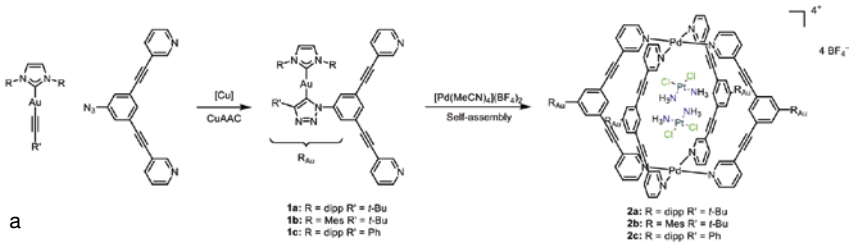
Our main aim is to develop metal-based compounds for biological and biomedical applications. In detail, the research program focuses on the design of novel *organometallic gold compounds* as possible anticancer agents or as chemical probes to study the function of target biomolecules, including proteins and nucleic acids.

From coins to wedding rings, from stained glass windows to Olympic medals, gold has been highly prized for millennia. Nowadays, organometallic gold compounds occupy an important place in medicinal chemistry due to their unique chemical and anticancer properties. The possibility of “fine-tuning” the stability of organometallic gold complexes while maintaining their biological activity and reducing their side-effects is extremely attractive. Notably, regulating the redox chemistry of gold compounds and their ligand exchange reactivity via the optimization of an appropriate organometallic scaffold may constitute a strategy to achieve selectivity for a certain pharmacological target, a feature that is not often ensured by other types of molecules. Thus, gold compounds can be designed to be active against specific biomolecules with a great degree of target selectivity and innovative mechanisms of action. Within this framework, we used NMR spectroscopy and DFT methods, to study the reactivity and binding modes of heteroleptic gold(I) N-heterocyclic carbene (NHC) complexes of general formula NHC-Au(I)-alkynyl (Figure 1) with model thiols. The results show that the reaction leads, in most cases, to the nucleophilic substitution of the alkynyl ligand by the thiol group (Step I). Of note, the BzImi-Au(I)-alkynyl complexes, upon EtSH binding, can also undergo the detachment of the NHC ligand over time (Step II).

Discrete supramolecular constructs continue to attract important research interest because of their myriad of applications, including in biology. The biomedical application of supramolecular coordination complexes (SCCs) is still an emergent field of study, but the pioneering examples available so far exploiting their host-guest chemistry demonstrate their possible use as new generation of drug delivery systems for anticancer chemotherapeutics. In fact, the robustness of supramolecular metal-based complexes, particularly *metallacages*, allows incorporation of different functionalities in the same scaffold to enable imaging in cells, but also targeting and stimuli-responsiveness. Certainly, the myriad of possible metallacages and their almost limitless modularity and tunability, without significant synthetic penalty, suggest that the biomedical applications of such species will continue along this already promising path. In this context, we are presently developing new $Pd_2L_4$ cages (with L being bipyridyl ligands, Figure 2) as drug delivery systems for the anticancer drug cisplatin. Cisplatin occupies a crucial role in the treatment of various malignant tumors. However, its efficacy and applicability are heavily restricted by severe systemic toxicities and drug resistance, which demand further research in the optimization of metallodrug targeting and delivery strategies. Part of this work is conducted in collaboration with Dr. Alexander Pöthig (Catalysis Research Center, TUM) who is expert in the design of organometallic supramolecular systems.




1 | Reactivity of NHC-Au(I)-alkynyl compounds with EtSH used as model thiol.

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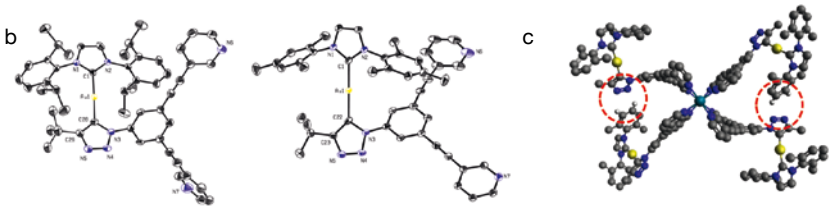


b c

2 | Scheme of supramolecular Pd2L4 metallacages exo-functionalized with cytotoxic gold moieties. a) General synthetic scheme. b) X-ray structures of cage precursors. c) DFT structure of heteronuclear Pd-Au metallacage.

Doctoral candidate Jens Oberkofler presented a poster on *"Supramolecular Heteronuclear Pd-Au Metallacages for Applications in Cancer Therapy"* at the International Symposium on Applied Bioinorganic Chemistry (ISABC15) held in Nara in June 2019, which was awarded the Elsevier *Journal of Inorganic Biochemistry* Poster Presentation Award. Furthermore, the research results of our Focus Group have been published in various international peer-reviewed journals and summarized in a number of review papers, as well as presented at national and international conferences and scientific meetings.

Overall, the ambition of our Focus Group includes not only providing targeted gold-based prodrugs with unprecedented activity and control, but also advancing the understanding of fundamental biological processes regulated by these compounds and their role in the development of diseases. Moreover, we aim at developing the promising field of supramolecular coordination chemistry for biomedical applications, particularly toward the design of novel targeted multimodal drug delivery systems.

Prof. Angela Casini was keynote speaker at the International Symposium on Applied Bioinorganic Chemistry (ISABC15, Nara, Japan, June 2019), one of the main events in the bioinorganic chemistry area, as well as at the Metallomics conference (Warsaw, Poland, June 2019). In May, she was also the plenary speaker of the Georgian Bay International conference on Bioinorganic Chemistry (CanBIC-7, in Parry Sound, Canada) and plenary speaker at the International Symposium on Metal Complexes (ISMEC 2019, Debrecen, Hungary). Of note, in November 2019 Angela was also invited to deliver the TGH Jones Memorial Lecture at the University of Queensland (Brisbane, Australia).

As a highlight of this year, in August 2019, Prof. Angela Casini received the prestigious ACS Inorganic Lectureship Award during a dedicated symposium held at the ACS annual meeting in San Diego. The award is an acknowledgement of her contribution to the development of bioinorganic chemistry.

*Publications by this Focus Group can be found in the section Publications of this report.*

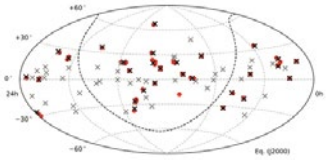
# Focus Group **Multi-Messenger Astrophysics and the United Nations Open Universe Initiative**

Prof. Paolo Giommi (Italian Space Agency) | Hans Fischer Senior Fellow
Theo Glauch (TUM) | Doctoral Candidate

Scientific Reports

Paolo Giommi

Host
Prof. Elisa Resconi
Experimental Physics with Cosmic Particles, TUM



1 | Map of the sky showing high-energy astrophysical neutrinos as crosses and counterpart candidates as red circles.

## Growing evidence for the connection between astrophysical neutrinos and active galaxies with relativistic jets

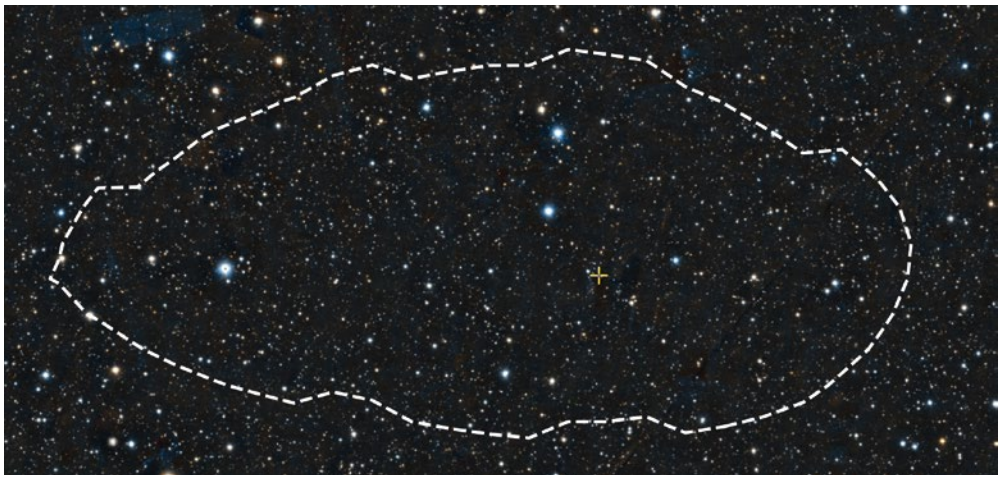
The origin of cosmic rays, the highest-energy particles reaching Earth from the Universe, is a century-old riddle. Victor Hess discovered them in 1912 and for this reason was awarded the Nobel Prize in 1936, but many questions about the origin of cosmic rays still remain unresolved. In the meantime, tremendous particle detectors have been built to measure the flux of galactic and extragalactic cosmic rays (protons and heavier nuclei), neutrinos, and gamma rays with energies up to ten million times larger than those attainable at CERN's Large Hadron Collider.

Despite the technical efforts, there are many general challenges in the identification of the sources of all of these particles:

- *Highly energetic cosmic rays* can only travel limited distances before being absorbed by radiation. Charged particles are deflected by magnetic fields and hence, even for the most energetic ones, their arrival directions are only loosely connected to their origin.
- *Neutrinos* can travel cosmological distances without being deflected, but they barely interact with matter. For this reason, their observation on Earth requires extremely large detectors that only recently have begun to operate.
- *Gamma rays* are produced in a large variety of processes, many of which may not be connected to neutrinos and cosmic rays.

In 2018, the IceCube Neutrino Observatory, together with several telescopes, announced the detection of the first source of neutrinos and gamma rays, an object named TXS 0506+056. The members of this Focus Group actively contributed to this discovery and played an important role in what followed. While the IceCube observation provides the main pieces of the puzzle, the Focus Group exploited all the additional astronomical data available in an attempt to arrive at a single coherent picture. In our follow-up work at TUM-IAS, we used the tools and data services provided by the OpenUniverse platform and found that TXS 0506+056 is a very special type of blazar, a supermassive black hole with a jet of accelerated particles pointing toward us. Through a detailed analysis of all the multi-wavelength electromagnetic data from radio up to the highest gamma-ray energies (spanning 16 orders of magnitude), we managed to confirm the association and to characterize the object as a so-called masqueraded BL Lac. These objects – a subclass of blazars – have long been suspected to be a promising source of cosmic neutrinos as they are capable of accelerating particles up to the highest observed energies. While all of these results are a milestone for the field of multi-messenger astronomy, there is still the open question: What are the counterparts of more than 70 additional high-energy, and most likely astrophysical, neutrinos detected by IceCube?

In order to address this question, we applied an improved version of our previously developed analysis pipeline to all of these events. Despite the apparent simplicity of the analysis methods, this comprehensive work rests on a foundation of broad and deep collaboration: This combines the long experience of our TUM-IAS Focus Group, which includes the founder of the OpenUniverse Initiative, with that of



2 | Optical image showing the region of sky corresponding to the neutrino alert of September 22, 2017. The white, dashed area indicates the uncertainty in the neutrino arrival direction, an area of sky including thousands of stars. The position of the astrophysical object identified as the source of this neutrino, TXS 0506+056, is at the center of the yellow bars.

senior astronomers from the ESO and scientists from the Collaborative Research Center “Neutrinos and Dark Matter in Astro- and Particle Physics” (SFB 1258) at TUM. The OpenUniverse platform provides the largest collection of publicly available astronomical data and innovative analysis tools, which allowed us to conduct a detailed analysis of the neutrino error regions and identify objects with features similar to TXS 0506+056. In Figure 1 we show a map of the sky where crosses indicate neutrino arrival directions and red circles the corresponding counterpart candidates. Each neutrino comes with a positional uncertainty of up to several degrees covering a large area of the sky, including thousands of astronomical sources, as shown in Figure 2. Here we show, for illustrative purposes, an image that is connected to the detection of the first neutrino source TXS 0506+056, with the dashed white line representing the directional uncertainty. While there are many bright and extended objects – mainly stars and galaxies – the source itself is the point-like object between the yellow bars, hardly visible by eye. After a detailed analysis of all the regions, our results, recently submitted to a refereed journal, show that despite the common assumption in the field, there are several promising astrophysical objects that coincide with IceCube neutrinos. Using a dedicated statistical test, we found that the probability of a non-connection of these sources with the neutrinos can be excluded by more than 99.99%. In turn, this means that these objects account for more than 20% of IceCube’s high-energy neutrinos.

While all of these results are exciting, we still have not exploited the full power of the available data. For future work we are planning to move away from existing gamma-ray catalogues and run our own statistical analysis pipeline on the publicly available data of the Fermi-LAT gamma-ray telescope. Most importantly, our implementation of the analysis can be run in real time, with all the results of the pipeline available to anyone shortly after the neutrino has been detected. In this way we can provide very valuable information, crucial for more precise follow-up observations using various telescopes around the world, to help realize the full potential of multi-messenger astrophysics as the key to understanding high-energy cosmic radiation.

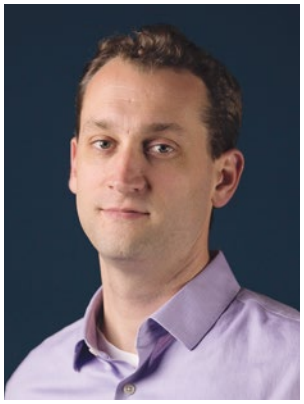
*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Population Epigenetics and Epigenomics**

Prof. Frank Johannes (TUM) | Rudolf Mößbauer Tenure Track Professor
Prof. Robert J. Schmitz (University of Georgia) | Hans Fischer Fellow
Dr. Rashmi Hazarika (TUM) | Postdoctoral Researcher
Talha Mubeen (TUM) | Doctoral Candidate

Scientific Reports

Frank Johannes



Robert J. Schmitz

Host
Population Epigenetics and Epigenomics, TUM

## Exploring plant DNA elements and spontaneous epigenetic variation

The Population Epigenetics and Epigenomics Focus Group studies how genes are turned on and off in plant genomes. The full DNA sequence complement (genome) of numerous plant species is quickly surfacing, revealing the location of genes. Missing from these efforts, however, is the location of DNA sequences that are critical determinants for controlling whether a gene is turned on or off. It is important to identify the location of these sequences as they possess an important source of genetic variation that leads to trait variation in key crop species. Once these sequences are identified, the genetic variants located in them can be linked to variation in the expression level of genes and could be used in breeding programs to improve crop performance.

A few years ago, we made a breakthrough by adopting a method for use in plant species that was originally used to study animals. This method enables the detection of these controlling sequences, as they are more accessible than non-controlling DNA sequences to an enzyme that integrates sequences into DNA. In our original study demonstrating the applicability of this method in plants, we used the model plant species *Arabidopsis thaliana*. During the last year, however, we have applied this method to leaf samples from many important crop species including maize, soybeans, asparagus, and barley, to name a few examples. These studies revealed that these controlling DNA sequences can be located very far away from their target gene and that the distance was correlated with the total genome size of the plants that we studied. We are continuing these efforts on a wider range of tissues/organs in a number of crops to reveal important DNA controlling elements that underly important traits.

In parallel, we also study how chemical modification to the DNA sequence (DNA methylation) can lead to turning off the gene. Much of the effort in this area is focused on how development or the environment affects these chemical modifications. Our group is unique in that we specifically focus on spontaneous changes to DNA methylation that accumulate naturally. In the past we have demonstrated that they accumulate, but the origins of these changes remain unknown. One major hypothesis is that they form as a by-product of reproduction when DNA is inherited from one generation to the next. To test this hypothesis, we isolated DNA from eight different branches of a long-lived perennial poplar tree that is ~350 years old. We were able to trace back the accumulation of changes to DNA methylation to a common ancestral cell and determine the extent of spontaneous DNA methylation variation. It is important to note that we discovered these variations in DNA methylation exist even though none of the samples were collected from across generations. These results show that spontaneous changes to DNA methylation that sometimes are linked to gene expression and trait variation, accumulate as a result of cells replicating their DNA within generations and not between generations.

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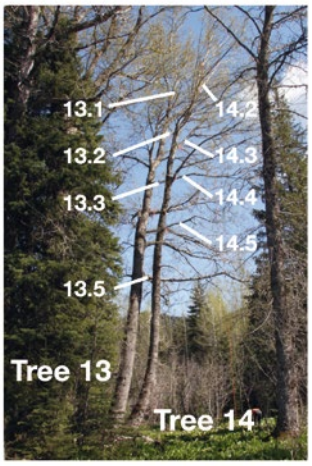


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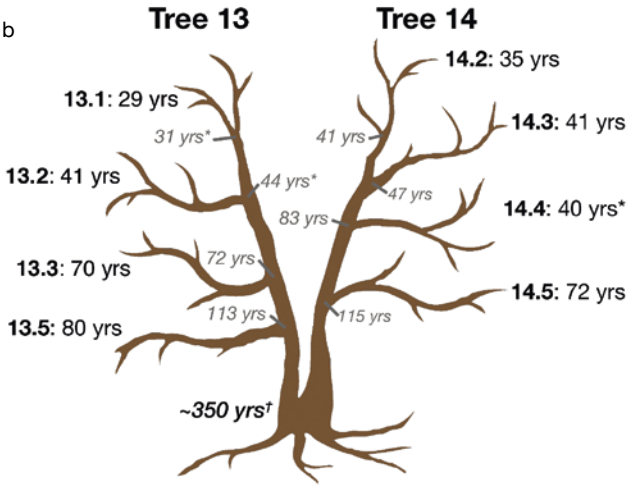



1 | Photograph and schematic drawing of the tree we studied. This wild poplar, located in Mt. Hood, Oregon, experienced a decapitation event ~300 years ago. Tree 14 re-sprouted from the stump and ~80-100 years later Tree 13 re-sprouted. (a) Leaf samples were collected from the labeled terminal branches.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

*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Structural Membrane Biochemistry**

Prof. Franz Hagn (TUM) | Rudolf Mößbauer Tenure Track Professor
Dr. Inguna Goba (TUM) | Postdoctoral Researcher
Melina Daniilidis, David Goricanec, Elisabeth Häusler, Kai Klöpfer, Kolio Raltchev, Laura Sperl, Andrea Steiner (TUM) | Doctoral Candidates

Scientific Reports

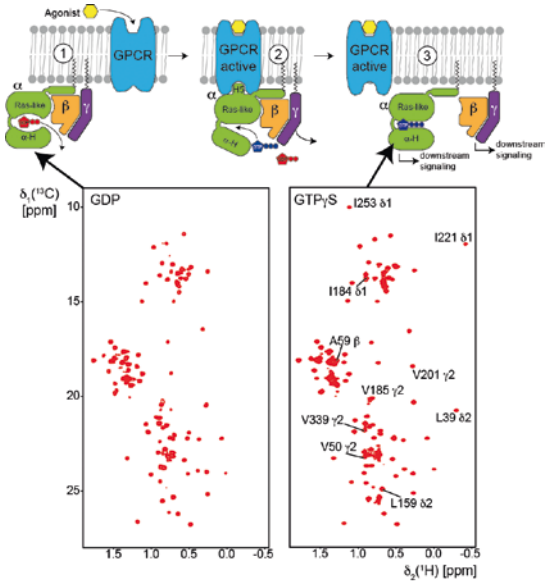
Franz Hagn

Host
Structural Membrane Biochemistry, TUM

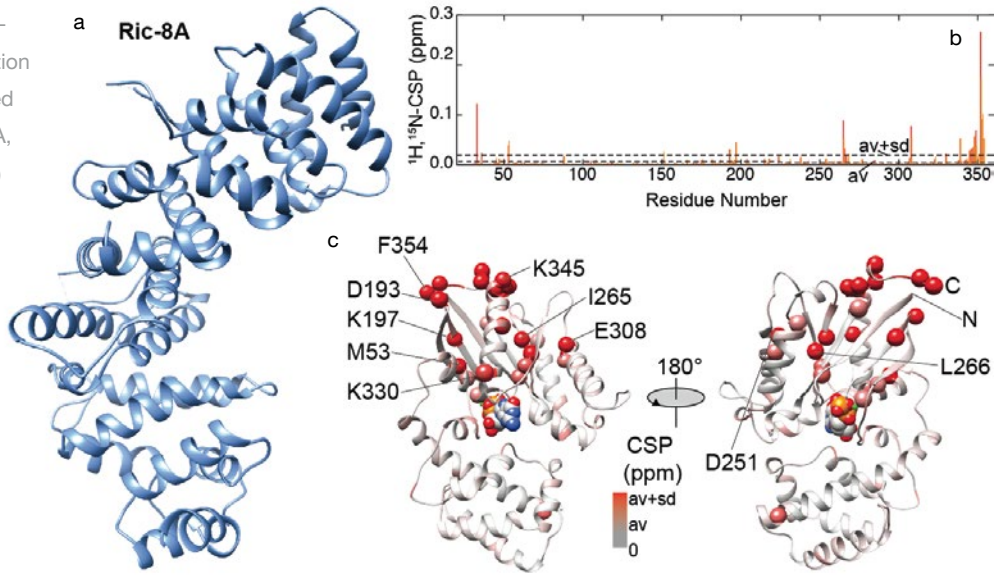
## Solution-state NMR spectroscopy of membrane proteins and their complexes in a native environment

The Focus Group Structural Membrane Biochemistry is dedicated to investigating the structure, dynamics, and interactions of membrane proteins in a native lipid environment. As a main method, we employ nuclear magnetic resonance (NMR) spectroscopy conducted at the Bavarian NMR Center (BNMRZ) at TUM. We are also heavily involved in the development and application of so-called phospholipid nanodiscs, a novel, detergent-free and lipid-based membrane mimetic [1]. Such advanced membrane mimetics can be used to investigate membrane proteins and their complexes in a “native-like” environment. With this strategy, we are able to obtain realistic information on structural, dynamical, and functional features that regulate cellular signaling across biological membranes, leading to a better understanding of the molecular signatures of these poorly understood processes. Since membrane proteins are the targets of around 60% of all currently marketed drugs, the insights obtained in our studies will facilitate the rational design of novel pharmaceuticals.

Besides our ongoing studies on mitochondrial membrane proteins [2], one particular field of interest is deciphering the mechanism of G-protein activation by G-protein coupled receptors (GPCRs) and other nucleotide exchange factors. The basic model of G-protein activation by a GPCR is depicted in Figure 1. Once an activating ligand (agonist) binds to the GPCR, the receptor undergoes an allosteric structural transition leading to the interaction with a heterotrimeric G-protein, consisting of α, β and γ subunits. This interaction leads to structural and dynamical changes within the G-protein α subunit and subsequent to exchange of GDP by GTP, followed by dissociation of the G-protein from the GPCR and separation into the G-protein α and the βγ subunits. These activated protein components then further engage in interactions mediating downstream signaling. Using NMR, we were able to characterize the G-protein α subunit and identify specific dynamical changes that are induced by the exchange of GDP by GTP [3] (Figure 1). On the basis of this work, we can now determine the structural features that are required for G-protein activation by a GPCR. In the lab, together with the group of Andreas Plückthun at the University of Zurich, we have established a suitable GPCR system, neurotensin receptor, that can be produced in bacteria and labeled with stable isotopes for NMR investigations [3].




1 | Mechanism of nucleotide exchange of a G-protein induced by a G-protein coupled receptor (GPCR). Using NMR, we can monitor the structural and dynamical signatures of the G-protein in atomic detail.




2 | Structure of the G-nucleotide exchange factor Ric-8A and its interaction with a G-protein alpha subunit probed by NMR. (a) X-ray structure of Ric-8A, adopting an ankyrin repeat fold. (b,c) NMR chemical shift perturbation experiments with isotope-labeled G-protein-alpha suggest that Ric-8A binds to the C-terminal tail of G-alpha, similar to the mode-of-action of a GPCR.

In addition to an in-depth characterization of G-protein activation by a GPCR, we are investigating the mode of action of non-GPCR nucleotide exchange factors that regulate G-protein activity in the cytoplasm without stimulation from outside the cell. One such exchange factor, Ric-8A, also exhibits chaperone functionality and is required for functional production of G-alpha subunits in mammalian cells. This functionality can be activated by phosphorylation in the cytoplasm. Thus, in collaboration with the lab of Steven Sprang at the University of Minnesota, we investigated the structural characterization of this functionally versatile exchange factor [4]. The obtained crystal structure of Ric-8A shows an $\alpha$-helical ankyrin repeat fold (Figure 2a), and subsequent NMR experiments revealed that binding of Ric-8A to the G-protein $\alpha$ subunit takes place at its C-terminus, very similar to the binding site of GPCRs (Figure 2b, c). However, in the obtained NMR spectra, we could also observe a loss of signal intensity of G-alpha upon the addition of Ric-8A, in line with the assumption that the chaperone Ric-8A stabilizes a molten globule-like state of the substrate G-alpha. Despite the availability of a variety of crystal and EM structures of GPCRs and G-proteins, our research will provide novel insights into the dynamical features of G-protein activation by NMR that cannot be captured by other methods at high resolution, in particular if molten globule or dynamical states are present.

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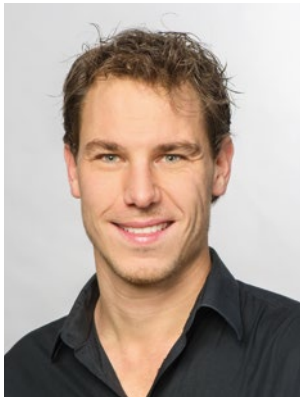
*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Supramolecular Chemistry**

Prof. Job Boekhoven (TUM) | Rudolf Mößbauer Tenure Track Professor
Dr. Chandan Maity, Dr. Marta Tena Solsona (TUM) | Postdoctoral Researchers
Raphael Grötsch, Benedikt Rieß, Caren Wanzke (TUM) | Doctoral Candidates

Scientific Reports



Job Boekhoven

Host
Supramolecular
Chemistry, TUM

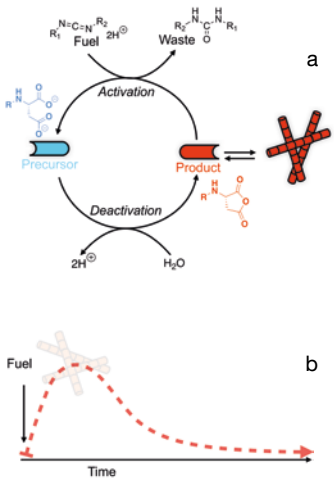
## Self-assembling molecules using chemical reactions

In the Supramolecular Chemistry Focus Group, we design molecules such that they can temporarily bond with each other via so-called non-covalent interactions. As a result, these molecules stack on top of each other to form larger structures, a process called self-assembly. Examples of these assemblies include large filaments or the liquid crystals in your liquid crystal display. Biology also uses non-covalent interactions and self-assembly to create larger structures such as proteins, organelles, or the cell. The question we ask ourselves is, why is biology so much better than we are at creating self-assembled structures?

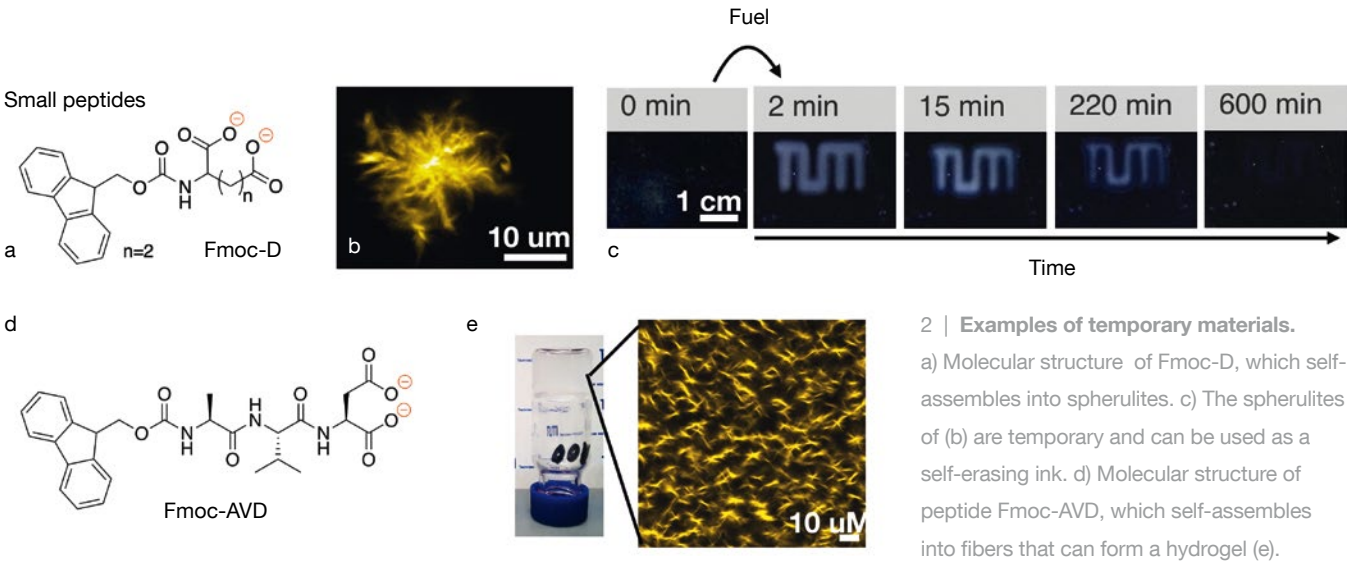
Part of the reason is that biology uses non-equilibrium self-assembly, whereas we usually make our materials in equilibrium. Living materials, like the cell, are not thermodynamically stable but require the constant influx of energy (a cell will require nutrients to survive). As a result, most biological assemblies are controlled by the kinetics of energy consumption and dissipation.[1,2] They thus possess unique properties unattainable when using supramolecular materials in equilibrium. These unique properties, including self-healing, adaptivity, and spatial or temporal control, can be of great interest when considering new strategies for the development of supramolecular materials.

The aim of our work is thus to understand the fundamental details of non-equilibrium energy-dissipative self-assembly. We design molecules such that they can self-assemble when driven by chemical reaction, very similar to the way biology self-assembles its molecules. With that approach, we aim to understand better why and how biology regulates structures and their function with chemical reactions. We also aim to create materials with more life-like properties, for example, materials that make autonomous decisions. Finally, we envision that such knowledge can help us better understand the fundamental principles of life, which in turn helps us better understand our own origin and suggests possible steps toward the synthesis of life.

We use a chemical reaction cycle as the engine for our molecular assemblies (Figure 1a). That reaction cycle “burns” up a chemical fuel, just like a car engine. The energy that is obtained by that cycle is temporarily stored into product molecules. These product molecules are designed such that they can self-assemble. However, given their temporary nature, the assemblies will spontaneously disassemble. In other words, these assemblies will emerge when we add fuel but collapse without it. That process is starting to look a lot closer to biological assemblies, like the cell.




1 | a) Scheme of the chemical reaction cycle for the fuel-driven formation of a transient product. The dicarboxylate precursor (blue brick) is converted into an anhydride product (red brick) by consumption of a carbodiimide (fuel). The aqueous anhydride is unstable and rapidly hydrolyzes back to the original precursor. Because of the loss of charges when anhydride is formed, the product self-assembles upon certain concentration. b) The result of the chemical reaction cycle is that the product and its associated properties are only temporarily present after the addition of fuel.




2 | **Examples of temporary materials.** a) Molecular structure of Fmoc-D, which self-assembles into spherulites. c) The spherulites of (b) are temporary and can be used as a self-erasing ink. d) Molecular structure of peptide Fmoc-AVD, which self-assembles into fibers that can form a hydrogel (e).

We introduced a chemical reaction cycle that fulfills the above requirements.[3–9] It uses carboxylic acid derivatives as precursors and carbodiimide-based condensing agents as fuel. When the fuel is added, the carboxylic acids are converted into metastable anhydrides, which rapidly hydrolyze back to carboxylic acids, restoring the equilibrium. During their limited lifetime, however, the anhydrides self-assemble into a desired supramolecular material. This supramolecular material is, as a result of the continuous formation and degradation, dynamically formed and only present for as long as the fuel remains. In this way, we tuned the lifetime of our assemblies by changing the components in the chemical reaction cycle, such as the amount of fuel added.

In the past years, we have shown that the chemical reaction cycle can be used to create materials with a finite and tuneable lifetime. We demonstrated that this could be used as a self-erasing ink or a hydrogel that self-abolishes.[3] In more recent work, we have shown that the assemblies can also be used to deliver drugs with tunable release profiles; that is, we can set how fast and for how long a certain drug is released from its carrier (see patents). Taken together, we have used our approach of non-equilibrium self-assembly to control the decay profile of materials.

*Publications by this Focus Group can also be found in the section Publications of this report.*

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# Focus Group **Synthetic Biochemistry**

Prof. Kathrin Lang (TUM) | Rudolf Mößbauer Tenure Track Professor
Marko Cigler, Maximilian Fottner, Marie-Lena Jokisch, Kristina Krauskopf, Susanne Mayer, Anton Murnauer, Marie-Kristin von Wrisberg, Vera Wanka (TUM)
Doctoral Candidates

Scientific Reports

Kathrin Lang

Host
Synthetic Biochemistry
TUM

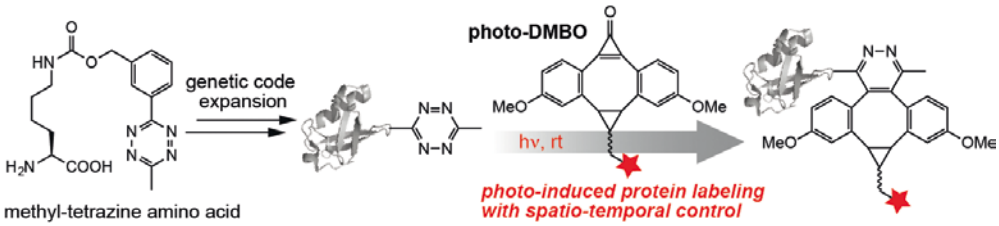
## Expanding the genetic code: Chemistry in living systems

The Focus Group Synthetic Biochemistry conducts research in the interdisciplinary area between chemistry and biology and combines organic chemical, biochemical, biophysical, structural, and cell biological techniques to develop new tools for studying and controlling biological systems. We are especially active in enabling and advancing approaches to expand the genetic code to endow proteins with chemical functionalities beyond the 20 proteinogenic amino acids, and in developing new *in vivo* chemistries that are amenable to and selective within living systems. We are convinced that such a combined approach is ideally suited to address unmet challenges in studying and manipulating biological processes with a new level of spatial, temporal and molecular precision.

Nature uses a limited set of 20 amino acid to synthesize proteins. In recent years it has become possible to genetically encode an expanded set of designer unnatural amino acids (UAAs) with tailored chemical and physical properties into proteins in bacteria and eukaryotes by reprogramming the genetic code and rewiring the translational machinery. These strategies have started to have a big impact on biological studies, as they enable diverse applications, including approaches for imaging and probing proteins, controlling and manipulating protein activity, and engineering and designing new protein function and protein therapeutics. [1–3]

One direction in our research concerns development and site-specific incorporation of UAAs bearing bioorthogonal handles that allow the selective and rapid functionalization of proteins with biophysical probes and small molecules within living cells under physiological conditions. [1] This allows diverse applications, including approaches for probing and imaging proteins in vivo, as well as controlling and manipulating their activity in living cells. Furthermore, within the last year we have developed novel chemistries that use external stimuli such as light to induce bioorthogonal reactivity. We have devised a novel light-induced Diels-Alder cycloaddition reaction between tetrazine-bearing UAAs that can be incorporated into proteins and caged strained cycloalkyne compounds (photo-DMBO, Figure 1). [4] *In situ* light activation of photo-DMBO conjugates allows rapid labeling of tetrazine-modified proteins in living E. coli. We are convinced that this new chemistry offers exciting opportunities to modify proteins in living cells in a spatio-temporally controlled manner, and we are currently benchmarking it for the study of receptor activation in mammalian cells.

A second line of research we are pursuing involves development of crosslinking chemistries to study and validate protein-protein interactions. We have developed approaches for the co-translational site-specific incorporation of UAAs bearing functional groups that are inert under physiological conditions but covalently link positions that are brought into proximity as a result of protein-protein interactions and protein complex formation. Such proximity-triggered crosslinking approaches (chemical crosslinking) allow covalent stabilization of low affinity and transient protein complexes in living bacteria and mammalian cells. We have pioneered their use to aid structure elucidation of previously inaccessible transient, low-affinity protein complexes. [5–6] In future studies we want to expand this approach to map cytosolic protein-protein interactions and to decipher new enzyme targets in protein profiling studies.




1 | Incorporation of tetrazine-bearing UAAs and their photo-activated labeling with photo-DMBO conjugates.

In a third line of research, we are pioneering approaches in which site-specifically introduced UAAs serve as a platform for a chemoenzymatic reaction, in order to install post-translational modifications such as ubiquitylation. Nearly all proteins in eukaryotic cells are at some point in their life span tagged with the small protein ubiquitin (Ub). Ubiquitylation plays crucial roles in a variety of eukaryotic cellular processes, such as protein degradation, DNA repair, nuclear transport, endocytosis, and chromosomal organization. Hence it is not surprising that many different human diseases, including different types of cancer, are being linked to dysfunction of ubiquitylation pathways. The modification of proteins with Ub is catalysed by a complex enzymatic machinery. The human genome encodes over 1000 different enzymes that are necessary for different ubiquitylation pathways, making it very difficult to study effects of individual ubiquitylation events. We have recently developed a novel and robust chemoenzymatic approach, dubbed *sortylation*, to site-specifically modify proteins with Ubls – both *in vitro* and *in cellulo* – in an inducible fashion by combining genetic code expansion, bioorthogonal Staudinger reduction, and sortase-mediated transpeptidation. [7] Our approach relies on the site-specific incorporation of a lysine derivative with an isopeptide bond linking its ε-amino group to a glycylglycine dipeptide (creating amino acid GGK) and its sortase-mediated transpeptidation with an engineered Ub mutant that contains a C-terminus with two amino acid mutations. The generated Ubl-conjugates display a native isopeptide bond and bear two point mutations in the linker region that confer resistance toward deubiquitinases, while retaining structural and physiological integrity and binding affinity for Ub-specific proteins. This novel approach overcomes current limitations for generating ubiquitin conjugates of complex, non-refoldable protein targets under native conditions and makes it possible for the first time to trigger ubiquitylation in living mammalian cells, providing a powerful tool to dissect and interrogate biological functions of Ub-dependent signaling pathways with temporal control.

Looking to the future, our aims lie in understanding mechanisms of complex biological processes such as ubiquitylation through the application of synthetic molecules with tailored functions and properties. In particular, we plan to extend approaches for endowing proteins with new chemical moieties and thereby re-engineer and design new protein functions. This will open up many possibilities for synthetic biology, drug design, biomaterials, and gene therapy.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Understanding How Cancer Drugs Work**

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

Scientific Reports

Bernhard Küster

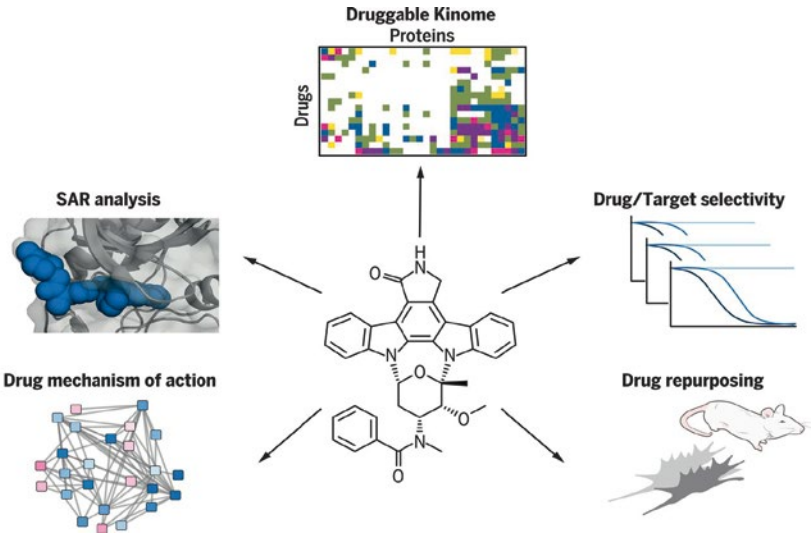
The Focus Group dedicates its research efforts to understanding how cancer drugs work with a view to elucidating the basis for undesired side effects, understanding how resistance occurs and, more importantly, to repurpose these often very effective medicines for use in other indications. To accomplish this, the group takes an interdisciplinary approach combining methods from biology, chemistry, and analytical sciences to generate large-scale molecular data for approved drugs and advanced clinical compounds in cancer model systems. Quantitative proteomics and bioinformatics are of particular importance in these endeavors as these approaches enable the parallel and quantitative measurement of thousands of proteins in a single experiment.

## Elucidating the effect of cancer drugs in preclinical model systems

In the past few years, our research efforts revolved around investigating the effects of kinase inhibitors on cancer cells. Here, we constantly optimize a chemical proteomics technology called Kinobeads to identify how many and which proteins are inhibited by these molecules and to obtain insights into their molecular modes of action. In 2019, have published a new version of this technology [1] and are in the process of profiling >1,000 clinical and academic kinase inhibitors. Also, we initialized an ERC Advanced Grant project (TOPAS – Tumor Proteome Activity Status), in which we study the intracellular effects of clinical kinase inhibitors on sarcoma cells. A team of biochemists and bioinformaticians will work on finding out which protein modifications are influenced by certain kinase inhibitors and how this information can be used to better understand why some drugs do or do not work for cancer treatment.

Recently, we have expanded our research to other treatment strategies, notably the use of epigenetic drugs such as HDAC inhibitors, different treatment strategies in pancreatic cancer and therapeutic antibodies that are often understudied even though they are extensively used in cancer care. Shedding light on the molecular effects of these therapeutics will improve our understanding of how they work in cancer cells and, we hope, enable the development of better therapies in the future.

Another milestone in 2019 was the completion of a project in which we measured the steady-state proteomes and phosphoproteomes of a large number of cancer cell lines and integrated this information with phenotypic drug response data. This allowed us 1) to identify proteins and phosphorylations that correlate with treatment sensitivity or resistance and 2) to predict the response of a cell line toward a certain treatment. We hope that such investigations will eventually guide the design of individual treatment regimens for cancer patients.




1 | The Focus Group Understanding How Cancer Drugs Work aims at characterizing the multifaceted molecular effects of therapeutics. Using chemical proteomics, we want to elucidate how drugs work, understand (un)desired effects, resistance mechanisms, and drug repurposing options. Figure reproduced from [2].

## Translation of preclinical research into clinical decision-making

As of 2019, we actively work toward the clinical translation of mass spectrometry-based proteomics and our research interests in clinical cancer drugs. We collaborate with the molecular tumor boards in Munich and Heidelberg, where treatment recommendations for individual cancer patients who have failed standard treatment are derived from their own molecular data. To strengthen the translational aspect of our work further, we are coordinating an interdisciplinary research consortium called CLINSPECT-M, which aims to establish mass spectrometry-based proteomics in clinical routine diagnostics and to better understand Alzheimer's disease, stroke, multiple sclerosis, and brain cancer.

## Events and activities

The Carl von Linde Senior Fellowship enabled us to extend and strengthen our research program in many ways. Most importantly, it provided time – specifically for grant writing and building new collaborations with academic and industrial partners. For example, Prof. Küster spent five weeks in the San Francisco area to interact with colleagues at the University of California San Francisco, Stanford University, Genentech, and ThermoFisher Scientific to name a few. In particular, we have built strong new ties to the group of Jack Taunton at UCSF, a world-leading expert in chemical biology. In turn, Jack spent five weeks with our group in Freising to learn about mass spectrometry. Professor Taunton's visit was partially sponsored by the TUM-IAS, and he duly gave a presentation at the Institute's headquarters for the university's chemical biology community.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Inclusion and Diversity in Physics**

Dr. Sara Lucatello (INAF Osservatorio Astronomico di Padova)
Anna Boyksen Fellow

Scientific Reports

Sara Lucatello

Host
Prof. Laura Fabbietti
Experimental Physics, TUM

## Unconscious bias in physics: Recognizing and mitigating it

The metrics used to assess a scientist's capability in the fields of natural sciences can be reduced to numerical indexes of seemingly easy and unbiased comparison, reinforcing the assumption that the scientific community values talent equally, regardless of the individual owning such expertise.

However, the under-representation of women and, more generally, the lack of diversity in hard sciences, is a long-standing issue which suggests that the metrics adopted are not as unbiased as assumed (see, e.g., [1] and [2]) and that in fact women, racial minorities, and people from socio-economically underprivileged backgrounds have a harder time successfully pursuing an academic career (see, e.g., [3]). The problem is of particular severity in Germany, with the under-representation of women in hard sciences being consistently more pronounced than in most EU countries across all academic levels.

Awareness of the problem of under-representation of women and lack of diversity is no doubt improving. The widespread belief that this matter does not affect the scientific community is still a reality, however, and specific initiatives pushed forward at the national, institutional, or funding agency level are met with reluctance and occasional resentment by the majority of the community, further hindering improvements in the climate and the inclusiveness of that group.

One of the crucial problems in eradicating the deeply rooted belief that hard sciences are unbiased is that of directly reaching the community and providing information they consider relevant to them in an appropriate format. Our Focus Group intends to take advantage of our privileged position as members of the physics and astrophysics community to gather and examine the relevant data on this issue and convey the information in a format suitable to the audience. Our goal is to improve awareness of the conscious and unconscious biases affecting the selection and evaluation systems in natural sciences, particularly in physics and astronomy in Germany, and to implement initiatives directed at improving the climate in the natural science departments at TUM and other research institutions in Munich.

Creating a fair system and an equitable environment is a fundamental step in improving diversity, which is linked to innovation (see, e.g., [4]). This is of crucial importance at this time, as the next decade will see a large influx of second-generation immigrants in postsecondary education, due to the still ongoing migratory wave that started a few years ago. During 2019, the activity of the Focus Group Diversity and Inclusion in Physics was twofold. On the one hand, we have been working to organize events aimed at improving the awareness of conscious and unconscious bias in academia.

On February 6, 2019, as part of the Collaborative Research Center “Neutrinos and Dark Matter in Astro- and Particle Physics” (SFB 1258) general meeting in Munich, we held an unconscious bias training event that was attended by more than 100

physicists from various German institutions and at all career stages. The event included the presentation of relevant statistics and data and discussion of best practices to mitigate the effect of unconscious bias in the academic environment.

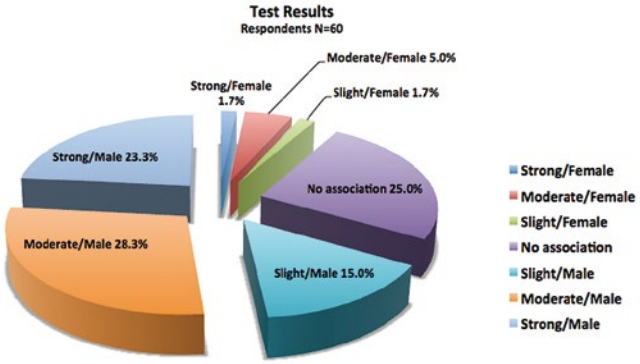
As part of the training, participants were encouraged to anonymously take the science-gender unconscious association tests, the results of which were presented during the TUM-IAS General Assembly, May 23–24, 2019. One of the relevant findings is reported in Figure 1. A similar event held at ESO on February 13 was attended by more than 50 scientists and support staff members. Both events were quite successful, with considerable engagement from the participants.

Our Focus Group was also invited by the faculty of physics at the Ponteficia Universidad Catolica de Chile in Santiago to serve as experts in unconscious bias in academia. We organized three separate day-long training events (June 17–19): one for the physics and astronomy faculty, which the vice-rector also attended, one for postdocs, and one for students, for a total of more than 100 attendees. A photograph taken during this event is shown in Figure 2.

Finally, in June we organized a very successful and well attended Special Session on Diversity and Inclusion at the annual meeting of the European Astronomical Society. With over 1200 attendees from more than 50 countries, this is the largest astrophysics conference held in Europe.

On the other hand, we have been taking steps toward the administration of an on-line survey aimed at examining the demographics of physics and astrophysics communities in Europe, with particular attention to German institutions. During 2019, we worked on survey design, in collaboration with social scientists and experienced researchers in the field, and on coordinating with various institutions and organizations (e.g., the European Astronomical Society) to distribute the surveys through their mailing lists. Data gathering through the on-line survey is expected to start in early 2020.

*Publications by this Focus Group can also be found in the section Publications of this report.*




1 | After unconscious bias training, members of the SFB were invited to take the Harvard Implicit Association Test on science and gender (https://implicit.harvard.eduimplicit/takeatest.html), which aims at assessing the presence of an unconscious association of science with males and liberal arts with females, and then to report their results anonymously. Possible results are: strong, moderate or slight association of males with science and females with liberal arts; no association; and strong, moderate or slight association of males with liberal arts and females with science. More than 65% of the respondents reported some degree of unconscious association of males with science and females with liberal arts.

2 | Unconscious bias training event for faculty members in physics and astronomy at the Ponteficia Universidad Catolica de Chile in Santiago, on June 17 2019.

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# Focus Group **Early Biomarkers of Prenatal Stress**

Prof. Marta C. Antonelli (University of Buenos Aires) | Hans Fischer Senior Fellow
Ritika Sharma (TUM) | Doctoral Candidate

Scientific Reports

Marta C. Antonelli

Host
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Women's Clinic at TUM,
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Klinikum rechts der Isar

## Main aims

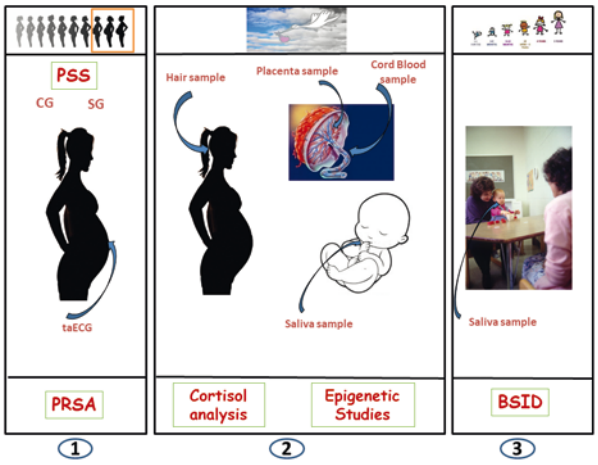
Our main objective is to test the feasibility of identifying early non-invasive pre- and postnatal biomarkers of brain programming due to intrauterine stress exposure. We propose that a combination of non-invasive physiological measures of the stress response system that are unequivocally linked to prenatal stress could be employed as predictive biomarkers of the child's neurodevelopmental outcome.

The stress response system can be divided into an acute response, which involves the rapid activation of the autonomic nervous system (ANS), and a delayed response mediated by the hypothalamic–pituitary–adrenal (HPA) axis. Most importantly, these maternal stress responses shape the development of the infant's stress response system, a phenomenon referred to as "fetal programming." The quest to find a prenatal measure that might have a preventive clinical significance has led us to hypothesize that the coordinated roles of the ANS and the HPA in the integrated stress response can be monitored non-invasively using electrocardiogram (ECG) and ECG-derived maternal and fetal heart rate (mHR, fHR). The HPA axis also promotes the physiological stress response leading to the release of glucocorticoids (GC). Glucocorticoids can act to directly modulate gene transcription affecting structural proteins in the brain and can also affect transcription through epigenetic changes [1]. Epigenetic mechanisms change the gene activity or expression, altering the chromatinic organization without modifying the DNA genetic code. The most highly studied and best characterized epigenetic marker, DNA methylation, involves a direct covalent, chemical modification of a cytosine base lying sequentially adjacent to a guanine base (thus a CpG dinucleotide) [2].

Therefore, we hope to achieve two main objectives: to analyze the impact of PS on ANS activity by deploying advanced methods of FHR monitoring, specifically phase-rectified signal averaging (PRSA) and assessment of maternal-fetal heart rate synchronization; and 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 (Figure 1).

## Relevance and impact

Pregnancy is a significant time in a women´s life, but it can also be very challenging. During the gestational period a pregnant women, like any other person, 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 are 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




1 | All pregnant women visiting the outpatient ward of Department of Obstetrics and Gynecology at TUM's University Hospital Klinikum rechts der Isar in their third trimester were administered the Cohen Perceived Stress Scale questionnaire (PSS-10), with a short information brochure about the study attached. A score was obtained and a PSS-10 below 19 categorized them in the Control Group and a PSS-10 score equal to or above 19 categorized them in the Stress Group.

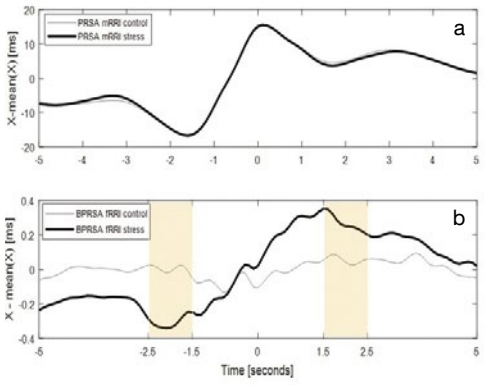
1) Two and a half weeks after screening, obstetricians perform a transabdominal ECG (taECG) recording; the data obtained will be used for PRSA analysis.
2) On the day of parturition, 3 cm of hair strands were collected from the posterior vertex region on the head. Based on an approximate hair growth 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 from 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), which evaluates the infant's cognitive, motor, and language skills. During the same visit, a new saliva sample is taken for the epigenetic analysis.

challenges will determine the child's ultimate health status. The concepts derived from these studies contributed to the emphasis on maternal health as a global priority for the World Health Organization (www.who.int/pmnch) and the International Monetary Fund (www.imf.org/external/np/exr/facts/mdg.htm), with the idea that nurturing care in early life is essential to enable children to become healthy and productive citizens with adequate intellectual skills, creativity, and wellbeing [3,4].

As stated by Rakers et al., [5] we believe that the effects of maternal stress on fetal development are mediated by a “multiple stress-transfer mechanism acting together in a synergistic manner.” We therefore propose that a combination of unambiguously correlated signals and markers (predictive biomarkers) will help to detect “at-risk children” as early as possible in order to take the decision to initiate early stimulation programs, whenever no prevention measures focused on the mother can be taken in a timely manner.

## Achievements

The relationship between mHR and fHR might provide important information about the functional status of fetal ANS [6]. 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) [7] and applied to trans-abdominally acquired fetal ECG (fECG) [8]. Our first results show that prenatal maternal stress identified in the third trimester by a validated questionnaire (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. We could detect periodic mHR decreases reflecting typical patterns of maternal breathing. Interestingly, GC fetuses remained “stable” during these periods, whereas fetuses of stressed mothers showed significant decreases of fHR (Figure 2). We hypothesize that this response is induced by the mechanical stimuli of diaphragm excursion that changes the uterine pressure. In conclusion, we validated our hypothesis that prenatal stress-induced programming is reflected in mHR and fHR biomarkers of ANS activity. The biomarkers we identified can be harnessed for early detection and follow-up of children affected by prenatal stress [9]. Early detection of altered neurodevelopmental trajectories opens new possibilities for designing more timely and effective interventions to improve outcomes of pregnancy affected by PS.




2 | Bivariate phase-rectified signal averaging (BPRSA) analysis of RR intervals.

a) PRSA signal X for maternal RR intervals (RR interval: the time elapsed between two successive R-waves of the QRS signal on the electrocardiogram) (mRRI). The anchor point definition, namely all heart rate deceleration, reflects the central oscillation of X.
b) The response of fetal RR intervals (fRRI) on the maternal decreases. The signal of the control BPRSA shows a significantly lower response than the BPRSA curve for the fetus of a stressed mother. Also shown is the time span used for the quantification of fetal stress index (FSI) (yellow).

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Engineering Immune Cells for Therapy**

Prof. Kathrin Schumann (TUM) | Rudolf Mößbauer Tenure Track Professor
Saskia Kolb (TUM) | Doctoral Candidate

Scientific Reports

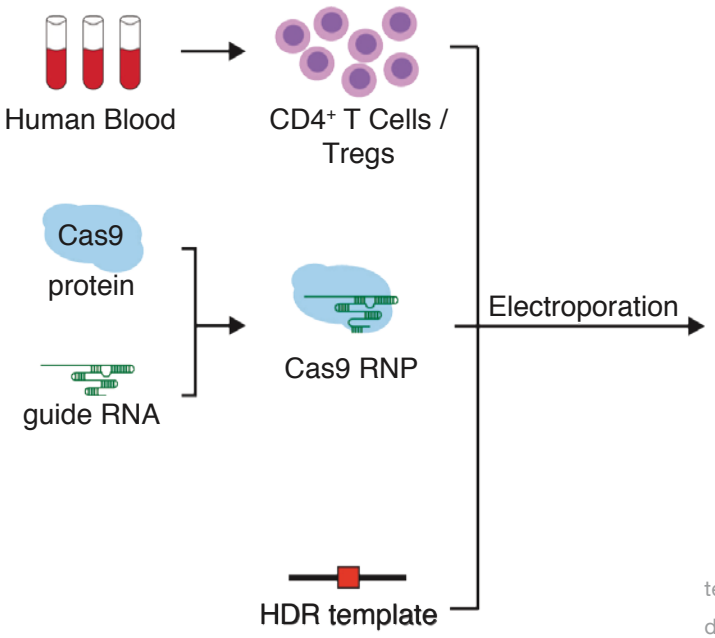
Kathrin Schumann

Host
Engineering Immune Cells for Therapy, TUM

## Using CRISPR screens to understand human regulatory T cell identity

Our immune system protects us from a broad range of pathogens while preventing misguided or exaggerated immune responses that could harm the body. Regulatory T cells (Tregs) play a central role in these processes by sustaining immunological self-tolerance and homeostasis through suppression of autoreactive effector T cells. Absence or depletion of Tregs results in the development of immunodysregulation polyendocrinopathy enteropathy X-linked (IPEX) syndrome, which manifests in multi-organ autoimmunity. Multiple forms of Treg malfunction have been observed in common human autoimmune diseases, including decreased Treg numbers, defective Tregs, and Tregs with destabilized cellular identity. In contrast to their protective role in autoimmune diseases, Tregs can contribute to tumor growth and metastasis by suppressing the cytotoxic CD8+ T cell anti-tumor response. In autoimmunity stabilized Tregs and in tumors “pro-inflammatory” Tregs with T effector functions would be beneficial. For these reasons Tregs are a promising target for cell therapies for both cancer and autoimmune diseases. However, our understanding of how human Tregs transcriptionally maintain their cellular identity is still scarce. So far Tregs have been mainly characterized in mouse models due to technical limitations. We developed Cas9 ribonucleoproteins (RNPs), consisting of recombinant Cas9 protein loaded with chemically synthesized gRNAs, as a powerful tool to generate gene knock-outs and gene knock-ins, and to perform genetic screens in a novel, pooled format or an arrayed format. We are now applying these technologies to dissect transcriptional regulation in human Tregs isolated out of the peripheral blood – cells that are a potential source for therapeutic approaches. Our Focus Group is now systematically analyzing which transcription factors are crucial for maintaining Treg cell identity and how these effects compare to pro-inflammatory conventional T cell subsets.

FOXP3 is the Treg master transcription factor and is fundamental for the functionality and stability of this special cell type. However, there are a multitude of transcription factors that in concert or in parallel with FOXP3 to shape the Treg transcriptional signature. We perform Cas9 RNP screens to knock-out transcription factors that are predominantly expressed in Tregs compared to other T cell subsets and analyze how the deletion of transcription factors changes the pro- or anti-inflammatory features of this special cell type. So far we have tested 40 different transcription factors, including the well characterized Treg-transcription factors FOXP3 and Helios as positive controls. By integrating single-cell RNA-seq data, we are starting to identify genetic modules controlled by individual transcription factors that regulate Treg survival, proliferation, metabolism, and suppressive function.

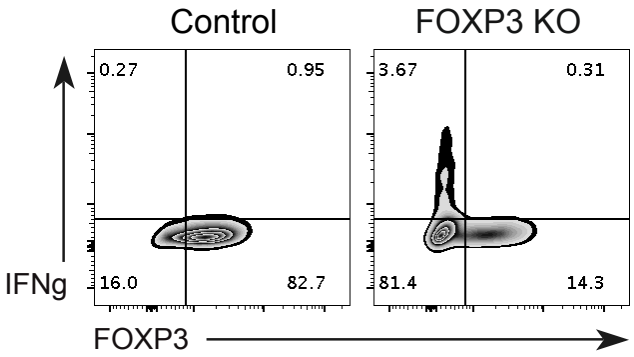



1 | Schematic workflow of CRISPR/Cas9 editing of primary human T cells (including Tregs). Knock-out T cells can be generated by nucleofection of primary human T cells with Cas9 ribonucleoproteins (RNPs). For gene knock-ins Cas9 RNPs are combined with a DNA template with an altered DNA-sequence ("HDR-template") to introduce for example fluorescent markers or patient-derived mutations into the genome of the cell.

We are especially interested in dissecting the function of two transcription factors identified in this screen, SATB1 and HIVEP2, which co-activate a large gene module in Treg cells. Interestingly, this gene module also includes genes known to be crucial for Treg cellular functions such as TET2 and HIF1alpha. We will now systematically dissect how these transcription factors affect Treg function and investigate whether their transcriptional pattern is Treg-specific or can be found in multiple T cell subsets. Furthermore, we will identify the genes directly regulated by these transcription factors.

Our goal is to identify transcription factors that are crucial to maintaining Treg cell identity and then apply this knowledge to engineer Tregs with distinct features for advanced cellular therapies.

*Publications by this Focus Group can be found in the section Publications of this report.*




2 | Fluorescence-activated cell sorting (FACS) data of CRISPR-edited human regulatory T cells. After FOXP3 ablation, Tregs start to produce the pro-inflammatory cytokine IFNg.

# Focus Group **Computer Simulation of Charge Transport in Organic Semiconductors**

Prof. Jochen Blumberger (University College London) | Hans Fischer Fellow
Patrick Gütlein (TUM) | Doctoral Candidate

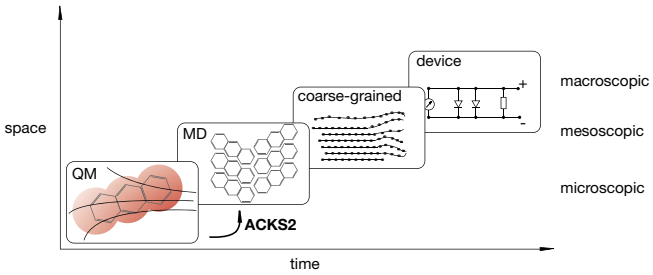
Scientific Reports

Jochen Blumberger

Hosts
Prof. Peter Müller-Buschbaum
Functional Materials, TUM
Prof. Karsten Reuter
Theoretical Chemistry, TUM

## *Ab initio* based polarization correction in force field methods: The ACKS2 method

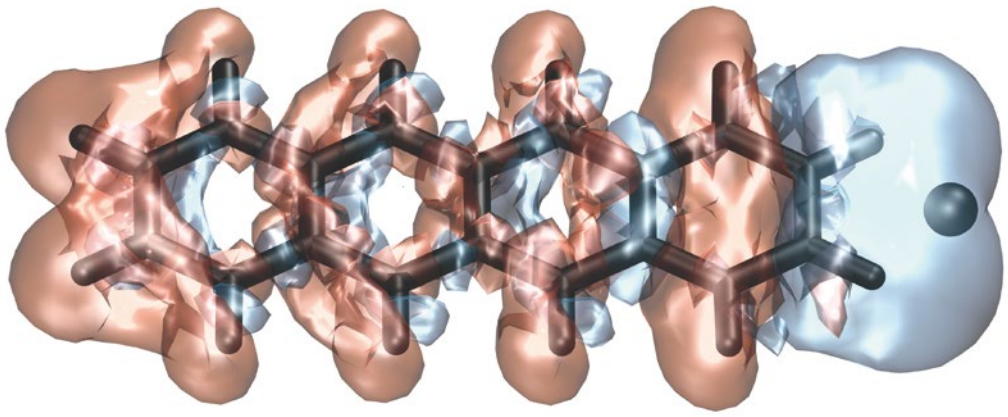
Organic semiconductors (OSs) are among the most thrilling materials discovered in the past decades. Light-weight, flexible and relatively easy to produce from renewable fabrication resources, OSs combine many desirable properties for modern applications such as thin-film electronic devices. Important and disruptive state-of-the-art technologies include light sources, e.g., organic light emitting diodes, and light-harvesting technologies such as organic photovoltaic devices.




1 | Illustration of a multiscale approach in material modeling. The ACKS2 model provides efficient quantum-mechanic level derived electronic polarization for force field simulations.

Unfortunately, the loss of electric conductivity poses a serious downside for these newly found OS materials compared to default inorganic compounds, and addressing this is crucial for modern electronic devices. The quest to identify new promising OS compositions and systematically improve their electric conduction properties requires a proper understanding and accurate theoretical modeling of charge carrier localization and transport. Despite recent progress, the current understanding of charge transport in organic molecular crystal and amorphous phases is still very limited. The motion and transient localization of electrons and electron holes, typical charge carriers, is subject to integral processes on very different time and length scales, which renders the theoretical representation a very difficult and expensive task. In classical multiscale modeling approaches, the microscopic charge transport properties of organic molecules are upscaled to macroscopic electronic device setups and currents, with statistical coarse-grain methods bridging the mesoscale gap.

On an atomic and molecular level, OSs are subject to the non-negligible dielectric response of the surrounding environment. The presence of charge carriers induces polarization of nearby organic molecules, which in turn influences localization and transport of charge carriers. These dynamical, many-body electronic rearrangements span over many molecules due to the small dielectric screening in organic semiconductors. This effect is particularly pronounced in densely packed materials such as OSs, as the electronic states are strongly coupled to nuclear motion, while typical operation conditions of electronic devices at ambient (or elevated) temperatures lead to strong molecular vibrations. In this situation, the recently proposed atom-condensed Kohn-Sham density functional theory approximated to second order (ACKS2) [1] approach could represent a computationally undemanding yet accurate technique to evaluate the electron density response to electric



2 | Density functional theory-based electron density response of an anthracene molecule to the presence of an idealized point charge carrier. The ACKS2 model offers a cheap tool to account for the main features of this very complex, corrugated polarization

fields in organic semiconductor materials. Molecular electronic polarization is captured by a simple linear expansion of the density change in an atom-centered Gaussian-type orbitals basis.

Over the past three years, we systematically worked toward the ACKS2 model as a general electronic polarization correction to force field techniques. We initially introduced a new Cartesian Gaussian-type basis set representation of the perturbation response and established a purely ACKS2-based evaluation of polarization energies, which is crucial in simulations of dynamical processes and charge transport. [2] Fundamentally, we validated the linear response properties for a representative set of hydrocarbon molecules akin to organic semiconductor materials by choice of various simple electrostatic field perturbations, yielding very good reproduction of the density functional theory reference. While this was a crucial first step, we further facilitated the application of ACKS2 by introducing a fragment scheme.[3] Deconstruction of a simulation cell enables us to evaluate the ACK2 parameters independently for each individual fragment, eventually improving the numerical scaling of the method as well as upgrading the ACKS2 parameter transferability. Through an approximate electrostatic coupling between the fragments, we are able to account for polarization in dielectric dense media, again validated by a density functional theory response of small hydrocarbon molecular dimers.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Collective Quantum Dynamics**

Prof. Michael Knap (TUM) | Rudolf Mößbauer Tenure Track Professor
Dr. Fabian Grusdt (TUM) | Postdoctoral Researcher
Annabelle Bohrdt, Johannes Feldmeier, Clemens Kuhlenkamp, Alexander Schuckert, Elisabeth Wybo (TUM) | Doctoral Candidate

Scientific Reports

Michael Knap

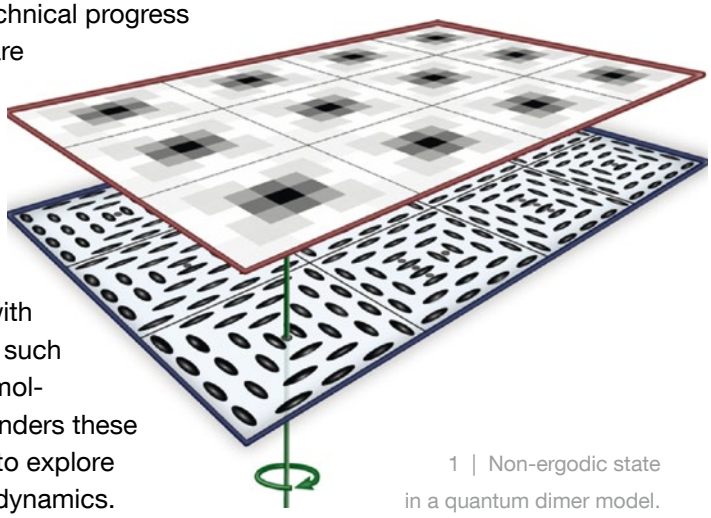
Host
Collective Quantum Dynamics, TUM

## Collective quantum dynamics: Teamwork of quantum particles

The research in our Focus Group aims at a broad range of questions from condensed matter theory such as exotic quantum material, ultracold quantum gases, and light-matter systems. Interactions and correlations in condensed matter systems often manifest in striking and novel properties. These properties emerge from collective behavior of the quantum particles and cannot be understood from the perspective of a single particle alone. In that sense, quantum particles can achieve new goals by forming teams. Many examples of collective quantum dynamics can be found in nature, including superconductors, quantum magnets, and superfluids. Our group develops both analytical and numerical techniques to elucidate the effects of strong interactions and emergent collective behavior. An important factor of our research is its immediate relevance for experiments, which leads to close collaboration with experimental groups all over the world.

## Correlated quantum systems out of equilibrium

Recent conceptual and technical progress makes it possible to prepare and explore strongly correlated non-equilibrium quantum states of matter. The tremendous level of control and favorable time scales achieved in experiments with synthetic quantum matter, such as ultracold atoms, polar molecules, or trapped ions, renders these systems ideal candidates to explore non-equilibrium quantum dynamics.

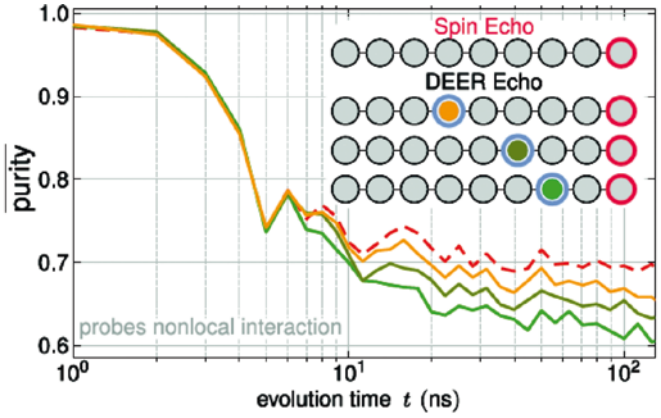


1 | Non-ergodic state in a quantum dimer model.

In a recent work [1], we study theoretically the dynamics in a constrained quantum dimer model. It has been an outstanding question how constraints that arise from strong interactions and geometric frustration can influence the far-from-equilibrium quantum dynamics. Using high-performance exact numerical simulations and analytical techniques, we show that in some parameter regimes this system does not display thermalization on numerically accessible time scales. On the basis of the model's kinematic constraints, we uncover a mechanism of relaxation that rests on emergent, highly detuned multidefect processes in a staggered background, which gives rise to slow, glassy dynamics at low temperatures even in the thermodynamic limit.

## Disordered many-body systems

Disorder has a drastic influence on transport properties. In the presence of a random potential, a system of interacting electrons can become insulating: a phenomenon known as many-body localization. However, even beyond the vanishing transport such systems have very intriguing properties. For example, many-body localization describes an exotic phase of matter that is robust to small changes in the microscopic Hamiltonian. Moreover, fundamental concepts of statistical mechanics break down in the many-body localized phase. In a recent collaboration with John Martini's group from UC Santa Barbara and Google [2], we have characterized the local integrals of motion of many-body localized superconducting qubits. Due to the ability to create superposition states of the qubits, a detailed investigation of the fundamental constituents was possible.




2 | Demonstration of interaction effects between localized integrals of motion.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Electrochemical Interfaces in Batteries**

Dr. Filippo Maglia (BMW Group) | Rudolf Diesel Industry Fellow
Dr. Peter Lamp (BMW Group) | Alumnus Rudolf Diesel Industry Fellow
Lennart Reuter (TUM) | Doctoral Candidate

Scientific Reports

Filippo Maglia

Peter Lamp

Host
Prof. Hubert A. Gasteiger
Technical
Electrochemistry, TUM

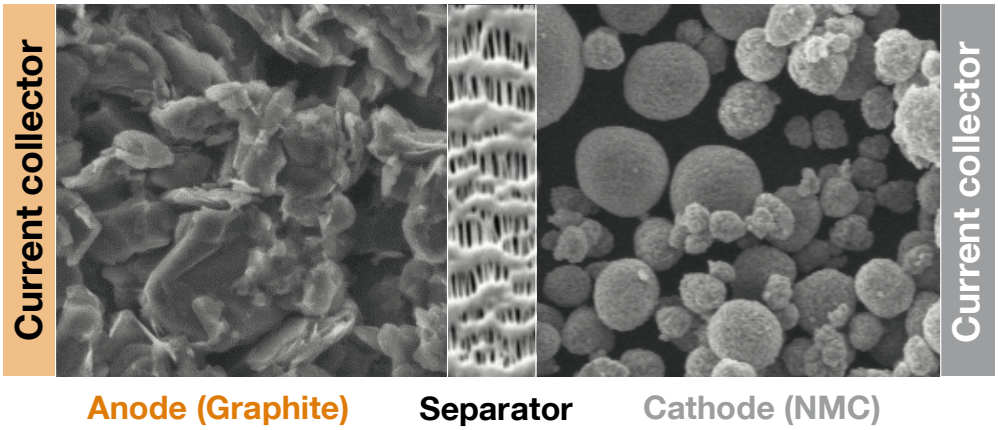
Major obstacles that must be overcome for battery electric vehicles to be competitive against combustion engine vehicles have been identified: limited driving range, high cost, extended charge period, and capacity fading. The Focus Group Electrochemical Interfaces in Batteries addresses the last two issues, namely the limited rate capability and limited lifetime of lithium ion batteries (LiBs).[1]

The efficiency of energy conversion and energy storage processes in LiBs is almost entirely determined by the richness of interfacial processes. The most widely investigated interface in LiBs is the solid-electrolyte interface (SEI), which forms at the negative electrode by electrolyte decomposition. After cell production, batteries undergo an extensive formation procedure, where the passivating SEI layer is developed. The SEI has the unique feature of being permeable toward the diffusion of $Li^+$-ions but electronically isolating. Thus, it simultaneously allows lithium intercalation and prevents further electrolyte reduction at the interface between the negative electrode and the electrolyte. The formation of the SEI, though, is achieved at the cost of an irreversible loss of lithium in the lithium reservoir.

During battery cycling, the SEI ages via catalytic decomposition by transition metals as well as thermal and mechanical stresses.[2,3] Therefore, a resistant SEI is imperative for LiBs with superior lifetime. The stability of the SEI upon dissolution and degradation is strongly related to the capacity retention of the battery. Despite playing a pivotal role in LiBs' performance and durability,[4] a detailed mechanistic understanding of the nature of SEI formation and its structure remains elusive, which makes the development of new electrolyte systems and SEI formation protocols a largely empirical process.[5]

The main aim of our work is the fundamental understanding of the structure-function relationship of the anode interface in lithium ion battery systems. In a previous study, we investigated the formation of the SEI using well defined model systems including metal single crystals, highly oriented pyrolytic graphite (HOPG), glassy carbon in a rotating disk electrode, and graphene.[6] These studies provided precious qualitative insights into SEI formation, composition, and morphology. A quantitative description will be now pursued, which requires the use of electrolyte/active mass ratios that closely represent that of industrial battery cells. Moreover, we aim at understanding the role played by impurities and electrolyte additives as well as the formation protocols in the SEI formation process.

To achieve our goals, among other techniques, we make large use of on-line electrochemical mass spectrometry (OEMS). With this method we can quantitatively monitor the gaseous species evolved during the first few charge cycles of our batteries, where the SEI formation takes place. [7,8]. The analysis of the gas evolution is the key to disclosing the SEI formation mechanism on different anode materials and for different electrolyte systems.




1 | Schematic representation of lithium ion battery components consisting of a graphite anode, layered $LiNi_xMn_yCo_zO_2$ (NMC) cathode material, and a polymeric separator.

**Project Target**

Understand the influence of the anode SEI on the performance and durability of real Li ion batteries

Current Focus Group, Filippo Maglia (BMW Group)

**Project Target**

Development of high energy-density cathode materials for electromobility applications

Previous Focus Group, Peter Lamp (BMW Group)

## References

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[2] R. Jung et al., "Nickel, Manganese, and Cobalt Dissolution from Ni-Rich NMC and Their Effects on NMC622-Graphite Cells", Journal of The Electrochemical Society, vol. 166, no. 2, pp. A378–A389, 2019.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Quantum Matter**

Dr. Marc Janoschek (Paul Scherrer Institut) | Hans Fischer Fellow
Franz Haslbeck (TUM) | Doctoral Candidate

Scientific Reports

Marc Janoschek

Host
Prof. Christian Pfleiderer
Topology of Correlated Systems, TUM

## Ultrahigh-resolution neutron spectroscopy of quantum matter

The properties of condensed matter emerge from the underlying atomic-scale interactions. For example, the thermal conductivity in an insulator is governed by the bonding forces between atoms which determine how atoms may vibrate in the crystal and, hence, transfer heat or energy. Similarly, “quantum matter” is any novel phase that is characterized by interactions that are inherently “quantum” in nature. Such quantum materials are broadly considered to have vast potential future applications ranging from power management and transmission to quantum computation and novel versatile sensors, and even for applications that go beyond what we can currently imagine [1].

Our Focus Group investigates quantum matter that emerges in the vicinity of magnetic instabilities – that is, phase transitions between magnetically ordered and nonmagnetic states. Such magnetic instabilities are typically characterized by violent magnetic fluctuations. When the instability occurs near to absolute zero temperature, those fluctuations are inherently quantum in nature, because there is no thermal energy available to excite thermal fluctuations. In turn, these zero-temperature instabilities – so-called magnetic quantum phase transitions (QPTs) – are ideal model systems to study quantum matter. Indeed, a potpourri of novel quantum matter phases is observed near QPTs, and it is widely accepted that the underlying quantum magnetic fluctuations are at their origin.

Here it is surprising that although quantum fluctuations only become important at temperatures approaching zero, the resulting quantum matter exhibits profoundly altered properties at finite temperatures and, in some cases, up to room temperature. In turn, quantum phase transitions have developed from a zero-temperature oddity to one of the most important issues in solid-state physics. Simultaneously, this highlights the relevance of quantum matter for future applications despite its low-temperature roots.

Over the previous two years our Focus Group has demonstrated that a new neutron spectroscopy method, with almost two orders of magnitude better energy resolution compared to previous techniques, makes it possible to reveal the signatures of the underlying quantum fluctuations [2]. Because neutrons carry a magnetic moment that can couple to magnetic fluctuations, similar to a small compass needle, neutron spectroscopy is ideally suited to investigate magnetic instabilities. The neutron resonant spin-echo (NRSE) technique, which we used here, encodes energy resolution in the neutron’s polarization to achieve ultrahigh energy resolution of about one 1 $\mu$eV (see Figure 1). This discovery is particularly relevant because to date generally very little quantitative information is available on magnetic quantum fluctuations, despite the fact that their importance for the understanding of quantum matter is widely appreciated.

a  b 

1 | a) The Neutron Resonance Spin-Echo (NRSE) Spectrometer RESEDA at the research reactor of the Heinz Maier-Leibnitz Zentrum (MLZ) [2]. b) The pressure cell used for our experiments designed to demonstrate control of quantum matter.

In our study, we investigated the material $UGe_2$, which is a candidate for a new form of superconductivity, so-called spin-triplet superconductivity, in which the Cooper pairs are formed in a distinctively different way compared to other superconductors [3]. This form of superconductivity is considered a candidate for realizing topological quantum computers. Topological quantum computing is distinct from current realizations of quantum computers in that it is inherently free from quantum decoherence [4]. The application of external and non-thermal control parameters such as high pressure has been demonstrated as an effective "control knob" to tune materials through QPTs. In turn, it is believed that this could also be used to control the underlying quantum fluctuations. Over the last year, our Focus Group has started to combine the NRSE technique with pressure tuning in order to demonstrate control of the quantum fluctuations. The pressure cell that was used for this purpose is shown in Figure 1. First experiments have already taken place; however, because the MLZ reactor where the spectrometer is situated was not operational during most of the year 2019, unfortunately only limited progress could be made. In conclusion, we have demonstrated that the new method NRSE is able to quantitatively determine the magnetic fluctuations that are at the heart of many quantum matter phases. This will enable us to establish a much more detailed understanding of quantum matter in the future.

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[4] M. Janoschek, "A magnetic field boost for superconductors", Nature Physics, vol. 15, no. 12, pp. 1211–1212, 2019.


*Publications by this Focus Group can also be found in the section Publications of this report.*

# Focus Group **Quantum Technologies**

Prof. Menno Poot (TUM) | Rudolf Mößbauer Tenure Track Professor
David Hoch (TUM) | Doctoral Candidate

Scientific Reports

Menno Poot

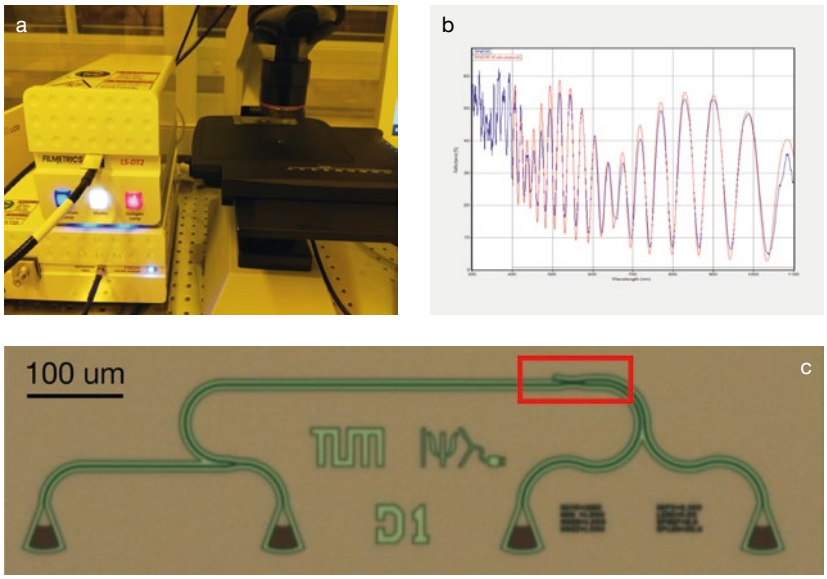
Host
Quantum Technologies, TUM

## Photonic quantum circuits and 2D optomechanics

One of the goals of our Focus Group is to generate, manipulate, and detect single photons on integrated photonic circuits, essential capabilities for performing universal quantum computation with linear optics. In 2019, we designed, fabricated, and measured a variety of chips with photonic devices. A big step forward is our new microscopic reflectometer, which we installed in the TUM Center for Nanotechnology and Nanomaterials (ZNN). It locally measures the precise layer thicknesses on transparent samples (Figure 1a). Using both D2 and halogen lamps, the reflectometer can measure the thicknesses of, e.g., our silicon nitride (SiN) layers with nm precision (Figure 1b). With this, we can now validate the correct etch times for our chips. The reflectometer setup was financed through the Munich Center for Quantum Science and Technology, and it is available to other groups.

Directional couplers are essential components for our photonic circuits (Figure 1c), necessary for single-photon operations on the chip and for quantum gates such as the two-qubit CNOT gate. The CNOT gate requires directional couplers with precisely 50/50 and 67/33 coupling ratios. For this, we fabricated chips with carefully designed directional couplers to find the ideal parameter set. The power crossing from the original waveguide to the one in its vicinity follows a $\sin^2$-behavior with increasing interaction length. This is shown in Figure 1d for a wavelength of 1550 nm, where every blue dot stands for one measured device. From this data, the ideal interaction lengths for given coupling ratios can be obtained, as shown in Figure 1e for the coupling ratios of 50/50 and 67/33 at our operating wavelength of 1550 nm (the wavelength used for most optical fiber telecommunications systems). The directional couplers form the basis of our future quantum optics circuitry, and current efforts are directed toward creating robust, dispersionless directional couplers and integrating these into larger quantum circuits.

Optomechanics is the other main research theme of our Focus Group. In 2019, we continued our work on vacuum setups for both on-chip and free-space optomechanics. In the latter case, the motion of two-dimensional membranes is read out perpendicularly using the reflected light from a HeNe laser. In collaboration with NTT Basic Research Laboratories (Atsugi, Japan) we studied the mechanics of chips with SiN membranes; see Figure 2a. By etching holes in SiN using RIE followed by wet etching of the underlying $SiO_2$, drums or membranes are made. The geometry depends on the position of the holes. Figure 2b shows the response of a large square membrane. Each peak corresponds to an eigenmode; the fundamental mode vibrates at 0.96 MHz and has an excellent quality factor of $1.0 \times 10^5$. It is also possible to make individual drums or linear arrays (Figure 2e). Figure 2d shows how the modes of a linear array of 15 drums evolve when the spacing between the holes is decreased. This way, the overlap between the individual drums grows, resulting in a clear widening of the band. Next steps are to study the spatial profile of each supermode and determine their quality factors. Another interesting feature of these arrays is their mode coupling. As Figure 2e shows, pumping one mode results in a clear shift in frequency in all probed modes. Surprisingly, this seems to influence the damping.




1 | **Reflectometer and directional couplers**

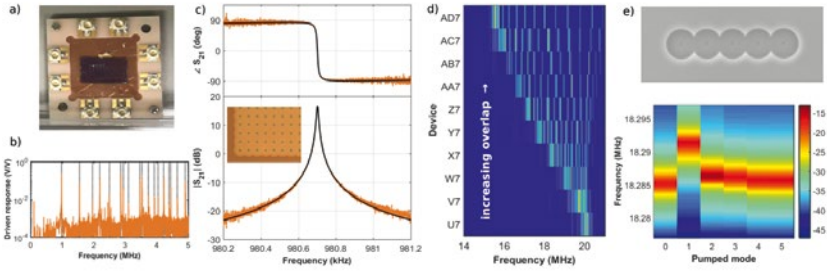
a) The reflectometer in the ZNN cleanroom.

b) Screenshot of a measurement. The fringes in the reflection spectrum (blue) are fitted (red) to determine the layer thicknesses of SiN and $SiO_2$, here measured as 319.77 nm and 3304.8 nm, respectively.

c) Device with a directional coupler (red rectangle).

d) Coupling ratio vs. the interaction length. Each data point is an individual device. The $\sin^2$ fit shown in gray fits the data very well.

e) Wavelength dependence of the coupling ratio of two devices which would show the desired coupling ratio of 50/50 and 67/33 at 1550 nm.




2 | **2D optomechanics**

a) Photograph of a chip (black, 6x10 mm) with silicon nitride drums mounted on a driving piezo and a circuit board with high-frequency connectors

b) Measured response of a 407x407 um membrane.

c) Zoom of (b) around the fundamental mode. The inset shows a micrograph of a part of the membrane.

d) Colormap of the response of different linear arrays with increasing overlap. The modes appear as light colors; the band widens with increasing overlap.

e) Scanning electron micrograph of an array with 5 drums (top) and the frequency shift of the second mode, when exciting the five modes in the first band to large amplitudes. The frequency shift due to mode coupling is clearly visible.

*Publications by this Focus Group can be found in the section Publications of this report.*

# Focus Group **Theory of Complex Quantum Systems**

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Lisa Hänggli, Cambyse Rouzé (TUM) | Postdoctoral Researchers
Martina Gschwendtner, Margret Heinze, Stefan Huber,
Alexander Kliesch (TUM) | Doctoral Candidates

Scientific Reports

Robert König

Host
Theory of Complex
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## Quantum information and computation

Since 2015, the Focus Group Complex Quantum Systems has been investigating to what extent quantum systems may be used to accomplish fundamental information-processing tasks. Of primary interest are communication, storage, and manipulation of quantum states, as well as computational problems for which quantum devices may provide advantages.

Decoherence is a major obstacle on the road toward robust quantum information processing. To understand the minimum technological requirements to enable larger-scale quantum information processing, we devise quantum error-correcting codes and fault-tolerance schemes resilient to general forms of noise. We also explore potential new applications of quantum devices, examining and comparing classical as well as quantum algorithms for certain computational tasks.

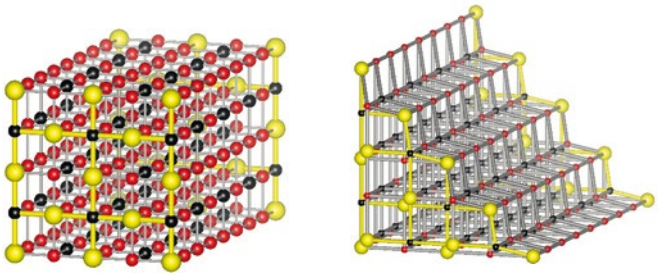
Our research lies at the intersection of mathematics, physics, and computer science. While we also pursue more fundamental statistical/mathematical questions related to many-body physics, the following areas are representative of the topics we study:

## Advantages of noise-tolerant quantum computation

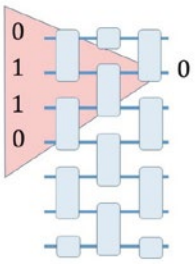
Recently, we have identified a computational problem that provides a separation between classical and quantum circuits: The problem can be solved using a simple constant-depth quantum circuit, but any classical circuit solving the problem requires at least linear depth. In contrast to existing statements about the power of quantum computing, the advantage in this case can be proven unconditionally. In particular, no complexity-theoretic assumptions (such as the assumption that factoring is hard for classical computers) are required.

In this statement, it was assumed that the quantum circuit is executed perfectly, i.e., without errors. However, any actual experimental realization of a quantum circuit will be prone to errors. One may therefore worry that this result is purely academic, i.e., of no practical relevance: Any quantum advantage could potentially disappear when the quantum circuit is noisy.

In [1], we have been able to address this shortcoming of our original result: We show that even non-ideal quantum circuits (with a realistic error model) provide a computational quantum advantage. The proposed algorithm is geometrically local in three dimensions, meaning that qubits need to be arranged on a certain lattice, and all gate operations are between nearest neighbors.



1 | **Computational architecture demonstrating a quantum advantage**
Left: Using a certain measurement pattern on a cluster state (a 3D array of qubits initialized in a particular entangled state) results in long-range encoded entanglement on the residual yellow qubits. Right: In a folded architecture, subsequent encoded logical gates may be executed using local operations only.




2 | **Constant-depth quantum circuits and their lightcones**
Each output bit of a classical constant depth circuit is determined locally by input bits in its lightcone. In contrast, constant-depth quantum circuits can exploit the phenomenon of quantum non-locality to perform computations that cannot be performed by their classical counterparts.

## Algorithms for quantum many-body physics and quantum information

Optimization problems are ubiquitous in both physics and computer science. For quantum many-body systems, computing or approximating ground state energy densities is one such task. It is generally highly non-trivial because the dimension of the state space scales exponentially with the number of qubits. In [2], we have constructed efficient classical algorithms for the case of n-qubit Hamiltonians involving general two-qubit interactions. These algorithms also provide guarantees on the achieved approximation ratios. They are based on randomized rounding of semidefinite programming relaxations.

While many simple operational problems such as hypothesis testing of quantum states may be expressed mathematically as semidefinite programs, some natural problems (such as channel coding) have more intricate structure. In [3], we designed an algorithm that solves semidefinite bilinear programs, making it possible to capture a larger range of problems of interest. We successfully applied this algorithm to the computation of so-called Dobrushin curves. These provide bounds on the information loss in scenarios where noise acts repeatedly, and arbitrary coding/recovering operations may be applied.

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*Publications by this Focus Group can also be found in the section Publications of this report.*

# Publications

# Publications



## Advanced Computation and Modeling



## Bio-Engineering and Imaging



## Communication and Information



## Control Theory, Systems Engineering and Robotics



## Environmental and Earth Sciences, Building Technology

## Fundamental Natural and Life Sciences



## Gender and Diversity in Science and Engineering



## Medical Natural Sciences



## Surface, Interface, Nano- and Quantum Science

# Advanced Computation and Modeling

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# Facts and Figures

## Where do the TUM-IAS Fellows come from?


Dr. Ioannis Brilakis
University of Cambridge
Prof. Krasimira Tsaneva-Atanasova
University of Exeter
Dr. Luca Magri
University of Cambridge
Dr. Christian Bick
University of Exeter
Prof. Jochen Blumberger
University College London
Prof. Angela Casini
University of Cardiff
Prof. Camilla Hollanti
Aalto University
Prof. Job Boekhoven
Prof. Jia Chen
Prof. Daniel Cremers
Prof. Hendrik Dietz
Prof. David Egger
Prof. Matthias J. Feige
Prof. Stephan Günnemann
Prof. Franz Hagn
Dr. Filippo Maglia
BMW Group, Munich
Dr. Marc Janoschek
Paul Scherrer Institut
Dr. Mirko Bothien
Ansaldo Energia Ldt.
Prof. Michael Bronstein
Imperial College London / Università della Svizzera Italiana / Intel Perceptual Computing / Twitter
Prof. Eleni Chatzi
ETH Zurich
Dr. Barbara Solenthaler
ETH Zurich
Prof. Takao Someya
University of Tokyo
Prof. Eitan Yaakobi
Technion
Prof. Lifeng Chi
Soochow University
Prof. Angelika Harbauer
Prof. Reinhard Heckel
Prof. Frank Johannes
Prof. Michael Knap
Prof. Susanne Kossatz
Prof. Robert König
Prof. Bernhard Küster
Prof. Kathrin Lang
Prof. Laura Leal-Taixé
Prof. Christian Mendl
Prof. Bjoern Menze
Prof. Rolf Moeckel
Prof. Kai Müller
Prof. Matthias Nießner
Prof. Menno Poot
Prof. Kathrin Schumann
Prof. Sebastian Steinhorst
Prof. Antonia Wachter-Zeh
Prof. Maya Schuldiner
Weizmann Institute of Science
Prof. Bernhard Schrefler
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Dr. Sara Lucatello
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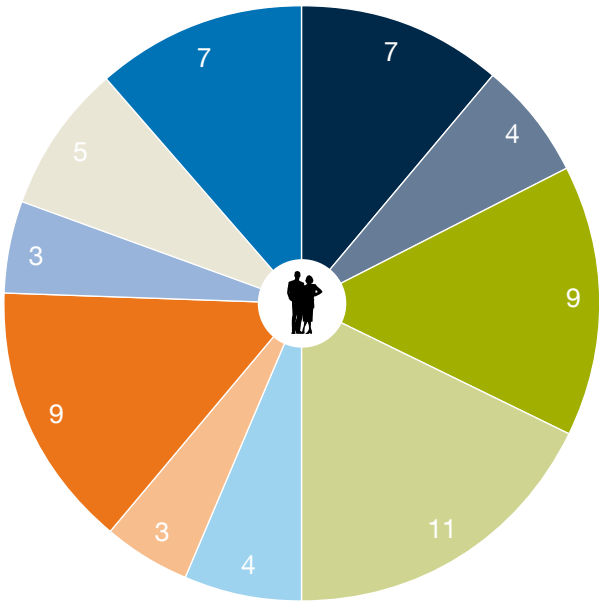
Prof. Giuseppe Savaré
Università degli Studi di Pavia
Prof. Susan Park
University of Sydney
Prof. Paolo Giommi
Italian Space Agency

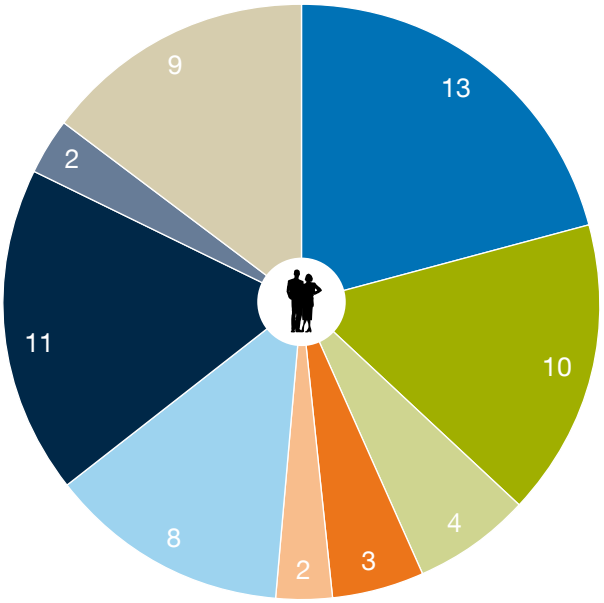
# Fellow Distribution

## Distribution of Active Fellows According to TUM Departments




- Chemistry
- Civil, Geo and Environmental Engineering
- Electrical and Computer Engineering
- Informatics
- Mathematics
- Mechanical Engineering
- Physics
- TUM School of Governance
- TUM School of Life and Food Sciences Weihenstephan
- TUM School of Medicine

## Distribution According to Research Areas




- Advanced Computation and Modeling
- Bio-Engineering and Imaging
- Medical Natural Sciences
- Communication and Information
- Control Theory, Systems Engineering and Robotics
- Environmental and Earth Sciences, Building Technology
- Fundamental Natural and Life Sciences
- Gender and Diversity in Science and Engineering
- Surface, Interface, Nano- and Quantum Science

# Finances

## Excellence Initiative, Excellence Strategy and TUM Budget

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. TUM was not only successful in both rounds of this nationwide competition (2006 and 2012) but even secured the title "University of Excellence" for the third time under the new program Excellence Strategy that has evolved from the Excellence Initiative. After having played a central part in the first two rounds TUM-IAS became established as a permanent institution of TUM which is financing TUM-IAS out of the general TUM budget. The Institute has also contributed to the proposal of the Excellence Strategy and is therefore receiving funding for its new initiatives. Moreover, TUM-IAS continues to receiving further third-party funding.

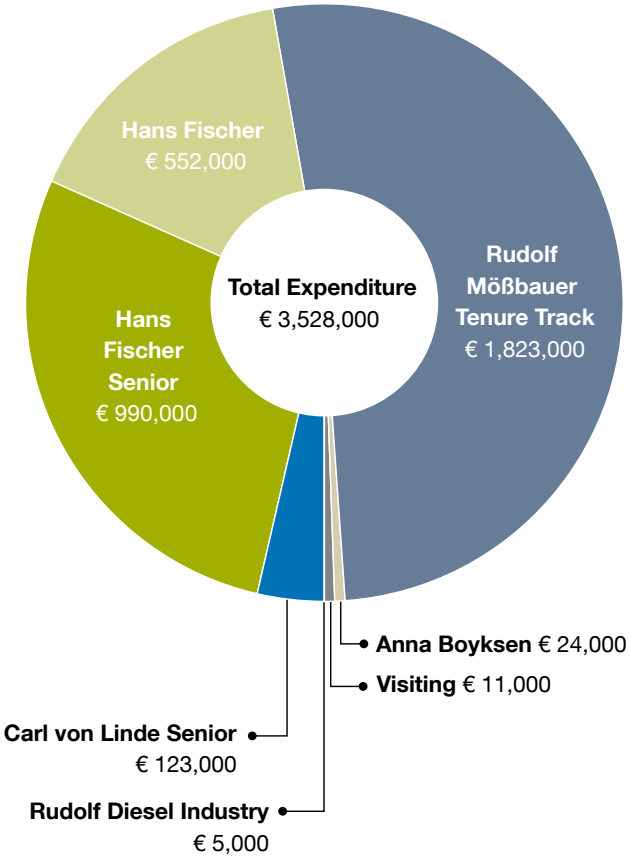
## TÜV Süd Foundation

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. So far, two Fellows were appointed under this scheme.

## Siemens AG

The Siemens AG provides funding for six Hans Fischer (Senior) Fellowships with over two million euros. The research focus is on the fields of "Simulation and Digital Twin" and "Future of Autonomous Systems/Robotics." The first two Fellows of this program have taken up their work in 2019.

Expenditure per Fellowship Category in 2019

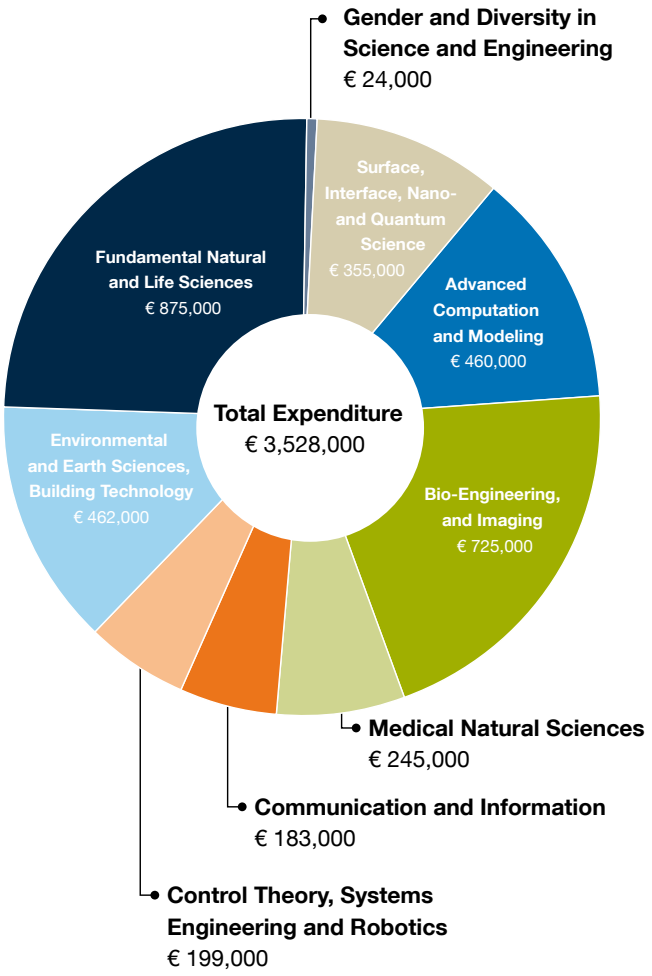



## Expenditure per Fellowship Category in 2019

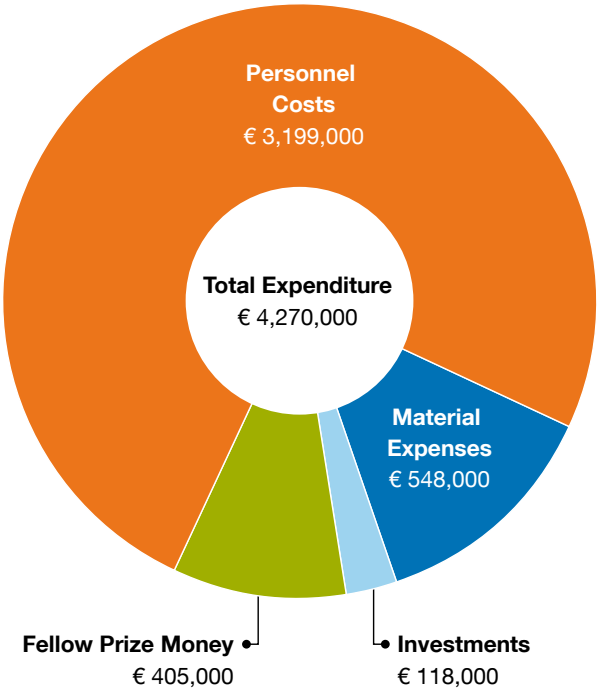
This chart illustrates the expenditure in 2019 for each Fellowship category. Most dominant in terms of costs (as has been the case since 2015) – with 52 percent of the total Fellowship expenditures – are the Rudolf Mößbauer Tenure Track Professorships. This program is devoted to the funding of outstanding, high-potential early career scientists who have already achieved a major scientific or technological breakthrough. The program was only established in 2013 (seven calls have been published between 2013–2019), and the financial data highlights the strong commitment to hiring these early-career talents as well as the significant investment the TUM-IAS makes in this Fellowship category.

The Hans Fischer Senior Fellowship comes in second in terms of costs and comprises 28 percent of the total expenditure for our Fellowship programs, whereas the Hans Fischer Fellowship represents the third largest category. These Fellowships represent an integral part of the TUM internationalization strategy and are immensely valuable in terms of the exchange of complementary expertise and the grooming of emerging fields.

## Expenditure per Research Area in 2019




## Total Expenditure in 2019




The Rudolf Diesel Industry Fellowship expenditures as well as the Anna Boyksen Fellowship expenditures, however, have been decreasing since 2018. The home institutions of the active Fellows are located in the European neighboring countries. The majority of the Rudolf Mößbauer Tenure Track Professors has spent their IAS budget by the end of 2018, which was the ending date of the Marie Curie COFUND Program. Therefore, the overall expenses in this Fellowship category dropped compared to 2018. This is also shown in the overall decrease of the Fellowship costs.

### Expenditure per Research Area in 2019

The chart on the left shows the TUM-IAS Fellowship expenditures grouped into the TUM-IAS Research Areas, including the Visiting Fellowship program, which is also grouped according to Research Areas. Interdisciplinary projects were classified according to their most dominant field. The Research Area with the highest expenditures was Fundamental Natural and Life Sciences, reflecting a high number of Rudolf Mößbauer Tenure Track Professors and Hans Fischer Senior Fellows working in this field.

### Total Expenditure in 2019

On the right chart, total TUM-IAS expenditure is displayed, including Fellowships, Visiting Fellowships, events, and management. The total expenditure decreased in comparison to 2018 (€ 5,349,000) reflecting mainly the decrease of the IAS budget allocated to the Rudolf Mößbauer Tenure Track Professors. The difference between the total expenditures per Fellowship category / Research Area and the total expenditure in 2019 is due to management and event expenses: € 681,000 for management and € 43,000 for event-related expenses.

Cover Image: Daniel Cremers and Emanuele Rodolà.

4, 6, 8, 14 (Steinberger, Kohout), 15 (Wahler, Schmidt), 24, 27–29, 44, 53 (Nießner), 57, 62, 66, 74, 86, 94, 102 (Clifton), 104, 133: Astrid Eckert.

9: Job Boekhoven

14 (Limmer): RINGFOTO Rauchfuss.

14, (Santos Kühn), 52, 53, 62,70, 82, 108, 116: Astrid Eckert/Andreas Heddergott.

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31, 33, 37: Sigrid Wagner.

37: Yuandong Pan.

38: (above) Julie Rousset.

38 (left): Andrea Maretto, Kéré Architecture.

38 (right): Kai-Uwe Bletzinger.

39: Chair of Food Chemistry and Molecular Science, TUM.

41: Susanne Steinkeller | ediundsepp.

42, 45: Simon Märkl.

43, 44: Uli Benz.

46: German-French Academy for the Industry of the Future.

53, 86: Frank Wojciechowski.

54: (above): Stacey Conti.

54: (down): Pablo Gainza.

55: TEDx Lugano.

63: P. Gainza et al, Journal Cover from Nature Methods, vol. 17, no. 2; illustration by Laura Persat; reprinted with permission from Springer Nature.

68: Dirk Bruniecki.

69 (left): B. Wirthl, J. Kremheller, B. Schrefler, W. Wall, “Extension of a multiphase tumour growth model to study nanoparticle delivery to solid tumours”, in: PLoS ONE, vol. 15, no. 2, 2020, e0228443, CC-BY 4.0.

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This figure is taken from the work “Partial Functional Correspondence” by Rodola, Cosmo, Bronstein, Torsello and Cremers that appeared in the Symposium on Graphics Processing 2016. It revolves around the challenge of analyzing and understanding 3d shapes. It shows the estimation of correspondence between a variety of 3D shapes (represented by the surface coloring). In particular, this work addresses the challenge of computing precise and robust correspondence even for cases when the respective shapes are only observed partially and under significant noise or perturbation (holes, missing parts, subsampling). The developed algorithm was the winner of the SHREC 2016 partial correspondence contest.

Reference: E. Rodolà, L. Cosmo, M. Bronstein, A. Torsello, D. Cremers, “Partial Functional Correspondence”, Comput. Graph. Forum 36, pp. 222–236, 2016.

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