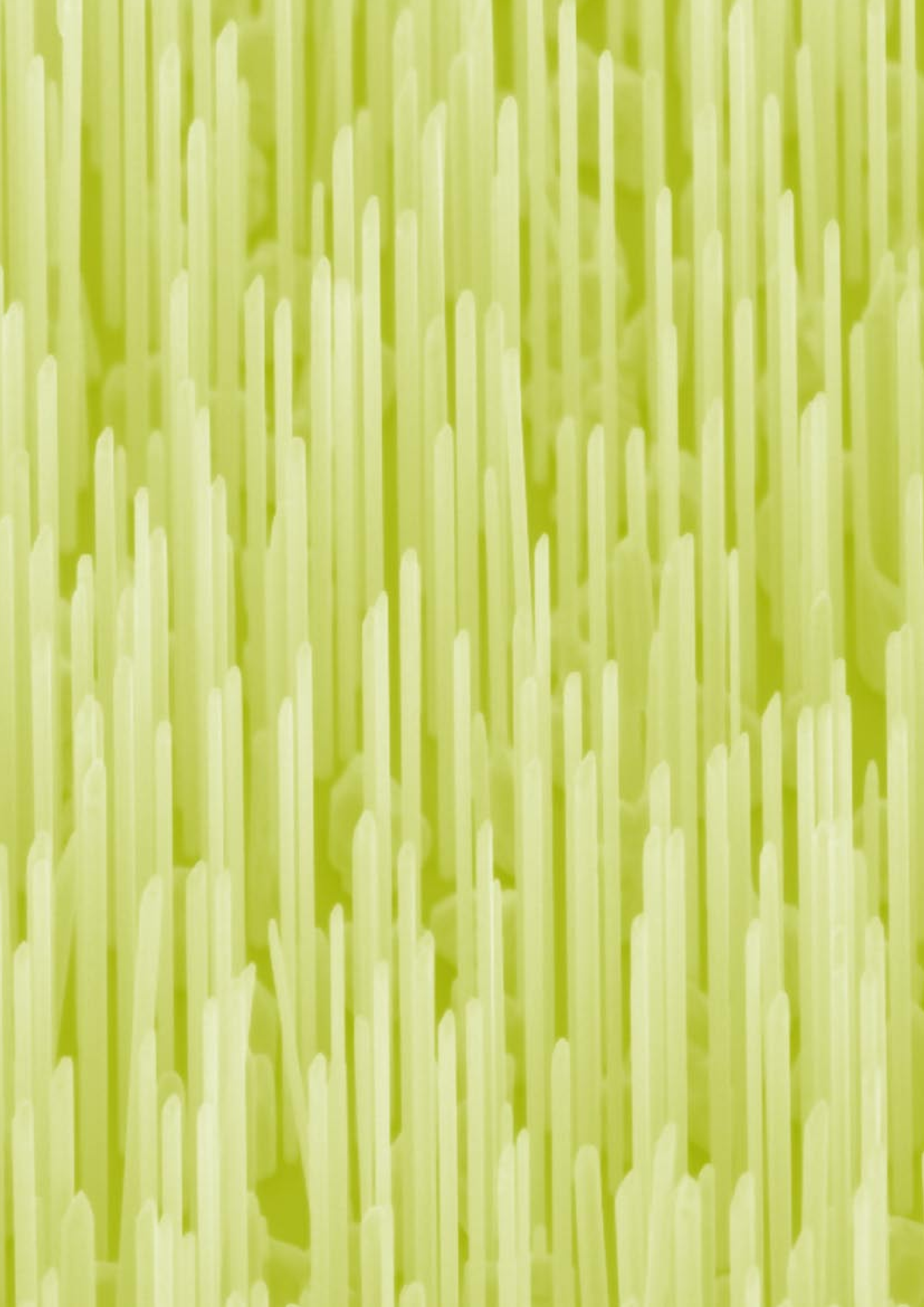
Annual Report

Technische Universität München

Institute for Advanced Study

2014



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TUM President's Foreword

Some familiar sayings are so often repeated and so widely attributed that their true origins can be lost. Nonetheless, I feel confident in asserting that this one never would have originated in Germany: "If you're not failing, you're not trying hard enough." Traditionally our culture, while nurturing excellent science and engineering, has shown intolerance toward failure and an aversion to risk – arguably inhibiting innovation. Thus an institution with the motto "Risking Creativity" might be expected to arise more naturally in the land of Thomas Alva Edison and Silicon Valley. And yet here it is, in the heart of Bavaria: the TUM Institute for Advanced Study.

There is a cultural transformation under way here, with the TUM-IAS in the vanguard. More than ever before, the world's leading universities compete for minds, means, results, and recognition in a global arena, gaining leverage through strategic partnerships. TUM has embraced this change, moving decisively to infuse excellent research and teaching with entrepreneurial thinking, an international orientation, and a bias toward bold action. Empowered from its founding to foster high-risk/high-gain research within a non-bureaucratic framework, the TUM-IAS has led the way in many respects.

At the same time, the TUM-IAS joins in major initiatives of the university in its own distinctive way. For example, Germany's first true tenure track is the centerpiece of the TUM Faculty Recruitment and Career System launched in 2012. In conjunction with this, the TUM-IAS introduced a new Fellowship that offers long-term career options, the Rudolf Mößbauer Tenure Track Professorship. The recruiting process, featuring an open call rather than a specific disciplinary profile, is bringing in a diverse group of high-caliber early-career researchers who are eager to take the risk of developing entirely new fields. Increasingly integrated with the larger TUM community, the TUM-IAS does not stand apart but rather marks a leading edge as the whole university advances.

Time also marches on, bringing the end of Gerhard Abstreiter's tenure as TUM-IAS director in the spring of 2015. I want to thank him, who clearly could have succeeded brilliantly in Silicon Valley or anywhere else, for choosing to make his career at TUM. One of the world's most innovative semiconductor researchers – most recently honored by the German Physical Society (DPG) with its highest award, the Stern-Gerlach Medal – he has also distinguished himself by building and reinforcing institutional excellence. The vibrant research environments of the Walter Schottky Institute, the Center for Nanotechnology and Nanomaterials, and the TUM-IAS all bear the mark of Gerhard Abstreiter's leadership.

Prof. Wolfgang A. Herrmann
President

TUM-IAS Director's Message

The main challenge of the TUM-IAS in the past year was the final implementation of the existing commitment based on the successful second round of the Excellence Initiative. A major task in this context was the appointment of 14 Rudolf Mößbauer Professors within the newly established TUM Tenure Track system. We had to select the best candidates out of about 500 applications in vastly different fields. The newly appointed early-career scientists broaden the research and teaching portfolio of TUM in exciting and highly relevant scientific and technological domains, especially at the border between classical disciplines.

In addition, quite a few new research Focus Groups were established in 2014 based on our well-established Fellowship programs. At present, we support a record number of more than 50 active Focus Groups covering a wide range of innovative and interdisciplinary fields. TUM-IAS is Fellow-driven, not thematically driven, and we initiate this by motivating TUM groups to submit Fellowship proposals and create Focus Groups, which are the basic research units of the TUM-IAS. The successful applications resulted in various new projects, which have been grouped into the following eight larger Research Areas:

- Advanced Computation and Modeling
- Biomedical Engineering, Bio-Imaging, Neuroscience
- Bio-related Natural Sciences
- Communication and Information
- Control and Robotics
- Environmental and Earth Sciences, Building Technologies
- Fundamental Physics
- Surface, Interface, Nano- and Quantum Science

These big themes emerge dynamically and may be changed and further developed over time.

With the Anna Boyksen Fellowship, we established a new program last year in order to strengthen activities on gender- and diversity-related topics in science and technology. Two such Fellowships have been granted so far.

The TUM-IAS has become an intellectual center on the Garching campus, and the newly established events became more and more popular, fostering more interactions between scientists from different fields. This includes especially the weekly Wednesday Coffee Talks, where scientists on all career levels gather at the Institute to chat, discuss, and listen to short talks on recent and relevant publications, which cover research results from all areas within TUM. We have had around 50 such talks so far, specifically prepared for a non-expert audience. The scientific Sunday Matinees, organized four times a year, attracted typically 100 people from the general public who wanted to learn "what those researchers in Garching actually do." The TUM-IAS has developed as a lively hub where scientists from the various TUM research fields get together to interact with each other as well as with researchers from international research institutions and from industry, discussing possible collaborations and participating actively in exploratory symposia, workshops, and seminars.

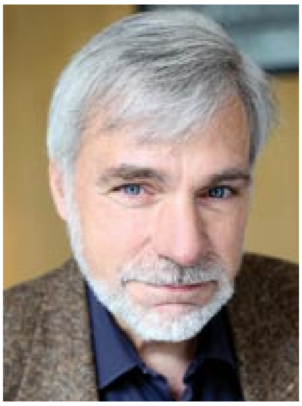
Time went by in a flash for my two-year term as director of the TUM-IAS. I want to thank the many people who contributed in different ways to the success of the Institute, inside and outside of TUM. My special thanks go to the administrative staff for their competent work and the excellent working atmosphere. It was a great pleasure to work with all of you and to serve TUM as scientific director of the Institute for Advanced Study, trying to stimulate and promote top-level research and international collaborations.

Prof. Gerhard Abstreiter
Director

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.



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Bielefeld University
Faculty of History, Philosophy and Theology
Institute for Interdisciplinary Studies of Science

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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

Advisory Council

The TUM-IAS Advisory Council consists of a member from the Max Planck Institute of Quantum Optics and TUM professors covering all important 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 about four times a year.

Members

Prof. Hans-Joachim Bungartz Chair of Scientific Computing,
Graduate Dean of the TUM Graduate School

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Prof. Horst Kessler Department of Chemistry

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Prof. Katharina Krischer Nonequilibrium Chemical Physics

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Event Manager / Web Coordinator

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Erika Höchtl
Secretary / Building Coordination (since October 2014)

Nina Jelinek
Secretary / Building Coordination (until September 2014)

Kristina Schwarzer
Project Manager IESP

Fellows

Carl von Linde Senior Fellows

2008 Prof. Horst Kessler
2011 Prof. Ingrid Kögel-Knabner
2013 Prof. Annette Menzel
2014 Prof. Martin Buss

Carl von Linde Junior Fellows

2011 Prof. Dongheui Lee, Prof. Angelika Peer
2013 Dr. Peer-Hendrik Kuhn

Hans Fischer Senior Fellows

2009 Prof. Stanley Riddell
2011 Prof. Silvio Aime, Prof. Polly L. Arnold, Prof. Daniel Gianola, Prof. Frank Kschischang, Prof. Christian Werthmann
2012 Prof. Stephen Goodnick, Prof. Dietmar W. Hutmacher
2013 Prof. Harald Brune, Prof. Zvonimir Dogic, Prof. Josef P. Rauschecker, Prof. Jelena Vuckovic
2014 Prof. John S. Baras, Prof. Dirk Bergemann, Prof. Gregory D. Hager, Prof. Tamas L. Horvath, Dr. Andreas Kronfeld, Prof. A. Lee Swindlehurst, Prof. Nicholas Zabaras

Hans Fischer Fellows

2012 Prof. George Biros
2013 Prof. Matthias Batzill, Dr. Christian Hirt
2014 Prof. Yana Bromberg, Prof. Tsung-Yi Ho, Prof. Stuart Khan, Prof. Suljo Linic

Hans Fischer Tenure Track Professors

2010 Prof. Hendrik Dietz

Rudolf Diesel Industry Fellows

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

Rudolf Mößbauer Tenure Track Professors

2013 Prof. Kathrin Lang, Prof. Bjoern Menze, Prof. Alessio Zaccone
2014 Prof. Jia Chen, Prof. Matthias Feige, Prof. Franz Hagn, Prof. Michael Knap, Prof. Robert König

Anna Boyksen Fellows

2014 Prof. Madeline E. Heilman

Alumni Fellows

Carl von Linde Senior Fellows

2007 Prof. Andrzej Buras, Prof. Arthur Konnerth, Prof. Reiner Rummel
2008 Prof. Claudia Klüppelberg
2009 Prof. Axel Haase
2010 Prof. Ulrich Stimming, Prof. Gerhard Abstreiter

Carl von Linde Junior Fellows

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

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. 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

Hans Fischer Fellows

2012 Prof. Franz Hagn

Hans Fischer Tenure Track Professors

2007 Prof. Thomas Misgeld

Rudolf Diesel Industry Fellows

2009 Prof. Khaled Karrai, Dr. Dragan Obradovic, Dr. Georg von Wichert
2010 Dr. Tsuyoshi Hirata, Prof. Gernot Spiegelberg, Dr. Matthias Heller, Dr. Chin Man W. Mok

Honorary Fellows 2014

Alexander von Humboldt Research Awardees

Honorary Hans Fischer Senior Fellows

Prof. Michel Géradin | University of Liège

Prof. Naira Hovakimyan | University of Illinois at Urbana-Champaign

TÜV Süd Stiftung Visiting Professors 2014

Prof. Mohamad T. Araji

Faculty of Architecture, Co-Chair for the Environmental Design Studios

University of Manitoba

Host: Prof. Werner Lang

Prof. Henry Sodano

Department of Mechanical and Aerospace Engineering

Department of Materials Science and Engineering

University of Florida

Host: Prof. Norbert Schwesinger

Visiting Fellows 2014

Prof. José Antonio Carrillo de la Plata
Department of Mathematics
Imperial College London
Host: Prof. Massimo Fornasier

Prof. Wendy Demark-Wahnefried
Department of Nutrition Sciences
University of Alabama at Birmingham
Host: Prof. Martin Halle

Prof. Sandrine de Ribaupierre
London Health Sciences Centre, Victoria Hospital
Department of Clinical Neurological Sciences
University of Western Ontario
Host: Prof. Nassir Navab

Prof. Roy Eagleson
Faculty of Engineering
University of Western Ontario
Host: Prof. Nassir Navab

Prof. Robert Guy Griffin
Francis Bitter Magnet Laboratory
MIT School of Science
Host: Prof. Bernd Reif

Prof. Gary L. Haller
Department of Chemical and Environmental Engineering
Yale University
Host: Prof. Johannes Lercher

Prof. Yuri Matiyasevich
St. Petersburg Department of Steklov Institute of Mathematics
Russian Academy of Sciences
Host: Prof. Ernst W. Mayr

Prof. Dianne Newell
Peter Wall Institute for Advanced Studies, Director (retired)
Department of History, University of British Columbia
Host: TUM Institute for Advanced Study

Prof. Klaus Schilling
Department of Informatics VII: Robotics and Telematics
Julius Maximilian University Würzburg
Host: Prof. Florian Holzapfel

Portrait: Rudolf Mößbauer Tenure Track Professors

Core elements of the winning institutional strategy that TUM crafted for the first and second rounds of the Excellence Initiative are united in a special category of TUM-IAS Fellowship that is, simultaneously, a Tenure Track Professorship. In the first phase of the Excellence Initiative, a central measure was the founding of the TUM Institute for Advanced Study, with its emphasis on stimulating the development of new fields of research at the university. The second phase introduced the TUM Faculty Tenure Track within a comprehensive recruitment and career system, offering internationally competitive career options with transparent, performance-based criteria and procedures. These impulses have come together in the Rudolf Mößbauer Tenure Track Professorship.

This Fellowship is named in honor of the former TUM professor who was awarded the 1961 Nobel Prize in Physics. Rudolf Mößbauer Tenure Track Professors are expected, like all other TUM-IAS Fellows, to develop vigorous independent programs and contribute to the intellectual life of the Institute and the university. Like all others on the tenure track, they come into TUM at the level of Assistant Professor with the possibility of tenure as Associate Professor after a positive evaluation (normally in the sixth year) and the potential for future advancement to Full Professor.

The Mößbauer Tenure Track Professorship is unique at TUM, however, in that each candidate has the chance to invent his or her own dream job. Instead of advertising positions carefully predefined by the academic departments, the university makes an open call – that is, open to any topic that might fit TUM's overall research portfolio and strategy – to be administered by the TUM-IAS. There have been three such calls to date, attracting a total of around five hundred applications.

Prof. Franz Hagn: *"It is a great privilege to be part of the interdisciplinary TUM-IAS community, especially as a young scientist who heavily relies on collaborations and fruitful scientific discussions. The Mößbauer Assistant Professorship gave me the opportunity to start my independent research program in the field of membrane protein structural biology at the Bavarian NMR Center at TUM and thereby complement the existing focus of the center. The professional support by the TUM-IAS staff was crucial for setting up my lab within just a few months. I really enjoy and appreciate the scientific freedom, the excellent research infrastructure and the extraordinary scientific community at TUM."*

Prof. Kathrin Lang: *"The Mößbauer Professorship gives me the possibility to establish autonomously – yet with support from renowned professors at TUM – my research field of synthetic biochemistry at the interface of chemistry and biology. I am enjoying very much the collegial and collaborative environment in the department of Chemistry, but the extra bonus of belonging to the TUM-IAS gives me the opportunity to reach out to colleagues whose research is a bit further away from my original experience. This has already led to new, exciting, and very interdisciplinary collaborations."*

By the end of 2014, four exceptional young scientists had joined the TUM faculty under this program. All four provide detailed overviews of their research elsewhere in this Annual Report. Prof. Franz Hagn (p. 100), who came to TUM from Harvard Medical School, focuses on nuclear magnetic resonance (NMR) spectroscopy of membrane proteins. Prof. Kathrin Lang (p. 102) was recruited from the MRC Laboratory of Molecular Biology in Cambridge, UK, and now leads research here in synthetic biochemistry. Prof. Bjoern Menze (p. 76), who joined TUM from ETH Zurich, pursues research in medical image computing, with potential applications in clinical neuroimaging and modeling of tumor growth. The research of Prof. Alessio Zaccone (p. 104) aims to understand the relationship between molecular interactions and the dynamical collective behavior of condensed matter systems; he came to TUM from the Cavendish Laboratory at the University of Cambridge, UK.

As different as their backgrounds and research programs are, these first four Mößbauer Tenure Track Professors describe the experience in similar terms: a transparent and unbiased recruiting process; an informal and multicultural atmosphere that makes it easy for members of the TUM-IAS community to connect and keep up with research in other fields; and a good balance between the security of working within a strong scientific environment and the creative challenge of branching out in new directions.

Prof. Bjoern Menze: *"My research is at the intersection of several disciplines, in particular between medical clinical research and computer science, but also at the intersection with medical physics and bioengineering. As the Mößbauer Professorship is not directly tied with one particular department or institute, it is particularly well suited for such interdisciplinary work. I think it's unlikely that any department would have made an effort to open a position for this type of research in the first place. Also, several links have developed because I had a chance to present my work within the TUM-IAS community. Even though I already spend a significant amount of time talking with people who are not from my department and with widely different backgrounds, the TUM-IAS is my personal window to all the other departments at TUM."*

Prof. Alessio Zaccone: *"The field of amorphous materials has a glorious tradition at TUM. After the retirement of Prof. Wolfgang Götze and before my appointment, this field was no longer represented; therefore I feel honored to revive this area of condensed matter theory in one of the places in the world that contributed most to it in the past. Thanks to my Mößbauer status I have the privilege of shaping the strategy of my own research. Yet while enjoying this intellectual freedom, I also have the opportunity to team up with cutting-edge groups at TUM working experimentally on the same materials and systems – from polymers and biomolecules all the way to metals – to see my mathematical predictions at work in the lab."*

Activities and Events

TUM-IAS General Assembly 2014

April 10–11

Many members of the TUM-IAS community have been involved for several years now; yet, sadly, not all of them have had the opportunity to visit our beautiful headquarters on the Garching campus. It was for this reason, among others, that we decided to hold this year's General Assembly in our own building for the first time. For two days, our building was buzzing with lively discussions and talks on interdisciplinary and future-shaping topics, such as the risks and opportunities of brain plasticity, battery lifetime and performance, human-robot interaction, and nanoscience for renewable energy sources. A poster presentation in which many 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 gain first-hand insight into wholly different research areas.

The General Assembly's conference dinner is always a good and festive occasion to announce new community members and to honor parting members. TUM president and TUM-IAS Board of Trustees chair Prof. Wolfgang A. Herrmann took the opportunity not only to welcome new Fellows, but also to thank a substantial number of Advisory Council members whose terms had come to an end (Prof. Andrzej Buras, Prof. Martin Buss, Prof. Sandra Hirche, Prof. Claudia Klüppelberg, Prof. Arthur Konnerth, Prof. Klaus Mainzer, and Prof. Ernst Rank). Each of them has been an invaluable part of our community for many years, and we sincerely hope to keep them all involved! In addition, it was time for him to say a very personal farewell to his parting fellow Board members (see picture on the right), some of whom had served with him from the very first days of the Institute.

Parting Board of Trustees members, left to right: Prof. Jürgen Mittelstraß, Prof. Klaus-Olaf von Klitzing, Dr. Christian Bode, Prof. Joachim Hagenauer, Prof. Burkhard Göschel, Prof. Angelika Görg, Hildegard Holzheid, Prof. Lars Pallesen, Prof. Frank E. Talke (with TUM president Prof. Wolfgang A. Herrmann, center, and TUM-IAS director Prof. Gerhard Abstreiter, second from the right). Not in the picture: Prof. Manfred Erhardt, Dr. Georg Schütte, and Prof. Peter Wilderer.

Fellows' Lunches

The TUM-IAS is proud of having Fellows and members from all research fields in the TUM portfolio – however, having a large community of talented people with many different specializations has no use if there are no opportunities for them to get together and find out about each other's expertise. It is for this reason that the TUM-IAS Fellows' Lunch has become a long-standing tradition: Once a month, we invite our community to share an informal lunch with us as well as to listen to a talk from one of the members. These talks are always explicitly addressed to an audience of scientists who are experts in fields other than the speaker's, thus enabling a computer scientist to understand a geneticist's project, or giving an architect an insight into biomedical imaging. When, after the lunch, we see new acquaintances lingering to discuss this month's talk or exchanging contact details, we know that once again, the Fellows' Lunch has served its purpose!

February 4

Imaged-Based Modeling of Tumor Growth
Speaker: Prof. Bjoern Menze | Rudolf Mößbauer Tenure Track Professor

March 6

Small Is Powerful: Challenges for Cooperating 1kg Spacecraft Systems
Speaker: Prof. Klaus Schilling (University of Würzburg) | Visiting Fellow

June 2

N-body Algorithms in Computational Science and Engineering
Speaker: Prof. George Biros | Hans Fischer Fellow

July 1

The Registry for Cradle to Cradle® Inspired Elements in Buildings – Celebrating Buildings with Positive Impacts.
Speaker: Martin Korndoerfer | Research Member Cradle to Cradle

Performative Architectural Typologies Integral to the Energy Equation
Speaker: Prof. Mohamad T. Araji (University of Manitoba) | TÜV Süd Stiftung Visiting Professor

October 2

Tell Me What You Do and I'll Tell You Who You Are: Exploring the Functional Basis of Microorganism Classification.
Speaker: Prof. Yana Bromberg | Hans Fischer Fellow

November 6

Friction Mechanics, onset of Sliding, and Laboratory Earthquakes
Speaker: Prof. Steven D. Glaser | TUM Distinguished Affiliated Professor

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

This lecture series was started at the end of 2013 to engage local residents – particularly high school students – in the scientific research activities on the Garching campus. The talks are specifically aimed at a non-scientific audience and are therefore an opportunity for interested members of the public to expand their scientific knowledge and engage in intellectual discourse.

In March 2014, Prof. Andreas Burkert of the Max Planck Institute for Extraterrestrial Physics gave the introductory lecture, “The black hole in the center of our milky way.” This was followed in June by “Is ois Nano? – Insight into nano sciences,” given by our very own director Prof. Gerhard Abstreiter. Further topics were “Experimentation with the coldest objects in the universe” (September) by Prof. Immanuel Bloch of the Max Planck Institute of Quantum Optics and “What can engineers contribute to the advancements in the medical field?” (November) by Prof. Wolfgang A. Wall, chair for Numerical Mechanics at TUM. A little out of the ordinary but all the more popular with the kids was the robot Roboy, who was presented to the audience in the drama “Roboy – To be or not to be humanoid” (May), followed by a talk by Prof. Rolf Pfeifer from the University of Zurich. Without exception, all talks were met with great interest and followed by a lively discussion. We thank everyone for the overwhelmingly positive response and look forward to continuing this lecture series.

Scientists Meet Scientists – Wednesday Coffee Talk

We began hosting the Wednesday Coffee Talks in the summer of 2013 with the intention of bringing together people from outside and within the TUM-IAS community to share experiences about their work and research. Since then, we have held over 50 talks by diverse speakers whose publications resulted in a press release by TUM, with the topics ranging from drug development to particle physics. There is always plenty of time before and after the talk for discussion and conversation, while enjoying a cup of coffee. The relaxed atmosphere has drawn together various people from all over the campus who now regularly attend the talks. These Wednesday get-togethers were met with great enthusiasm throughout 2014 and will certainly be continued.

January 15	Prof. Gerhard Abstreiter on nanowire lasers that could work with silicon chips, optical fibers, even living cells
January 22	Prof. Johannes Buchner on proteins safeguarding against cataracts
January 29	Prof. Thorsten Bach on photoreactions as a potential pathway to drug development
February 5	Prof. Ingrid Kögel-Knabner on how carbon content in soil influences today's climate models
March 26	Prof. Friedrich Simmel on the thousand-droplets test
April 2	Prof. Reinhard Kienberger on having developed a detector for the measurement of the waveforms of pulsed laser radiation which brings them one step closer towards perfect control of light waves
April 16	Dr. Tobias Madl on a chaperone that binds a protein which is responsible for Alzheimer's disease
April 23	Prof. Stefan Sieber on new mechanisms of action that open alternative approaches to antibiotics development
April 30	Prof. Ulrike Protzer on having discovered a new way of defense against the hepatitis B virus

May 7	Prof. Michael Bader on a computational record on SuperMUC: an earthquake simulation that tops one quadrillion flops
May 14	Prof. Jürgen Ruland on a "braking system" for immune responses
May 21	Dr. Nils Haag on having discovered a way to apply an astroparticle physics methodology to nuclear facility monitoring
May 28	Prof. Raman I. Sujith on multifractality in combustion noise: the prediction of an impending instability
June 4	Dr. José Antonio Garrido on a gateway to tuning diamond devices
June 11	Prof. Gerhard Abstreiter on the perfect penalty kick (World Cup edition)
June 25	Prof. Florian Holzapfel on brain-controlled aircraft
July 9	Prof. Peter Fierlinger on not having found any evidence of the Majorana nature of neutrinos
July 16	Prof. Bernhard Küster on having decoded the human proteome
July 23	Prof. Dirk Haller on having discovered that cell stress can inflame the gut
July 30	Prof. Gordon Cheng on the Walk Again project, which led to a paralyzed person kicking the World Cup's first ball
September 24	Prof. Thomas Hofmann on having decoded the molecular olfactory signatures of foodstuffs
October 1	Prof. Markus-Christian Amann on having created highly efficient nonlinear metamaterials for laser technology
October 8	Dr. Uwe Firzlaff on spatial orientation in bats
October 15	Prof. Stefan Schönert on observing the creation of solar energy for the first time ever
October 22	Prof. Andreas Bausch on having fabricated a moveable cytoskeleton membrane
October 29	Prof. Michael Groll on having found a way to inhibit the functionality of immunoproteasome
November 5	Prof. Klaus Schilling on the Rosetta spacecraft: The art of landing and drilling on a comet
November 12	Dr. Markus Becherer on how field-coupled magnets could replace transistors in some computer chips
November 19	Prof. Franz Pfeiffer on having improved the method of X-ray phase-contrast imaging by scrambling x-rays from a new source
November 26	Prof. Percy Knolle on having discovered a signaling pathway for T cell activation in the liver
December 3	Dr. Andreas Kronfeld on the origin of mass for everyday objects, and why they are made of matter and not antimatter
December 10	Prof. Joachim Hermsdörfer on what happens in our brain when we unlock a door
December 17	Prof. Wilfried Schwab on having discovered the mechanism for aroma formation in wine

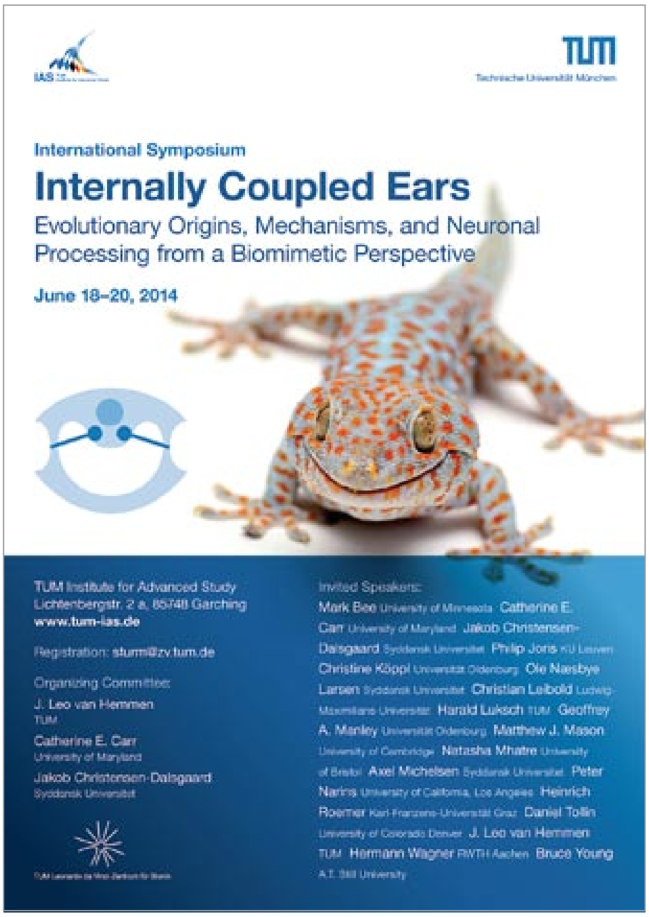
International Symposium on Internally Coupled Ears: Evolutionary Origins, Mechanisms, and Neuronal Processing from a Biomimetic Perspective

June 18–20

Organization: Prof. J. Leo van Hemmen (TUM), Prof. Catherine E. Carr (University of Maryland), Prof. Jakob Christensen Dalsgaard (University of Southern Denmark)

Animals have evolved a variety of adaptations to enhance spatial hearing, such as the external, often moveable ears of mammals, the facial ruffs of barn owls and the coupled ears of insects and reptiles. Coupled ears are well understood in insects; in 1941, Hans-Jochen Autrum (Berlin, later LMU Munich) showed that the coupling of locust ears greatly increased sound localization cues. The performance of coupled ears in vertebrates is less well understood. Large groups of the latter, such as frogs, lizards, birds, and crocodilia, have an air-filled cavity or an equivalent thereof, starting with a mere cylinder in frogs, which connects the left and right eardrums. Hence a natural but fundamental question is why so many orders possess a direct coupling between left and right tympanum. In short, why do they possess internally coupled ears or, for short, ICE? Exactly this question, in conjunction with potential biomimetic spinoffs, was the focus of the ICE Symposium at the TUM-IAS.
In principle, internally coupled ears enhance directional hearing because both sides of the eardrum are exposed to the sound waves and thus will respond to the difference in sound pressure on each side of the membrane. The resultant eardrum motion is thus a function of both the phase and intensity difference across the eardrum. The degree to which ears are coupled depends on the anatomy of interior coupling, the sound frequency, and the animal's physiological state.

In practice, however, the strength of the coupling between the ears has been called into question: Is it sufficient to modify eardrum motion? In birds, for example, an anatomical connection between the middle ears of birds exists through the interaural canal. In lizards, the coupling is even more pronounced, and the tympani are connected through the oral cavity. In alligators there are even several canals with an analogous coupling function. Though described in astounding detail by Owen as early as 1850, the resulting effects on the nature of sound localization have aroused intense study only recently. Although internally coupled ears have appeared in many vertebrate orders, they are far better understood in insects. Autrum (1941) was the first to point out their prevalent presence in insect hearing, though on a different scale and at higher frequencies.



At the symposium these issues were addressed in detail. This gathering of most of the contributors to the field made it possible to resolve the confusion, while recent theoretical analyses (van Hemmen, Michelsen) clarified several interlocking effects of structure and frequency. A further important advantage of the symposium that it brought together groups that could analyze interaural coupling in frogs (Narins), lizards (Carr, Christensen-Dalsgaard, Young), birds (Köppl, Næsbye Larsen, Leibold, Luksch, Wagner), lizards (Carr, Christensen-Dalsgaard, van Hemmen), alligators (Carr, Christensen-Dalsgaard, van Hemmen, Tollin), and even mammals (Joris, Manley, Mason, Tollin), so that the striking similarity between ICE in all these orders – as well as its contrast with most, though not all, of the mammals – became evident. Several surprising spinoffs arose naturally. Furthermore, insect experts (Mhatre and Roemer) were able to present a puzzling analogy between ICE in vertebrates and its equivalent in insects such as locusts and crickets.

In summary this symposium was the first of its kind to bring together the leading experts on ICE, arrive at a complete agreement on the terminology that ought to be used, and to highlight the universality of ICE in many animal orders and its underlying mechanisms. Only if we clearly grasp the mechanisms underlying ICE both experimentally and theoretically (i.e., mathematically) can we devise biomimetic applications to a full extent. It is fair to say that, with evolutionary hindsight, nature must have had good reasons to provide that many animals with ICE. The TUM-IAS played an essential role in bringing together so many prominent investigators working on ICE in so many different fields, enabling them to unify the underlying biological physics, and revealing how different orders in nature handle the ensuing neuronal information processing that is essential to auditory processing.

Liesel Beckmann Symposium 2014

November 3, 2014

Organization: Chair for Strategy and Organization, TUM

Solutions! New Ways of Working – Diversity in Organizations

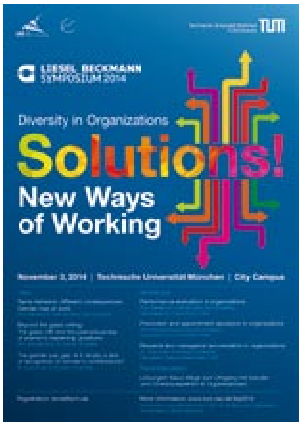
In 2014, the Liesel Beckmann Symposium, which generally aims to generate new ideas and concepts for gender and diversity related research at TUM and to help promote internal and external networking, focused on the topic of gender in organizations. Under the title "Solutions! Diversity in Organization: New Ways of Working," 181 participants followed the invitation from the TUM-IAS, TUM.Diversity, and the Chair for Strategy and Organization of the TUM School of Management to the city campus in Munich. Researchers from TUM and other universities and practitioners working on gender equality in organizations from TUM, other universities, and private organizations took part.

Researchers and practitioners discussed new solutions for introducing gender equality, particularly with regard to performance evaluations, promotion decisions, and rewards in organizations. The program included keynotes by internationally renowned scientists, parallel workshops, and a discussion including panelists from academia, politics, and private organizations. In between, participants used the networking breaks to connect with each other and exchange their experiences with gender and diversity in organizations.

Keynotes by internationally renowned scientists
After the welcome by Prof. Isabell M. Welpe (Strategy and Organization, TUM) and Prof. Klaus Diepold (Senior Vice President for Diversity and Talent Management, TUM), three keynotes introduced the participants to the latest research results on gender in organizations.

Keynote 1: "Same behavior, different consequences: Gender bias at work"
by Prof. Madeline E. Heilman.

Prof. Madeline E. Heilman is a professor of Psychology at New York University and a TUM-IAS Anna Boyksen Fellow by invitation of the Chair for Strategy and Organization. With her research focusing for more than 30 years on gender in organizations, Prof. Madeline E. Heilman is one of the most outstanding researchers in this field and has published throughout that time in international top journals such as the Journal of Applied Psychology. Based on this profound experience on the topic, her talk discussed the nature of gender stereotypes and their detrimental effects on women's career progress. It particularly addressed the question of why being competent and qualified provides no assurance to a woman that she will advance to the same organizational level as an equivalently competent and qualified man.



Keynote 2: "Beyond the glass ceiling: The glass cliff and the precariousness of women's leadership positions" by Prof. Michelle Ryan.

Prof. Michelle Ryan is a professor of Social and Organisational Psychology at the University of Exeter. In her keynote, she presented her research program on the glass cliff phenomenon, which was short-listed for the Times Higher Education Supplement Research Project of the Year in 2005 and was named as one of the ideas that shaped 2008 by the New York Times. While women are breaking through the glass ceiling in increasing numbers, they are more likely than men to be placed in leadership positions that are risky and precarious – that is, on the "glass cliff."

Keynote 3: "The gender pay gap: Is it simply a lack of recognition of women's contributions?" by Dr. Clara Kulich.

Rounding up the keynotes on gender in organizations, Dr. Clara Kulich from the University of Geneva presented her research on the gender pay gap. This research predominantly shows differences between male and female remuneration, controlling for a number of human-capital factors. Kulich's talk illustrated that investigations of the context in which pay disparities occur point to a complex interaction of factors that goes beyond a simple difference in pay.

Workshops on solutions

With the keynotes having presented and delineated the main challenges for achieving gender equality in organizations, the workshops aimed to foster discussion on how organizations can respond with appropriate solutions. In three parallel workshops (workshop 1: *Performance evaluations in organizations*, led by Prof. Madeline E. Heilman; workshop 2: *Promotion and appointment decisions in organizations*, led by Prof. Michelle Ryan; and workshop 3: *Rewards and managerial remuneration in organizations*, led by Dr. Clara Kulich), the symposium participants vigorously discussed with the scientific experts new ideas, measures, and approaches for promoting unbiased performance evaluations, promotion and appointment decisions, and reward allocations in organizations.

Panel discussion on Solutions! Diversity in Organizations: New Ways of Working

This discussion included panelists from academia, politics, and private organizations: Prof. Sabine Doering-Manteuffel (President, University of Augsburg); Dr. Rudolf Gröger (President, Munich Business School, and former CEO of O2); Dr. Beate Merk (Minister of State, European Affairs and Regional Relations); Prof. Gerhard Müller (Senior Vice President for Academic and Student Affairs, TUM); and Bettina Reitz-Luebbert (TV director, Bayerischer Rundfunk). Moderated by Prof. Isabell M. Welpe, they discussed reasons for the underrepresentation of women in leadership positions, changes and measures to foster the promotion of women into leadership positions, and the necessary immediate next steps for achieving gender equality.

International Expert Group on Earth System Preservation (IESP)

The International Expert Group on Earth System Preservation (IESP) is a global network of scientists, engineers, and members from governmental and non-governmental organizations. Its purpose is to contribute to advances in Earth system science through thematic-based conferences, workshops, seminars, lectures, and publications. It also serves as a liaison between experts, decision makers, and the public. The IESP promotes the exchange of knowledge and provides access to current scientific results. Its activities contribute to widespread policy debates by establishing a platform for discussion on sustainable development of ecosystems, economic and societal systems, and their interrelationships. The IESP network has more than 50 international members from the fields of sustainability research, energy and environmental sciences, resource technology, environmental engineering, climate dynamics, risk assessment, industrial ecology, political sciences, economics, and more. The IESP is supported by the Bavarian State Ministry of the Environment and Consumer Protection. In addition, the IESP is hosted by TUM-IAS, where the organizational staff is located. Prof. Peter Wilderer acts as chairman of the IESP.

Earth system science

The thematic-based activities of the IESP focus mainly on the promotion of scientific knowledge in Earth system science. The Earth system is to be understood as the sum of the planet's interacting physical, chemical, biological, and anthropogenic processes. As the human population is growing rapidly, the extent of anthropogenic impact is increasing as well, leading to problematic environmental changes: for example, global warming caused by excess emission of greenhouse gases. Obviously, humankind is changing the Earth system and its function, deeply affecting its dynamic, its stability, and its resilience. Therefore one of the most important concerns of the scientists of the IESP is how to protect the functioning of the Earth system in favor of the continued existence of life on Earth and decent living conditions for future generations.

IESP Events

October 2013– January 2014	International Online Workshop **Post-2015 Development Goals** Organization: IESP
April 23–25, 2014 Wildbad Kreuth	International Workshop **Global Stability through Decentralization?** **In search for the right balance between central and decentral solutions** Organization: IESP
May 6–7, 2014 IFAT Munich	Symposium **Intelligent Peri-Urbanization through Decentralization** Organization: IESP, Chinese Research Academy of Environmental Sciences (CRAES)
July 3, 2014 Augsburg	Colloquium **Microplastics in the Environment** Organization: IESP, Bavarian Environment Agency
September 8–12, 2014 TUM-IAS	International **Workshop on Environmental Modeling** Organization: IESP, TUM-IAS, LRZ

TUM-IAS Events

January 14

Seminar **NanoSIMS – A Tool to Discover Micro-Scale Processes from Geology to Life Science**
Organization: Chair for Soil Science
Speakers: Prof. Ingrid Kögel-Knabner | Carl von Linde Senior Fellow,
Dr. Carmen Höschen (Soil Science, TUM)

January 17

Lecture **Use of Hybrid Surgical Suites for Different Applications and Overview of Technical Solutions**
Organization: Prof. Michael Friebe | Rudolf Diesel Industry Fellow
Speaker: Dirk Sunderbrink (Siemens AG)

January 24–25

Bioprinting Workshop for Horizon 2020
Organization: Prof. Dietmar W. Hutmacher | Hans Fischer Senior Fellow

February 13

Kolloquium zu Ehren von Prof. Friedhelm Korte **Ökologische Chemie und Bauen**
Organization: Prof. Michael Braungart | Start-up Cradle to Cradle
Prof. Werner Lang (Energy-Efficient, Sustainable Building and Planning, TUM)
Prof. Harun Parlar (Chemical-Technical Analysis and Chemical Food Technology, TUM)

March 17–18

Munich Battery Discussions **Reliable High Energy Materials – Perspectives for the Future Energy Storage**
Organization: Dr. Peter Lamp | Rudolf Diesel Industry Fellow
Prof. Julia Kunze-Liebhäuser | Carl von Linde Junior Fellow
Prof. Hubert Gasteiger (Technical Electrochemistry, TUM)

March 23

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

Lecture Series „Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?“ **Das Schwarze Loch im Zentrum unserer Milchstraße**
Speaker: Prof. Andreas Burkert (Ludwig-Maximilians-Universität München; Max Planck Institute for Extraterrestrial Physics)

March 25

Inaugural Lecture **Quantum Nano-Photonics**
Speaker: Prof. Jelena Vuckovic | Hans Fischer Senior Fellow

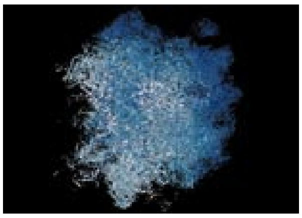
March 28

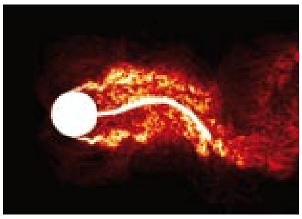
Opening Ceremony **TUM Center for Advanced PCE Studies**
Organization: Chair for Construction Chemistry, TUM-IAS

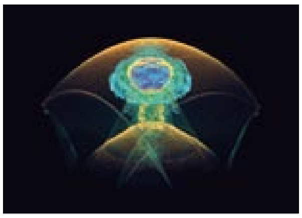
April 10–11

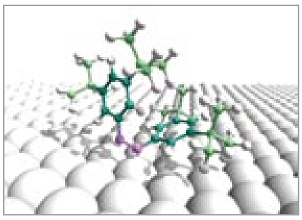
TUM-IAS General Assembly

May 7 Opening of the Exhibition **Science and Technology Meet Art – Computer Simulations**









May 8 Talk **Autonomie auf anderen Planeten: Die Raumsonden Rosetta, Huygens & Co.**
Organization: Forum Munich Aerospace
Speaker: Prof. Klaus Schilling (University of Würzburg) | Visiting Fellow

May 11 Lecture Series „Was machen eigentlich unsere Nachbarn, die Forscher in Garching?“ **Roboy – Humanoid sein oder nicht sein**
Organization: TUM Faculty for Informatics, TUM-IAS
Mini-Drama: Sasha Mazzotti, Philipp Siegel
Speaker: Prof. Rolf Pfeifer (University of Zurich)

May 12 Münchner Physik-Kolloquium **Recent Advances and Future Trends in Medical Computed Tomography**
Speaker: Dr. Thomas Koehler | Rudolf Diesel Industry Fellow

May 15 Kick-off Symposium **Interfaces of Two-Dimensional Materials: Graphene and Beyond**
Organization: Prof. Matthias Batzill | Hans Fischer Fellow
Prof. Johannes Barth (Molecular Nanoscience and Chemical Physics of Interfaces)

May 15 Talk **Environmental Augmentation**
Organization: Oskar von Miller Forum
Speaker: Prof. Mohamad T. Araji (University of Manitoba) | TÜV Süd Stiftung Visiting Professor

May 19 Lecture Series **Signal Processing and Time Frequency Analysis - Learn How to Analyze Experimental and Numerical Data**
Organization: Chair for Thermodynamics
Speaker: Prof. Arun K. Tangirala (IIT Madras) | Alumnus Visiting Fellow

May 22 Speakers Series "New Frontiers in Battery Science and Technology"
Solid Electrolytes as Battery Components
Organization: Dr. Peter Lamp | Rudolf Diesel Industry Fellow
Speaker: Prof. Jürgen Janek (Justus Liebig University Gießen)

May 28 TUM Informatik-Kolloquium **Scalable Nearest Neighbor Search Algorithms in High Dimensions**
Speaker: Prof. George Biros | Hans Fischer Fellow

June 1 Lecture Series „Was machen eigentlich unsere Nachbarn, die Forscher in Garching?" **Is ois Nano? – Einblicke in die Nanowissenschaften**
Speaker: Prof. Gerhard Abstreiter | TUM-IAS/Walter Schottky Institute

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

June 2 Talk **Piezoelectric Energy Harvesting through Nanostructured Materials**
Speaker: Prof. Henry Sodano (University of Florida) | TÜV Süd Stiftung Visiting Professor

June 3 Workshop **Reconstruction Technology in Medical Imaging**
Organization: Dr. Thomas Koehler | Rudolf Diesel Industry Fellow

June 9 CLEO:2014 Special Symposium in Memory of James P. Gordon
Organization: Dr. René-Jean Essiambre | Rudolf Diesel Industry Fellow, et al.
Location: San Jose, USA

June 18–20 International Symposium **Internally Coupled Ears – Evolutionary Origins, Mechanisms, and Neuronal Processing from a Biomimetic Perspective**
Organization: Prof. J. Leo van Hemmen (Theoretical Biophysics, TUM)
Prof. Catherine E. Carr (University of Maryland, College Park)
Prof. Jakob Christensen-Dalsgaard (University of Southern Denmark), TUM-IAS

July 17 Talk **Minimizing Interaction Energies**
Speaker: Prof. José A. Carrillo de la Plata (Imperial College London) | Visiting Fellow

June 25 **TUM-IAS Summer Faculty Day**

August 20

Speakers Series “New Frontiers in Battery Science and Technology”:
Reversible Li-Metal-Electrodes for Rechargeable Li-S and Li-Air Batteries
Organization: Dr. Peter Lamp | Rudolf Diesel Industry Fellow
Speaker: Prof. Martin Winter (University of Münster)

September 19

Eric Catalysis Colloquium **Methanol to Gasoline/Olefins Revisited**
Speaker: Prof. Gary L. Haller (Yale University) | Visiting Fellow

September 21–23

2nd Annual Helmholtz-Nature Medicine Diabetes Conference
Organization: Prof. Matthias Tschöp (Metabolic Diseases, TUM), et al.
Speaker: Prof. Tamas L. Horvath | Hans Fischer Senior Fellow, et al.

September 28

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

Lecture Series “Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?” **Experimentieren mit den kältesten Objekten des Universums**
Speaker: Prof. Immanuel Bloch (Max Planck Institute of Quantum Optics)

October 6

International Workshop on **Advanced Robotics PLUS**
Organization: Prof. Martin Buss | Carl von Linde Senior Fellow, CoTeSys

October 6–10

Synbreed Summer School **From SNPs to Gene Networks**
Organization: Focus Group Statistical and Quantitative Genomics

October 9–10

EUBET2014: **Applications of Effective Field Theories to Particle Physics, Condensed Matter and Quantum Optics**
Organization: Prof. Nora Brambilla (Theoretical Particle and Nucelar Physics, TUM)

October 11

Tag der offenen Tür
Talk **Is ois Nano? Mit einer Einführung in das TUM Institute for Advanced Study**
Speaker: Prof. Gerhard Abstreiter | TUM-IAS/Walter Schottky Institute
Talk **Was blüht uns in Zukunft? Der Einfluss des Klimawandels auf allergieauslösende Pflanzen**
Speaker: Dr. Susanne Jochner (Ecoclimatology, TUM)

October 14

Inaugural Lecture **Sliding Friction and the Onset of Earthquake**
Speaker: Prof. Steven D. Glaser (University of California, Berkeley) | TUM Distinguished Affiliated Professor

October 21

Inaugural Lecture **Distributed Learning in Collaborative Control and Decision Making**
Speaker: Prof. John S. Baras | Hans Fischer Senior Fellow

October 24–25

3rd International Symposium: Exercise and Cancer 2014 - Impact on Prevention and Prognosis
Speaker: Prof. Wendy Demark-Wahnefried (University of Alabama at Birmingham) | Visiting Fellow, et al.

October 26–30

SpinMol Conference
Organization: Prof. Harald Brune | Hans Fischer Senior Fellow, et al.
Location: ETH Zurich

October 27

Münchner Physik-Kolloquium **Structurally Disordered Materials: From Fundamental Physics to Applications**
Speaker: Prof. Alessio Zaccone | Rudolf Mößbauer Tenure Track Professor

November 3

LIESEL BECKMANN SYMPOSIUM 2014

Liesel-Beckmann-Symposium 2014: **Solutions! New Ways of Working: Diversity in Organizations**
Organization: Chair for Strategy and Organization, TUM-IAS
Speakers: Prof. Madeline E. Heilman | Anna Boyksen Fellow
Prof. Michelle Ryan (University of Exeter)
Dr. Clara Kulich (University of Geneva)

November 6

Inaugural Lecture **Applications of an Expanded Genetic Code - The Power of Bioorthogonal Chemistry**
Speaker: Prof. Kathrin Lang | Rudolf Mößbauer Tenure Track Professor

November 18

Talk **Wide-bandgap Semiconductors for Electronic and Photovoltaic Applications**
Speaker: Prof. Stephen Goodnick | Hans Fischer Senior Fellow

November 23

Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?

Lecture Series "Was machen eigentlich unsere Nachbarn, die Forscher, in Garching?" **Ingenieure in der Medizin – Einblicke in Computational Biomedical Engineering**
Speaker: Prof. Wolfgang A. Wall (Computational Mechanics, TUM)

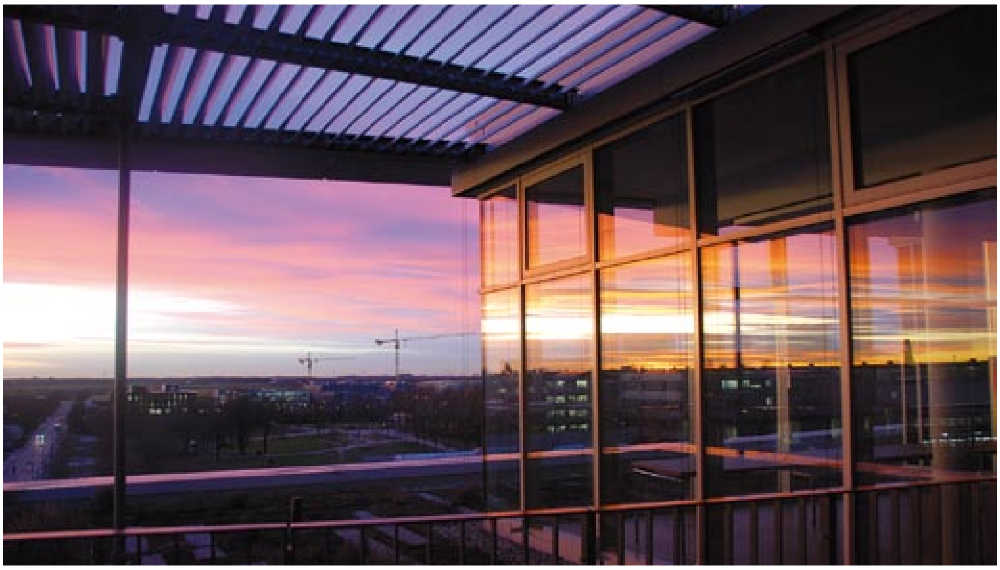
November 26

Kick-off Symposium **Lattice Gauge Theory and Effective Field Theories**
Organization: Dr. Andreas Kronfeld | Hans Fischer Senior Fellow

December 3

Talk **MFI-based Catalysts for Oligomerization of Olefins for Diesel Fuel**
Speaker: Prof. Gary L. Haller (Yale University) | Visiting Fellow

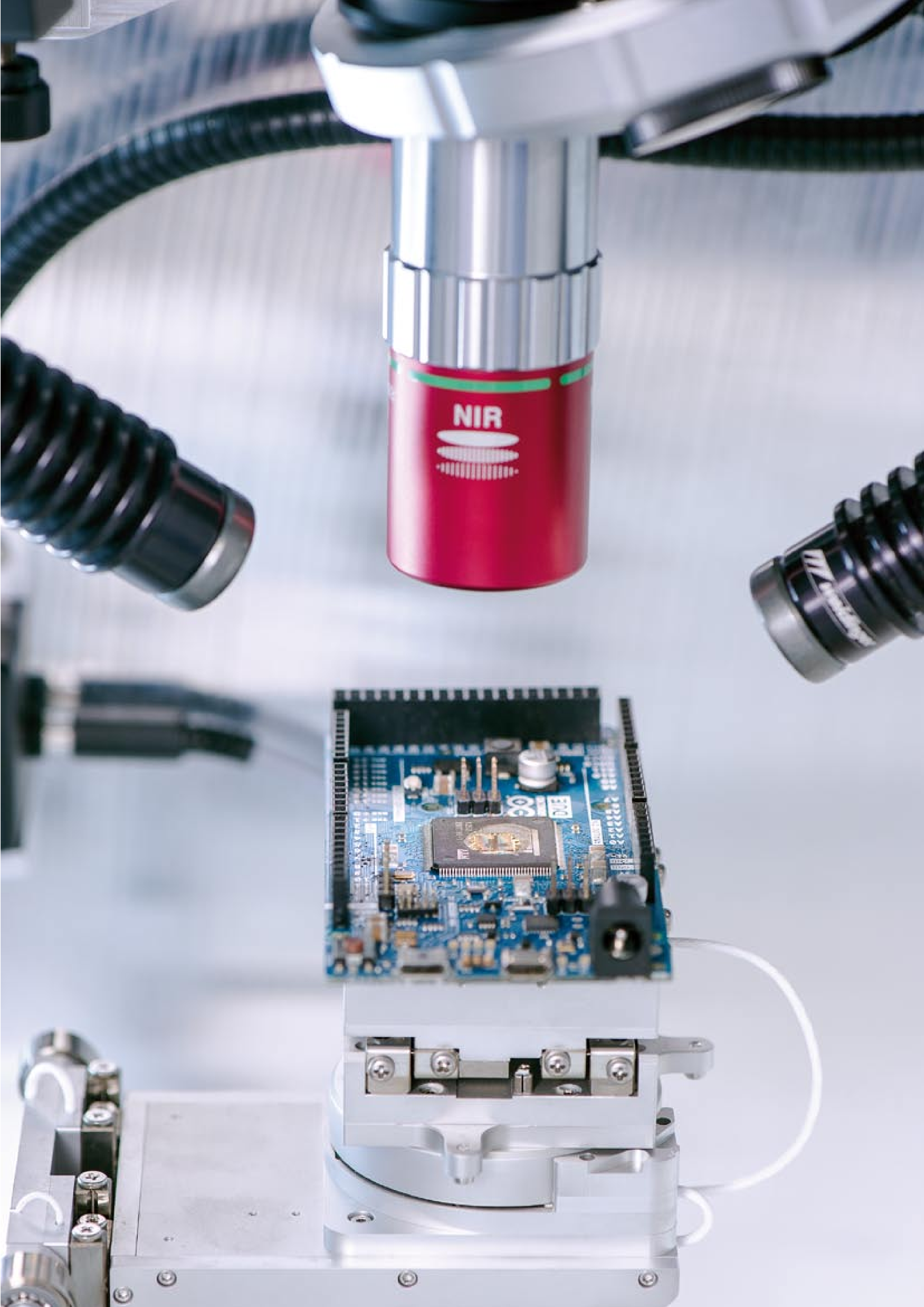
December 3 **TUM-IAS Winter Faculty Day**



December 10 Inaugural Lecture **Brain Plasticity: Risks and Opportunities**
Speaker: Prof. Josef P. Rauschecker | Hans Fischer Senior Fellow

December 10 – 11 Munich Workshop on **Information Theory of Optical Fiber**
Organization: Focus Group Fiber-Optic Communication and Information Theory: Prof. Gerhard Kramer, Dr. Luca Barletta, Dr. Mansoor Yousefi (Communications Engineering), et al.

December 11 Speakers Series "New Frontiers in Battery Science and Technology"
Lithium Distribution and Diffusion Paths in Solid State Electrolytes and their Challenges in Terms of Structural Compatibility in Solid State Batteries
Organization: Dr. Peter Lamp | Rudolf Diesel Industry Fellow
Speaker: Prof. Helmut Ehrenberg (Karlsruhe Institute of Technology)


NIR

In Focus

C-H Activation Chemistry

Fiber-Optic Communication
and Information Theory

On the trail of nature's solutions

From a group interview by Patrick S. Regan (PSR) with Hans Fischer Senior Fellow Polly L. Arnold, University of Edinburgh (PLA); Prof. Fritz E. Kühn, TUM (FEK); and doctoral candidates Max McMullon, University of Edinburgh (MM); and Julia Rieb, TUM (JR).

PSR: Your group is focusing wide-ranging expertise in chemical synthesis and catalysts on new approaches to activating carbon-hydrogen bonds. What's the aim?

PLA: We want to show how, working together, we can more easily make compounds that break some of the hardest bonds to break, in molecules that we currently burn when we should be using them to do useful things.

PSR: Molecules such as oil and natural gas?

MM: We want to use the resources that we have in the correct way, with maximum efficiency. At the moment we burn a lot of methane as a by-product, but if we could transform the molecules – for example, activating the bonds of the molecules to make them easier to transport – then that's a higher-value product. That's the aim of the project.

FEK: The final goal is to activate C-H bonds, particularly in methane. Methane is a very abundant molecule on the earth, as methane hydrate or as natural gas. If you transform methane gas into methanol, alcohol, it becomes a liquid and can be much more easily transported. The art is to stop the oxidation of methane after the oxidation to methanol and not go all the way through to carbon dioxide. If you have methanol, you can use it as a liquid fuel, on the one hand, or as a starting material for a variety of value-added chemicals.

PLA: Fossil fuels and biorenewables all contain a large number of very similar carbon-hydrogen bonds. The molecules have carbon skeletons with carbon-hydrogen bonds all over them. The bonds aren't the strongest bonds known, but the compounds are very symmetrical, and selectively choosing just one carbon-hydrogen bond and then converting that – either in the absence or presence of other potentially useful functional groups of other atoms – that's the hard thing to do. So if you have methane, you just have a perfect tetrahedron with very inaccessible, identical carbon-hydrogen bonds. To get just one, that's the real trick.

If you have a very good catalyst that functions at low temperature – so if we really do make a good asymmetric molecule, as we are trying to do with cerium – that can pick up selectively just one carbon-hydrogen bond, there might be interesting fine chemicals or more complex molecules where, instead of ignoring every other carbon-hydrogen bond, we can treat those as the functional group. So we could selectively pick out a carbon-hydrogen bond in a very complex structure and then would not have to go through all the atom-inefficient processes of putting in other groups earlier on in the synthesis. So we can do a late-stage transformation and make exactly the drug molecule that we want, with perfect atom economy. All the basic molecules start with carbon-hydrogen bonds everywhere, so to control the carbon-hydrogen bond in the presence of all sorts of atoms is extremely useful in a variety of ways.

FEK: Nature can do this. Nature can transform methane into methanol. But mimicking the natural compounds, the enzymes, is difficult, because usually they have an organometallic element but then a lot of biochemistry around it. These bio-ligands we cannot yet synthesize easily. So what we need are molecules that are easier to make than those natural compounds but achieve similar purposes. There are several metals at hand that are common enough, and promising enough, to be used. Our groups utilize different approaches with different metals, but we can compare how close they come to the solutions of nature.

PSR: And you are working with solutions, aren't you?

PLA: There are some really high-energy solid-state processes where instead of just burning a hydrocarbon you can partially transform it – which is pretty much what we're trying to do – but it's a lot more aggressive. For us, taking a solution approach, where everything is all dissolved up together, gives us perfect control – not only allowing us to trap every intermediate product as we go along so we understand what we're doing and then can design a better one, but also enabling us to do this at low energy, so we can behave more like nature does.

Polly L. Arnold

PSR: How do you gain that kind of insight into a reaction?

PLA: Say you're looking at the transient intermediate that forms when you bring one of these traditionally inert small molecules, one of these hydrocarbons, right up to the metal center – and it just starts to form that interaction. Sometimes you can trap these in a crystalline form. You can look at the structure and see how you might want to design or redesign your molecule to get that perfect approach and then get enough electron density from your metal into that small molecule to break up that carbon-hydrogen bond – just that one and not the others. Crystallizing these is hugely important for us, and that's one of the things that our sorts of chemistry allow us to do.

PSR: What are you after besides lowering the energy threshold for a reaction?

Fritz E. Kühn

FEK: Allowing pathways that otherwise would not be available, or that would be available only with more difficulty. So if we examine different molecules, we can also open up new ways in which we can do a reaction that, before, was energetically not favored and just didn't happen. This can also lead to somewhat different pathways, and we have to see if we get side products, do we get what we want, in which direction does the whole thing go. Of course we need to know more about the reaction pathways, we need to know intermediates. If we have just the starting and product molecules, there would be a lot of possible ways, and when we modify the process, it would just be trial and error. The more we know of the steps in between, the more tailor-made our catalysts can be.

PSR: What kinds of alternatives are available?

PLA: To convert single carbon-hydrogen bonds you can take a big bed of solid-state material and heat it up to 800 degrees, so fast that only some of the bonds transform – and that's not going to work for a fine chemical. Or you can work with very expensive, very rare metals on the right-hand side of the periodic table – such as palladium and platinum, metals that don't exist very much in the earth's crust. Cerium and iron, the metals that our labs focus on, are ubiquitous, very cheap, and practically non-toxic. The drug companies will take many extra steps to avoid using palladium; if it gets left in a drug, it's very toxic. But cerium and other lanthanides are ten times less toxic than iron, which already is regarded as being non-toxic or nearly so.

FEK: Iron is one of the most common elements. It's not, in most of its compounds, toxic, because nature has had time to cope with it and use it safely for various purposes. Some of the less common elements either are toxic to living beings or have little influence on biological processes.

PSR: And now your Focus Group has brought together the Edinburgh lab's experience working with lanthanides and the TUM lab's experience with iron. How does this work in practice?

JR: In my master's thesis at TUM, I worked with metalorganic complexes of iron. When I switched to this project, we decided to keep my ligands, the organic framework around a metal center, and try them with these unusual metals. We don't know so much about them, but they seem to do very interesting chemistry. We kept my ligands, and took these metals, and we tried to combine the expertise. My focus is just to explore if there is any possibility to activate these inert molecules with cerium organometallic complexes, so-called NHC-complexes. Using my ligands I already worked with makes it a little bit easier.

PLA: We have been developing a large variety of the sorts of frameworks that you would think could bind, particularly working in my group, the lanthanide ions. We've also both been interested in opportunities perhaps to put two metals together. If we could combine the cerium and iron that we have so much expertise in, using the same large organic ligand structures that we've been working with, we might see cooperativity from compounds that people haven't been able to isolate before. This is something that's really quite different to what other people are doing. One of the simplest ways to build up from this is to take both types using ligands and see just how we combine first iron and then cerium in there. We're finding that you need to have a much bigger ligand framework for that – which we could predict – but it's also thrown up other interesting routes. Julia was able to come to our lab, where we have a smorgasbord of reagents that can insert just that metal ion in a whole different range of starting materials.

PSR: Is this like a chemical library, or a toolbox?

PLA: Yes. She was able to take some ligand into the glovebox and go along the shelves and just pick one reagent after another and have a look. In almost all cases the solutions went purple, and then in almost all cases they decomposed. However, we identified a couple that didn't, and things began to look good, so Julia was able to come back here into the iron expertise area, with the different ligand set, knowing which cerium compounds she wanted to focus on while she was here. And then she could draw on Max's expertise by keeping contact, to help characterize what was going on.

PSR: And is this the kind of thing that you really can't do yet, or that you can't accelerate, through computational chemistry?

FEK: To a certain degree, yes. The problem is, we have a toolbox with a lot of tools, and we do not know what all of them can do. And by putting them together, we try to find how much we can predict and see what we might be able to use for something we are not aware of yet. It's like building something with very versatile building blocks, which can do more than we already know. Of course we can make predictions based on what we know. But we always have, so to say, an exchange between what we already know and what we think we could achieve. If we don't know what kind of intermediates we have, it's like having two valleys, and you just know that there are mountains in between, but you don't know the mountain passes, and you might not exactly know the height of the mountains. If you just try to get to the other side of the mountain ridge without additional information, the theoretician may find one way, but there could be other pathways that lead over lower passes and would be easier to walk.

PLA: Max and I wouldn't dream of trusting our own calculations on the metals we use, because we're working right at the bottom of the periodic table, where the nuclei are so densely packed that relativistic effects apply. It's very difficult to know how to even start the calculations. It's really not our area of expertise. Calculations on iron for example are much more straightforward, because all the atoms in those calculations are so much lighter. So we actually collaborate a lot with computational chemists.

PSR: And physicists?

PLA: Yes. To try and understand where the electrons are, and to help them better explain the bonding in these materials, which are also nuclear waste-relevant. But for us, computation has never been a predictive option. So it's nice to make weird molecules that help the computational chemists improve their models.

FEK: Maybe I can tell you another anecdote to explain how problematic this is. In the 1960s, after Ernst Otto Fischer and Geoffrey Wilkinson had determined the structure of ferrocene, for which they got the Nobel Prize, they wanted to make other compounds of that type. Fischer's method was to draw a molecule on a sheet of paper, show it to a co-worker, and say: "Make it. I don't know how." And then the coworker started trying. Wilkinson thought this would be a waste of time and already had a theoretician calculating whether a molecule would be possible. In one particular case his theoretician told him the molecule he wanted could not exist, for it would not be stable. So his coworkers didn't even try to make it, while Fischer's group was able to make it, and published it. When Wilkinson came into the library of the university where he regularly checked the periodicals, he came upon this publication. And Wilkinson had a temper.

He got mad about this, he threw the journal on the floor and jumped on it, and you can still see Wilkinson's footstep on this article. This story shows that theory is not always the best approach – even today, and particularly with the heavier elements, for example the actinides and the lanthanides. With the lighter ones it's easier now, for several reasons.

PLA: There are monsters out there.

JR: Yes.

PLA: We actually had an argument last week.

JR: Exactly. We are trying right now to do a calculation on the molecules I'm trying to synthesize, and because of these relativistic effects we had to simplify the ligand framework. But that small change could be very important, just possibly exactly this part of the ligand and this metal could be very important. But we had to simplify it because it would consume so much time to do this calculation, so it's a problem. It's probably the best way to have the compounds, know it's working, and *then* try to do computational chemistry on it.

PLA: It's actually quite funny to have Julia sitting in Fritz's office going: "No. No. I don't want to do that calculation." That was very good. That means she's coming into her own as a scientist.

PSR: Julia, you and Max are facing a classic challenge for doctoral research. It should be bold and original – yet at the same time you should be able to get results within a few short years. How do you find the right balance when doing something that's daring, interesting, and potentially high-impact but also has a high risk?

JR: From the start I knew that it would be a very challenging project, because these organometallic compounds with cerium are very air-sensitive, they are moisture-sensitive, and they require extremely careful handling. I love the challenge, even though at times it's really frustrating. Most of the time, unfortunately, it doesn't work, just because it's still so much trial and error. You have an idea and you try something out, and many times what comes out is something different you were not thinking about. But even that is a very interesting aspect of the research.

Julia Rieb

PSR: Finding out why something you tried has failed?

JR: Exactly. What's different there? I wanted this compound, and I got another one. Why? Or maybe, how do I get it there? Right now I am working on synthesis of the cerium NHC-compounds. And so my problem is sometimes, because such a compound is not very stable, how will I stabilize it and crystallize it.

MM: That's the nature of our work. Our focus is on making the reactive molecules themselves and, using the ligand framework and quite unusual metals, to effectively reduce the energy barrier for reactions. When those things succeed and you get chemistry that is really interesting or molecules with a really interesting activity, part of the challenge is to find out why.

FEK: Of course, our job is also to carefully observe each doctoral candidate to make sure he or she does not come out with nothing. In some cases we

Patrick S. Regan

have to shift the main topic a bit or add something else for the PhD thesis. Another point is, sometimes something totally unexpected comes out. This has happened a lot through the history of chemistry. For example, the carbenes and the carbynes were found by accident by Ernst Otto Fischer's co-workers. He wanted something else, and he got these compounds, but these were interesting findings, so he asked his co-workers to continue in this direction and did not switch back to the original goal. This is also part of the art, to give a certain freedom and to judge which of the unexpected things might be interesting.

PSR: This brings us to another topic, connecting basic research with industry. You've mentioned both energy and pharmaceuticals. Do you always have in the back of your mind the question of how your research will influence or enable industrial processes?

FEK: These of course are very different aims. Energy has to be cheap, pharmaceuticals not necessarily. It depends on what you gain with them, and they can be comparatively expensive. So you can use rather exotic techniques and chemicals for pharmaceuticals as long as they do a very specific job. But for energy, you need cheap methods, you have to utilize broadly available things, otherwise it will be unaffordable for most of the human beings on earth. So you have to go a bit in different directions. But if a discovery turns out to be useless for one purpose, it may be useful for the other. And in research, when we know almost nothing, we have to learn on a very basic level to see in which direction it might develop and for what it might be useful.

MM: You want to have that link with potential applications, but also, understanding the reactions that we do is really helpful for everybody in the field. If you can understand what we do, if we can explain something, then it may help someone else in a different area or further down the line understand what's going on in similar processes. It's important that we collaborate with people, and actually understanding the reaction is just as important as making the molecules themselves. That really helps other people as well as us.

JR: Basically it is the same for me. I see my research as fundamental research, and I know that in the three years I have, it's almost impossible for me to go from zero to some useful applications in the pharmaceutical industry. I see my research as a small step toward this big goal.

PSR: One last question for all of you: Are there advantages to doing this collaboration within framework of the TUM-IAS that might not have been available to you otherwise?

FEK: It's not bureaucratic.

PLA: It's given us space to explore, and to think deeply, then talk to someone who's thinking deeply about exactly the same thing – which is rare.

JR: I'm very grateful that I was able to go to Edinburgh. I learned so much there and brought a couple of techniques back to TUM. Also, I think it's really great that we can work on the fundamental chemistry without much pressure put on us to get such high output, because fundamental research is high-risk. You need a little bit more space to do things creatively. It needs time.

Max McMullon

MM: I'd say the same thing. Being able to do fundamental research is kind of refreshing. You don't get that so often these days. Also, as chemists we're quite separated into our areas, and chemists in different fields don't necessarily get to work together a lot. But in this kind of relationship you can. You can collaborate much more easily and talk about things in a way you don't get to very often.

FEK: The TUM-IAS Focus Group is a starting point. I learned a lot about rare earth chemistry during this time and there is still a lot for me to learn, because I'm usually dealing with "ordinary" transition metals and not so much with the lanthanides and the actinides. After a while we can better see what we can do with these metals, what we can do with the ligands, in which direction we want to go, and we will publish some papers. And based on this we can apply for further funding and increase the size of the group.

PSR: So would you describe it as a chance to make a constructive disruption in the normal course of your work?

PLA: Yes.

FEK: You also have these meetings here with people from other fields, which I think otherwise is much more difficult to achieve. And then maybe through the exchange of ideas you can see, for example in medicine, materials science, or whatever, possible applications you have not been aware of before.

PLA: One of the things that's come out is lots of extra little collaborations around us. Friends and colleagues of both of our groups have begun to work together, and are submitting papers. I've been talking a lot about my TUM interactions back home, and since Edinburgh and Munich are twin cities, I've actually generated a lot of interest locally. Not just Edinburgh, but also Heriot-Watt and LMU are beginning to talk as a set of universities about doing something collaboratively. With the prospect of Horizon 2020 funding, I think this might actually be a very interesting springboard, to put us in a position to lead the way, because we have such connections.

Frank Kschischang, Mansoor I. Yousefi, Gerhard Kramer, Patrick S. Regan, René-Jean Essiambre and Luca Barletta

Laser light, glass fibers, digital data: Probing the limits

Based on an interview by Patrick S. Regan (PSR) with TUM Prof. Gerhard Kramer (GK); Hans Fischer Senior Fellow Prof. Frank Kschischang, University of Toronto (FK); Rudolf Diesel Industry Fellow Dr. René-Jean Essiambre, Alcatel-Lucent Bell Labs (RJE); Dr. Luca Barletta (LB) and Dr. Mansoor I. Yousefi (MIY), both TUM.

PSR: Optical communications technology is fairly mature now, isn't it? What kinds of open scientific questions are being addressed by this Focus Group?

GK: The technology is mature in many ways, although of course the companies that provide commercial systems – basically, the extremely high-capacity fiber-optic systems that serve as the backbone of the Internet – continue to push the limits. The thing is, the *theoretical* limits are, strictly speaking, unknown. And that has been one goal of our Focus Group's research, to investigate the theoretical capacity of communication over optical fiber in a rigorous way.

PSR: The basic framework for that, information theory, was created nearly 70 years ago by a paper Claude Shannon published in the Bell System Technical Journal: "A Mathematical Theory of Communication." To what extent is this research rooted in Shannon's original work, and to what extent does it branch off in new directions?

FK: Shannon really looms over the field, and everything it touches. I remember during an ISIT meeting, the IEEE International Symposium on Information Theory, on the 50th anniversary of that paper, a giant picture of Shannon was hanging on the stage, as if he was watching you giving your talk. One guy said it was too intimidating, and he turned it around. If people only knew – you could argue that Claude Shannon has had a bigger impact on the digitalization of life today than Steve Jobs or Bill Gates.

GK: Shannon's theory still forms the basis for defining a communication channel mathematically. But optical fiber is different from other transmission media, and the fiber channel requires a special approach.

MIY: We just hosted the first Munich Workshop on Information Theory of Optical Fiber, an international conference sponsored by the TUM-IAS. The main theme of the workshop was finding a fundamental limit of the optical fiber channel. So far we have estimates and we have lower bounds and so on, but still, several decades after the introduction of the optical fiber, no one yet knows the fundamental limit on information rate in this channel.The question is still open, and it is very important. It's the cornerstone of the world's communication networks.

RJE: Nonlinear effects need to be taken into account. Optical fiber is a very transparent medium, an extremely efficient waveguide made from ultra-pure silica glass. Modern fibers attenuate light by a factor of 2 every 15 kilometers. At about every one hundred kilometers, you need to insert an optical amplifier to bring the power back up. You can transmit light for hundreds or thousands of kilometers that way. Very small in diameter, 125 microns, it's comparable to the thickness of a human hair. It has a small 10-micron core that keeps light inside the fiber. And the light is so concentrated inside the core, there's such a high intensity there, that it changes the index of refraction of the material, for all the different users – there could be typically one hundred different "users" …

Gerhard Kramer

PSR: Meaning many different wavelengths of light carrying data simultaneously through a single fiber?

RJE: Different wavelengths, exactly, different frequencies. And because they all share the medium, with their own data, they start to interfere with each other, even if they don't overlap spectrally. Your distortion depends on the other user's data. And that creates distortion for you. And that's part of the reason for the Focus Group, to discover how much information can be sent in the presence of these distortions created by nonlinear effects.

PSR: The TUM-IAS framework has enabled you to bring together people with different expertise but common interests, younger as well as more senior, from industry as well as from universities. Where are the various Focus Group members "coming from" scientifically?

GK: Frank and I are information theorists, with somewhat overlapping research programs. For us at TUM, we have a large group, especially through the funding that's been available through my Humboldt professorship. We have active research on a very wide range of topics, mainly in reliable communications, secure communications, and data compression.

RJE: My background is in physics, more specifically nonlinear dynamics, chaos theory, and astrophysics as well. I have worked on solitons in the past, and nonlinear switching. At Bell Labs I also work, for instance, on more applied problems of optimizing the transmission of information over our commercial systems.

LB: I did my PhD in wireless communication. I started to study these problems during an internship with René at Bell Labs. Here, with the Focus Group, I'm studying certain kinds of disturbance in optical channels introduced by lasers. These components are not ideal, so they introduce noise, and it's a particular kind of noise. It's a noise with memory, a multiplicative noise, that is different from the usual additive noise. Phase noise arises not only from the lasers, but also because of the nonlinear effects in the glass fiber. Now, the main goal in communication is to detect the data that was transmitted, and so you want to compensate for noise that disturbs the communication. But to do this – or potentially even to use the noise to carry information – we need to understand the noise better than we do now. That's my focus.

MIY: I'm an engineer but with emphasis on the mathematical side. I did my PhD with Frank at the University of Toronto in Canada. Initially I intended to work on probabilistic and graphical models; I had no background in optical communications. For a year and a half I worked on network coding and related topics, before Frank suggested that I look at the fiber problem. I got attracted by the rich mathematics of the nonlinear dispersive partial differential equations that appear in this context. We also learned the nonlinear Fourier transform, which turns out to be an elegant and powerful tool for dealing with wave propagation in certain nonlinear media such as optical fiber. Then we started to see how we could actually use it to intelligently communicate over what's called the nonlinear Schrödinger channel.

PSR: How did this collaboration come together?

GK: The idea for the Focus Group started with Frank. Just when I was about to join TUM, Frank approached me at a conference and told me he had a sabbatical coming up. That was a natural fit. I was looking for topics at the time, and I felt it would be an opportunity to bring together an industry Fellowship and an academic Fellowship. If I put the two together, it was just natural to choose this topic, because it's very strongly industry-related. I had been working with René at Bell Labs, and Frank, I knew, was working on the fiber side and more, with a bit of a different spin, the coding side, coding from various perspectives. He had visited

Mansoor I. Yousefi

Bell Labs while I was there, and he had interacted with René already. It was a natural fit, and through the TUM-IAS it was very easy.

PSR: I gather you see this as the start of something bigger. Why now?

GK: It hasn't been studied much in the information theory community, which is really unfortunate, because the problems are challenging, they're very practical, and you have really good people who could contribute.

FK: There's a really good reason that we, information theory people, should come in now. And that's because the physics has matured to where the channel model is more or less agreed upon. The devices haven't changed, basically, the fiber itself hasn't changed in the last decade or so, but there

Frank Kschischang

have been improvements in the physical understanding of the channel. Now you need information theoretic progress to finish the story.

MIY: That's right. And again, importantly, we have this limited capacity at the core of the Internet, facing ever increasing, virtually limitless demand. That makes the information theory of optical fiber very interesting.

GK: Information theory, coding in particular, always comes in when you need to improve efficiency. Up to a point you can use much simpler methods, but once you start hitting these boundaries, you can *shift* the boundaries through more sophisticated methods. And this shifting is quite strong. It's always a good step beyond what you could do without it.

RJE: And the problem itself is actually very new to the information theory group, isn't it?

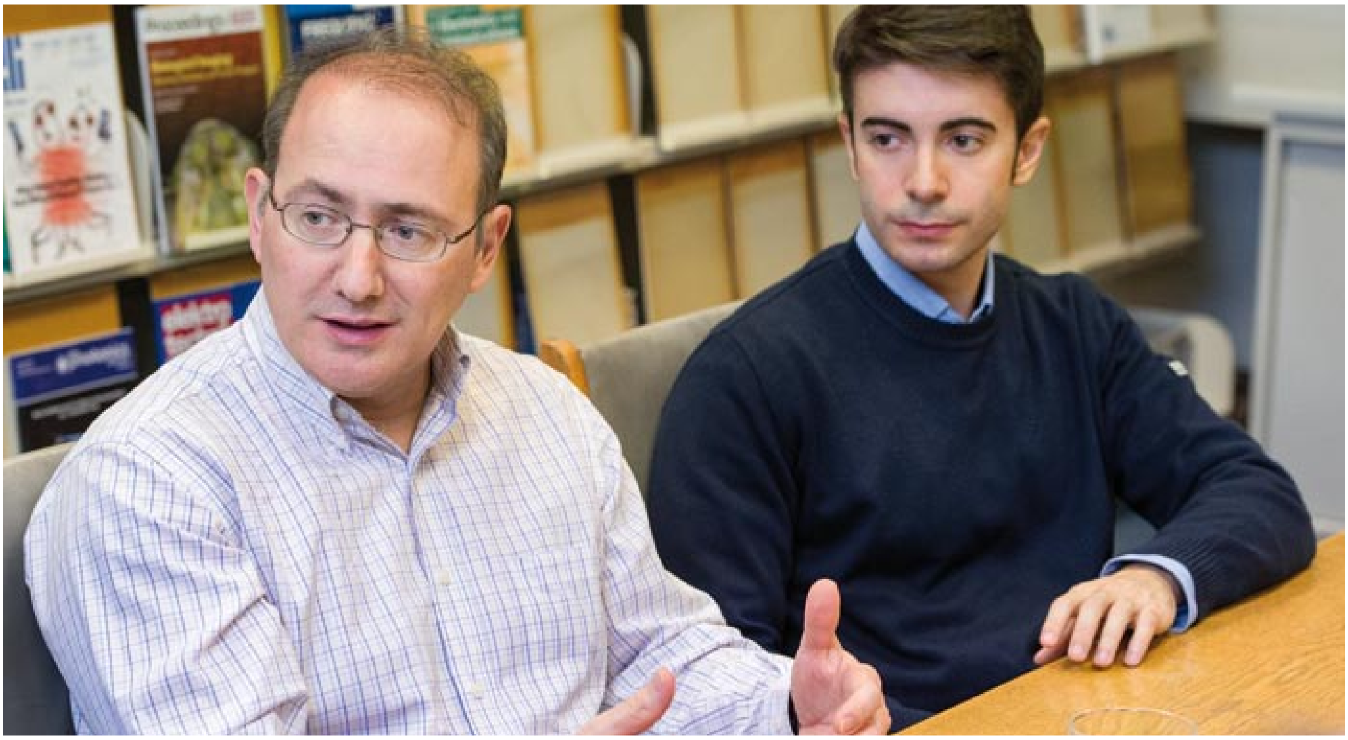
GK: It is.

RJE: Because there's something that you never dealt with. You cannot do a simple extension of what people have done with other media. It's very difficult to do. So at the fundamental level, it is also something that is open for a lot of discoveries and new understanding.

PSR: When Frank says that the physical model has improved, what does that mean exactly? Is it correct to say that what you mean by a model is a set of interlocking equations describing separate physical phenomena that interact?

MIY: A set of mathematical equations that have predictive capabilities. To predict what's going on, precisely enough to be useful in practice.

RJE: There are a lot of things happening in the fiber. The model we are using, it's a very good model, but it's still not exact. There are other phenomena – not only photons, there are also phonons, mechanical waves, and they interact and lead to some other effects that we neglect here – the question is, *can* we neglect them? And so all this goes into refining the model for our purposes. In fibers, as soon as you go to a certain level of power, it could be only five or six dB higher, something else is happening, and the model now starts to fail. So you actually have to know how the model changes, according to where you're pushing the limits.



René-Jean Essiambre and Luca Barletta

PSR: And are you looking also at optical amplifiers, components like that?

RJE: Absolutely. I'm not the most expert in that, but I do have some expertise in terms of all the noise that is generated. There are others, more expert than I am, that I can talk to. That way we bring the knowledge together, and then we figure out what is the proper model and what the limitations of this model are.

FK: That's right. We need the physicists to give us the model to some extent. Our starting point is the mathematical model, and we take off with the mathematical approach from that point. But we need people like René to tell us what the model really is and to delineate the applicability of the models, so we don't go and spend two decades solving the wrong model.

PSR: In some sense this whole pursuit takes off from a practical concern – a "capacity crunch" in the face of growing Internet traffic. How do you think this theoretical research might connect with technological applications in the future?

LB: I think a step could be, at least from my side, getting a better understanding of these channels with memory, and especially devising algorithms, practical algorithms for achieving capacity limits. It will be very important to devise low-complexity algorithms, because right now what theory suggests is to use very complex algorithms. So what happens if we use low-complexity algorithms? Will we still come close to the limits, or not? This is a good question to answer.

FK: This elegant nonlinear Fourier transform theory that Mansoor has developed not only helps us understand the limits, but also could suggest ways to achieve capacity closer to the limits.

MIY: Our work would predict that you can achieve these high data rates in the fiber if you use these particular methods. Looking forward, one direction is to continue the approach that we started. But we are looking at other ways as well. There's not just one way you can look at research problems.

PSR: Do the answers you're seeking have implications for system design, device design, economics of networking?

RJE: The optical hardware already is quite mature. We know how to do low-noise amplification. Coherent detection works very well.

GK: But maybe, I hope, the math will influence the design of some future devices. In relation to dispersion management, for example, it already has. So, for instance, you have to wonder if there could be new kinds of filters – rather than being wavelength filters designed for sinusoids – that might enable a so-called ROADM, a reconfigurable optical add-drop multiplexer, based on the math of the nonlinear Fourier transform.

FK: That's the number one burning question for us.

MIY: That is, whether or not the mathematics could enable you to do optical processing, for network routing, in the nonlinear Fourier domain.

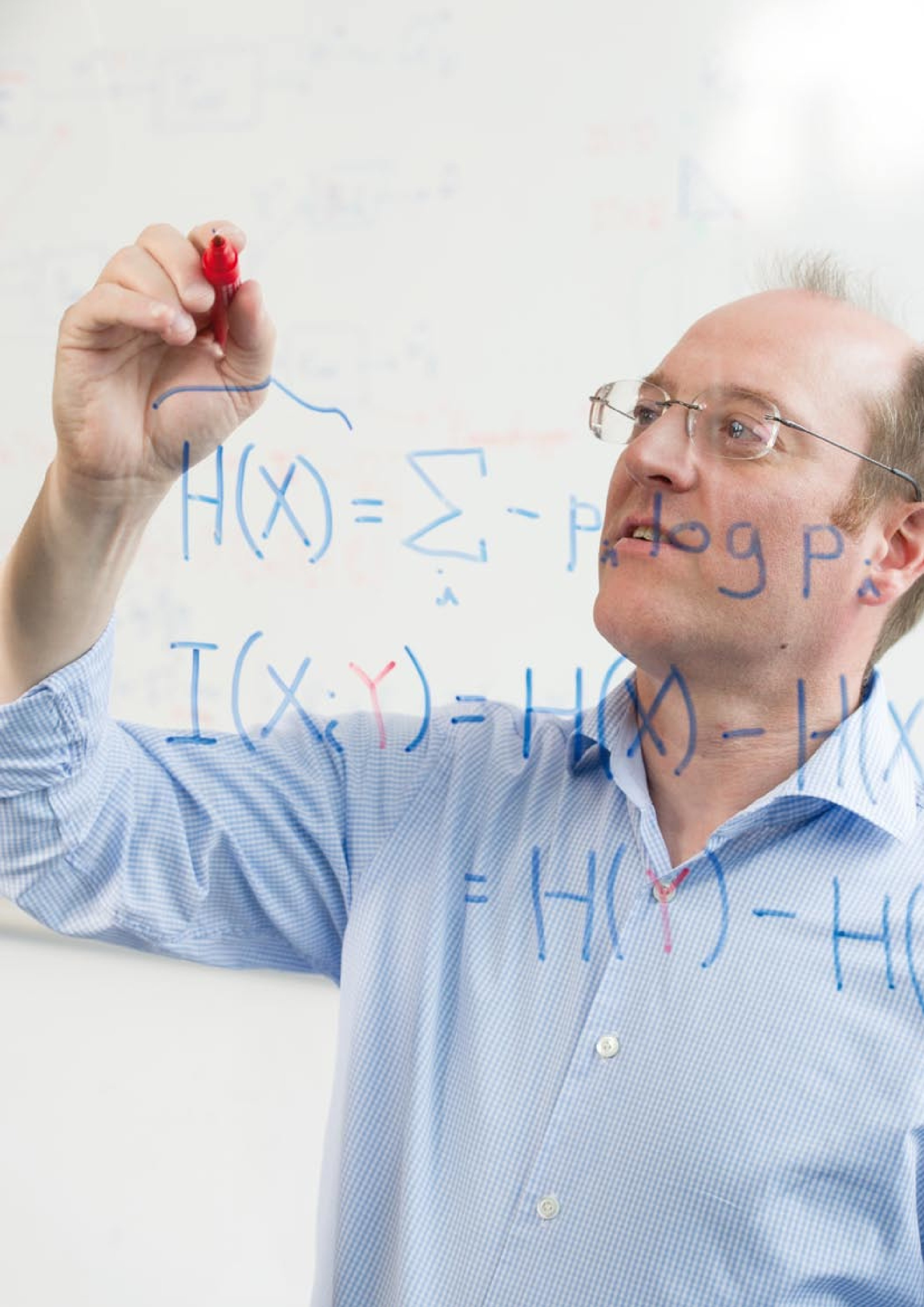
GK: There are different classes of equations, and every one of them has some applications. Whether for communications or not, you don't always know. But you get different solutions for different classes of equations.

RJE: And there are different materials. The fiber has a nonlinearity of a certain type, so-called Kerr linearity, because the glass is a disordered medium, an amorphous medium. There are media that are different. A medium might be found that is low-loss but has nonlinearity of a different kind. We don't know. In the future this may happen.

FK: And all this goes out the window.

GK: No!

RJE: We never know. We don't see it now, but we never know.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Scientific Reports

Advanced Computation and Modeling

Biomedical Engineering, Bio-Imaging, Neuroscience

Bio-related Natural Sciences

Communication and Information

Control Theory, Systems Engineering and Robotics

Environmental and Earth Sciences,
Building Technology

Fundamental Physics

Surface, Interface, Nano- and Quantum Science


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BCBV 1:1
BCBV 1:3
BCB 1:2
BC

Scientific reports of the Focus Groups

In this section, the TUM-IAS Focus Groups highlight their major achievements of 2014 or briefly describe their goals in the case of newly started activities. The more interested reader is referred to the original publications and reviews, which are listed in total in the publications section. The scientific reports are grouped according to our eight main research areas, namely

- Advanced Computation and Modeling
- Biomedical Engineering, Bioimaging, Neuroscience
- Bio-related Natural Sciences
- Communication and Information
- Control Theory, Systems Engineering and Robotics
- Environmental and Earth Sciences, Building Technology
- Fundamental Physics
- Surface, Interface, Nano- and Quantum Science

In 2014 we granted 14 new Fellowships in the categories Hans Fischer and Hans Fischer Senior, Rudolf Diesel Industry, and Carl von Linde Senior Fellowship. In addition, five more Rudolf Mößbauer Tenure Track Professors have been appointed. Not all of them are yet contributing a scientific report this year, as they started their activities only in fall 2014 or at the beginning of 2015. However, those new Focus Groups are already listed at the beginning of each section.

Advanced Computation and Modeling

New in this Research Area

Focus Group **Advanced Stability Analysis**

Dr. Bruno Schuermans (Alstom) | Rudolf Diesel Industry Fellow
Tobias Hummel | Doctoral Candidate
Prof. Thomas Sattelmayer, Thermodynamics, TUM

Bruno Schuermans

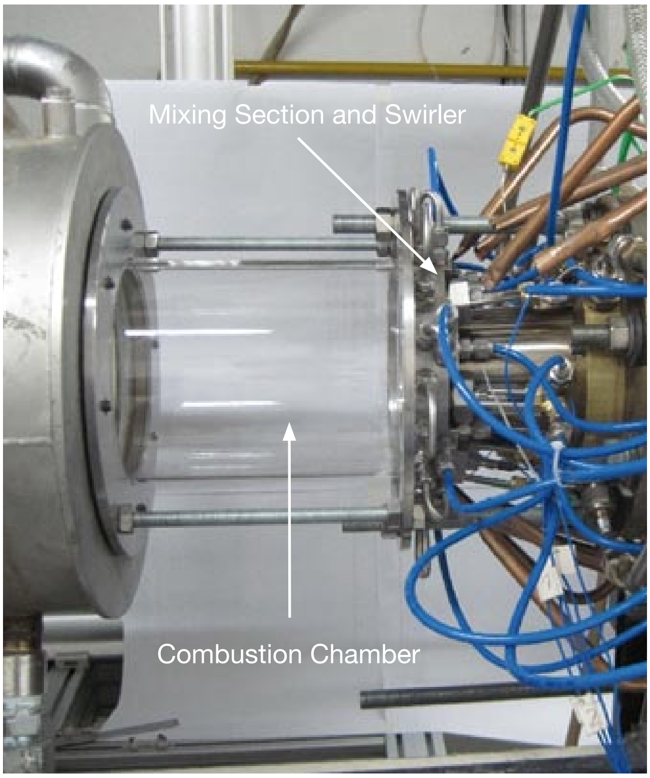
The successful transformation of our power generation landscape from dominantly conventional to renewable technologies crucially relies on the implementation of operationally flexible and clean gas turbines. The associated implementation of novel (i.e., turbulent lean premixed) combustion technologies is confronted with the combustion chamber exhibiting a sensitive susceptibility to thermoacoustic instabilities. Physically, these instabilities evolve from constructive, self-sustaining feedback couplings between the combustor's acoustic oscillations and the flame's heat release rate fluctuations, which manifest as pressure pulsations through the chamber. The pulsations can be detrimental to the engine's operational flexibility and may result in increased emissions of pollutants. Intensive research in recent decades has produced vast knowledge on low-frequency pulsations; the relevant physics and modeling methodologies are well understood and established, although numerous challenges still require solutions.

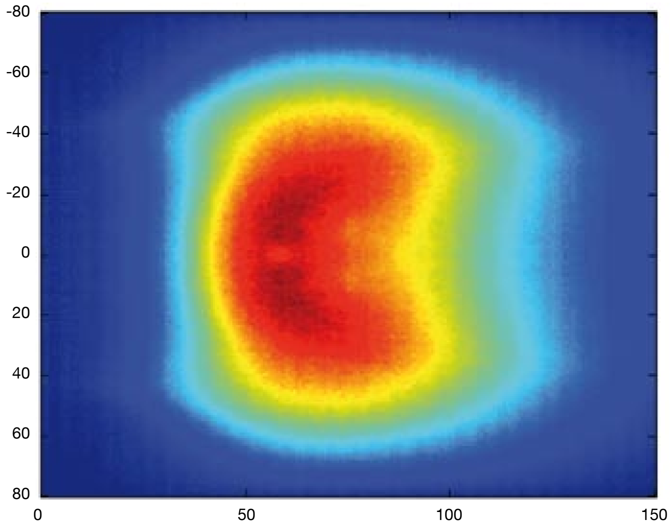
Recently, research on low-frequency pulsations has been enriched by doctoral students working with Alumnus Hans Fischer Senior Fellow Raman I. Sujith and TUM thermodynamics professor Wolfgang Polifke. They found a thermoacoustic instability mechanism caused by a so-called intrinsic feedback. This instability can be thought of as the flame's radiation of sound having a directly amplifying impact on its own heat release fluctuations. Thus, the intrinsic feedback loop may cause instability in a non-reflecting environment, i.e., where all sound waves generated by the flame are radiated away at the system in- and outlets, which is contradictory to the established thinking that thermoacoustic instability requires feedback with the global acoustic field.

Climbing up the regime from low- to high-frequency pulsations, comprehension of combustion chamber thermoacoustics due to the associated multi-dimensional oscillations poses yet another fundamental and ambitious task for the research community. At the end of 2013, Rudolf Diesel Industry Fellow Bruno Schuermans actively took up the challenge of unraveling high-frequency combustion instabilities in gas turbine combustors together with TUM thermodynamics professor Thomas Sattelmayer. An extensive collaboration network has been established including academic (TUM-IAS), industrial (ALSTOM & AG TURBO), and government (Federal Ministry for Economic Affairs and Energy / BMWi) research frameworks. This network accommodates five doctoral candidates conducting research at TUM with experimental, numerical, and analytical emphases.

Bruno Schuermans made frequent visits to the TUM campus in Garching during 2014. He and Thomas Sattelmayer have been fostering the ongoing development of a new experimental research combustor specifically designed to study high-frequency instabilities. At the same time, experimental research has been carried out on an existing test rig exhibiting these instabilities (figure 1) at the TUM Thermodynamics department, where physical observations have been explained and understood. Relevant findings have been directly channeled into the development process. Publications are in progress.

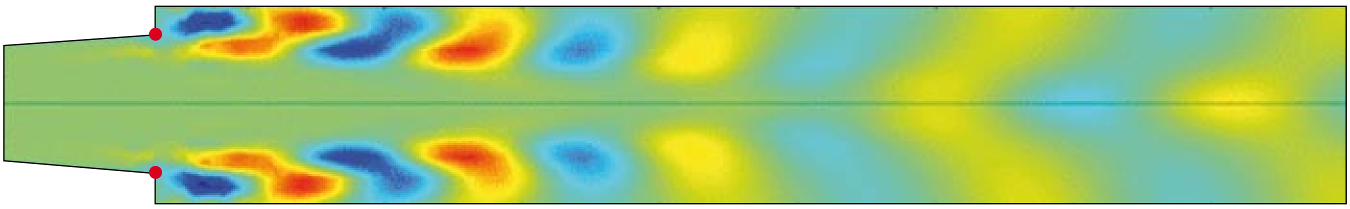
Alumni Members
Prof. Raman I. Sujith (IIT Madras) | Hans Fischer Senior Fellow
Ralf Blumenthal (Siemens AG), Sebastian Bomberg (TUM) | Doctoral Candidates
Prof. Wolfgang Polifke, Thermodynamics, TUM



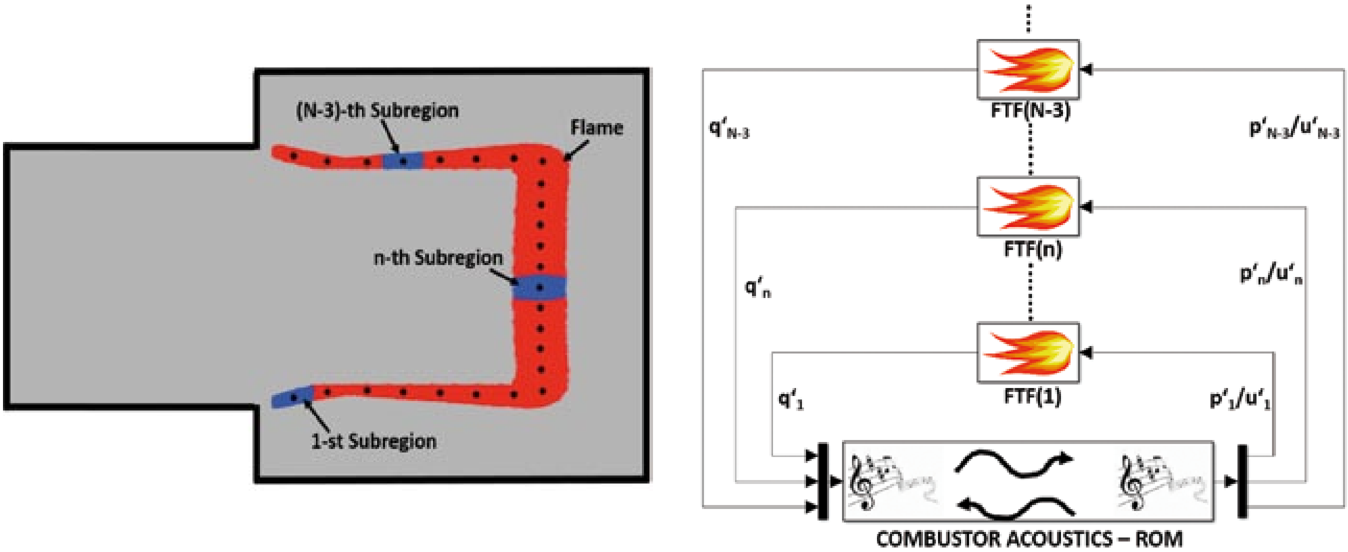


1 | Experimental rig at department of thermodynamics to study high-frequency thermoacoustics (right); OH-Chemiluminescence emission of flame is used to measure heat release fluctuations of the combustion process

A sophisticated aeroacoustic modeling methodology developed at TUM has been employed in the design stage of the new test rig as well as for the fundamental investigation of high-frequency acoustics. Specifically, the methodology solves the Linearized Navier-Stokes Equations (LNSE) in the frequency domain. Mathematically, the LNSEs govern complex interactions between mean-flow and acoustic perturbations such as vortex shedding (figure 2) leading to acoustic damping – a quantity that is useful for the prediction of a combustor's stability behavior.



2 | Modal field of vorticity disturbances: Acoustic oscillations couple with hydrodynamic flow instability at the edge of the area expansion (red dots). This process periodically (i.e. with oscillation frequency) triggers the formation of coherent vortical structures that are convected downstream by the mean flow and eventually dissipate.



3 | Schematic of flame division into a set of compact subregions in a simplified combustor geometry; Diagram of corresponding MIMO feedback loop to assess linear stability.

Furthermore, a low-order modeling tool capable of analyzing high-frequency thermoacoustic instabilities has been developed. Therefore, a truncation based Model Order Reduction (MOR) technique is employed on the LNSE. This procedure yields Reduced Order Models (ROM), which accurately reconstruct the acoustic wave propagation and damping as benchmarked by the high-order (N~100,000 – 500,000) LNSE system. The low order of these ROMs (N~100) allows for efficient dynamical analyses of gas turbine combustors using standard control theory procedures. The small wavelengths associated with high-frequency oscillations require the consideration of spatial non-uniformities of heat release fluctuations. Modeling these so-called non-compact heat release modulations is achieved by geometrically dividing the flame into a set of subregions (n=1,2,…,N), each of which can then be regarded as uniform/compact (cf. figure 3 and 4). Linear thermoacoustic stability is assessed by forming a Multi-Input-Multi-Output (MIMO) feedback loop with each subregion and the ROM (which describes the acoustics of the domain) by employing either analytical or experimental local flame transfer functions. A publication containing a demonstration of concept has been accepted [1].

Selected Publications

[1] T. Hummel, C. Temmler, B. Schuermans, and T. Sattelmayer, “Reduced order modeling of aeroacoustic systems for stability analyses of thermoacoustically non-compact gas turbine combustors,” in *ASME Turbo Expo 2015: Turbine Technical Conference and Exposition*, accepted.

[2] S. Bomberg, T. Emmert, and W. Polifke, “Thermal versus acoustic response of velocity sensitive premixed flames,” *Proc. Combust. Inst.*, vol. 35, no. 3, pp. 3185–3192, 2015. doi:10.1016/j.proci.2014.07.032 (2014).

Publications by this Focus Group can also be found on page 148.

Focus Group **High-Performance Computing (HPC)**

Prof. George Biros (University of Texas at Austin) | Hans Fischer Fellow
Arash Bakhtiari, Benjamin Uekermann, Valeriy Khakhutskyy | Doctoral Candidates
Prof. Hans-Joachim Bungartz, Scientific Computing, TUM

Tackling the multi-challenge, part 3: Scalable blood vessel simulations

George Biros

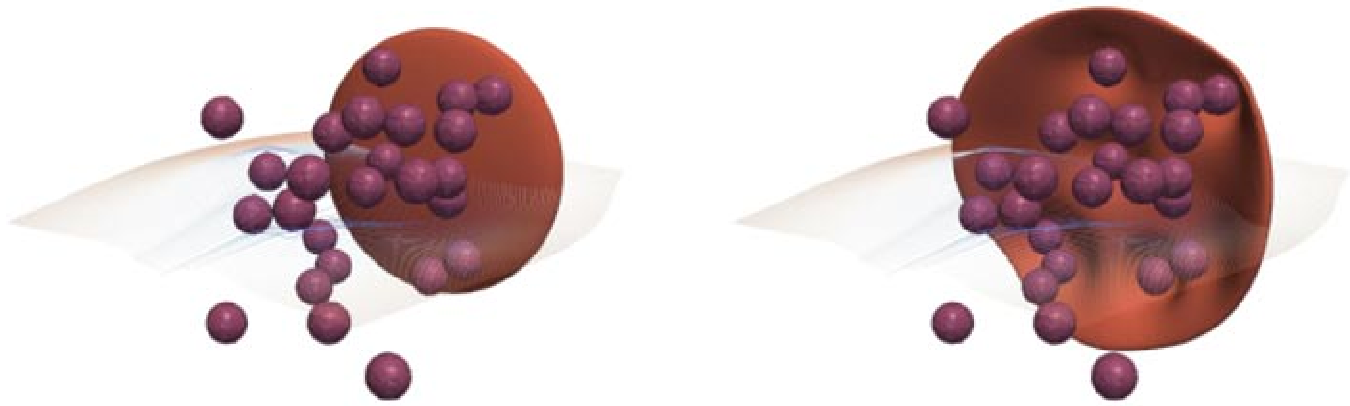
The Focus Group HPC—Tackling the Multi-Challenge, hosted by Hans-Joachim Bungartz, addresses the emerging challenges of high-performance computing in science and engineering. George Biros joined the group as a Hans Fischer Fellow to focus on the Multi-Core Challenge. His work complements the accomplishments of Alumni Fellows Miriam Mehl (now a professor at the University of Stuttgart) and Markus Hegland from ANU in Canberra, who were researching Multi-Physics and Multi-Dimensional Challenges. Besides George Biros and Hans-Joachim Bungartz, the Focus Group comprises doctoral candidates Arash Bakhtiari, Benjamin Uekermann, Christoph Kowitz, and Valeriy Khakhutskyy.

In 2010, George Biros won the Gordon Bell Prize for his accomplishments in simulation of blood vessels using 200,000 computational cores. His research in the Focus Group aims to build upon these results. In spring 2014, he visited TUM and initiated collaboration with Arash Bakhtiari, Hans-Joachim Bungartz, and Miriam Mehl. The team will develop fast solvers for transport in microcirculation. This will improve our understanding of transport of a substance due to fluid motion, for example, to control localized drug delivery and to understand oxygen transport in the alveole.

During this visit, the group developed a prototype of a novel advection equation solver in MATLAB. The solver is based on the semi-Lagrangian (SL) method, which provides an unconditionally stable numerical scheme. To minimize the memory and computational cost, the new solver employs an octree data structure.
Arash Bakhtiari implemented an efficient SL solver in C++ and at the end of the year continued his intensive collaboration with George Biros at the University of Texas at Austin. During his research stay, he worked on coupling of the SL solver with already existing distributed-memory parallelized static adaptive Chebyshev octree code developed at George Biros's research group in Austin. A Chebyshev octree representation of a function is a tree in which at every leaf the function is represented by the coefficients of its Chebyshev polynomials. Arash Bakhtiari also extended the octree code to support dynamic adaptivity: The tree structure is dynamically changing in each simulation time step to maintain its desired accuracy. In general, by using dynamically adaptive trees, one can avoid superfluous computations and reduce the computational cost.

George Biros's research group has developed a novel numerical scheme for solving Stokes equation in the unit box based on the volume integral equation formulation. By employing an adaptive fast multipole method for volume integrals, the scheme is algorithmically optimal. The solver is capable of computing the velocity fields of the Stokes flow through complex geometries such as porous media. This work was presented at the Supercomputing Conference 2014 [1]. Figure 1 illustrates an example of deploying the SL solver using the velocity field computed by the volume integral solver.

Alumni Members
Prof. Miriam Mehl (University of Stuttgart) | Carl von Linde Junior Fellow
Prof. Markus Hegland (Australian National University) | Hans Fischer Senior Fellow
Dr. Dirk Pflüger (University of Stuttgart) | Postdoctoral Researcher
Christoph Kowitz (TUM) | Doctoral Candidate



1 | Transport of a substance due to Stokes flow around a random distribution of spheres. The velocity field and the advection of the substance are computed by deploying the volume integral equations Stokes solver and the tree-based semi-Lagrangian advection solver, respectively.

At this point, the team has reached the first milestone of the project, the development of a highly efficient distributed-memory parallelized SL advection solver with dynamic adaptive Chebyshev octree data structure. To improve performance, the team plans to integrate the SL solver with hardware accelerators. The goal is to present the results of this research at the Supercomputing Conference 2015 in Austin. The team also plans to research the diffusion problem and to couple the advection-diffusion solver with the blood vessels simulation software.

Together with Miriam Mehl, Benjamin Uekermann continued the development of preCICE—a library for coupling multiple stand-alone simulation tools for fluid-structure- and fluid-structure-acoustic interaction scenarios. This year, the Focus Group developed a new fully implicit multi-coupling algorithm to simulate a new range of applications in a partitioned way [2]. PreCICE is used in several in-house and open-source codes in the context of the ExaFSA project, which endeavors to bring the fluid-structure simulations to the edge of exa-scale computing. Benjamin Uekermann and collaborators worked on coupling compressible flow to linearized acoustic equations. In spring, he stayed at the Barcelona Supercomputing Center and coupled the computational mechanics code Alya with preCICE [3].

Following the principle "Once a Fellow, always Fellow," Markus Hegland visited the TUM-IAS twice in 2014 to proceed with the intensive cooperation. In September, he joined Valeriy Khakhutskyy and Christoph Kowitz at the workshop on Sparse Grids and Applications, which he co-organized as a member of the scientific program committee. Also in 2014, Valeriy Khakhutskyy and Christoph Kowitz stayed at the ANU. Christoph Kowitz and collaborators worked on the application of the fault-tolerant combination technique on the plasma turbulence simulation code GENE. Markus Hegland and Valeriy Khakhutskyy researched scalable methods for high-dimensional data analysis with parallel additive models [4].

Selected Publications

[1] D. Malhotra, A. Gholami, and G. Biros, "A volume integral equation Stokes solver for problems with variable coefficients," in Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, 2014, pp. 92–102.
[2] B. Uekermann, B. Gatzhammer, and M. Mehl, "Coupling algorithms for partitioned multi-physics simulations," in Informatik 2014 Conference, 2014, pp. 113–124.
[3] B. Uekermann, J. C. Cajas, B. Gatzhammer, G. Houzeaux, M. Mehl, and M. Vazquez, "Towards partitioned fluid-structure interaction on massively parallel systems," in proceedings of WCCM XI / ECCM V / ECFD VI, 2014.
[4] V. Khakhutskyy and M. Hegland, "Parallel learning algorithm for large-scale regression with additive models," in ECML PKDD 2014, PhD Session, 2014, pp. 101–110.

Publications by this Focus Group can also be found on page 148.

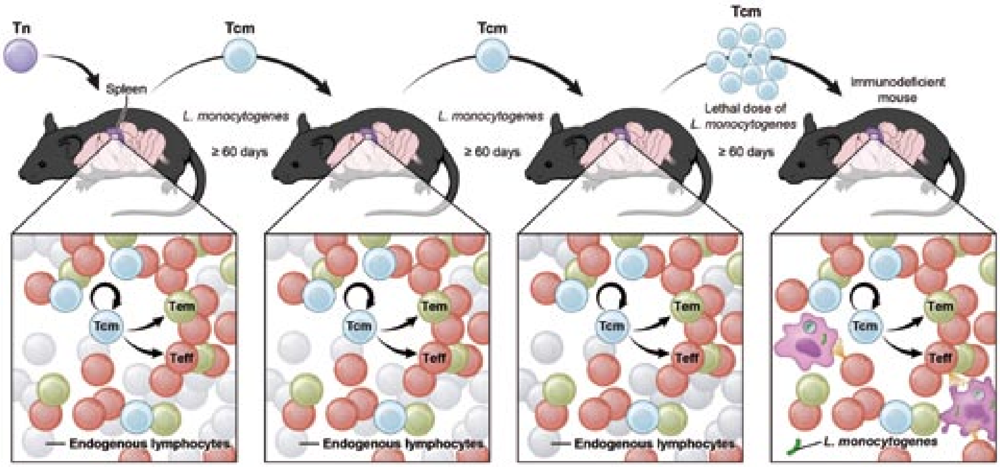
Biomedical Engineering, Bio-Imaging, Neuroscience

New in this Research Area

Focus Group **Clinical Cell Processing and Purification**

Prof. Stanley Riddell (University of Washington) | Hans Fischer Senior Fellow
Jeannette Bet, Paulina Paszkiewicz | Doctoral Candidates
Prof. Dirk Busch, Medical Microbiology, Immunology and Hygiene, TUM

Stanley Riddell



1 | Self-renewal and multipotency of a single central memory T cell (Tcm) across serial adoptive transfers and infection-driven re-expansions ensure full immunocompetence. Abbreviations are as follows: TN, naïve T cell; Tem, effector memory T cell; Teff, effector T cell.

The goal of our Focus Group is to develop unique, user-friendly, integrated cell-processing platforms to facilitate the preparation of effective and minimally manipulated therapeutic cells for highly individualized medical care. In the past year, studies performed by Focus Group members have elucidated fundamental properties of memory T cells that provide for life-long immunity and have defined a novel safety switch that serves dual functions in cell selection and elimination. The first-in-human clinical trials of novel cell therapies using Focus Group innovations have been initiated to evaluate safety and efficacy.

Identification of the "stem cell" responsible for immunologic memory
An important attribute of adaptive T cell immunity is that it provides the host with life-long protection from re-infection with the same pathogen. Like other organ systems, the longevity of this immunologic memory is thought to depend on cells with characteristics of stem cells that include the ability both to self-renew and to differentiate to other memory and effector cell subsets. Whether such a putative memory stem cell resided in an identifiable lineage had not been defined. In a landmark paper published in *Immunity* in 2014, doctoral candidate Patricia Graef and members of this Focus Group demonstrated using serial single cell transfers that the $CD8^{+}$ central memory (T_{CM}) cell, unlike other memory cells, has the attributes of a stem cell and provides long-lived protective immunity (figure 1). This observation has critical implications for selecting even very small numbers of T cells for adoptive immunotherapy to restore persistent immunity to pathogens and to engineer defined T cell subsets to recognize tumor cells. T_{CM} can only be identified by the expression of a constellation of cell surface markers, and clinical isolation protocols using Fab streptamers have been developed for clinical trials directed at restoring deficient immunity after allogeneic stem cell transplantation by infusing small numbers of donor-derived T_{CM}.

Regulation of survival of adoptively transferred T cells using a cell surface suicide switch

Adoptive immunotherapy with T cells selected or genetically engineered to recognize tumor cell antigens is emerging as a potent new approach for cancer therapy. Stanley Riddell, Hans Fischer Senior Fellow in this Focus Group, is leading clinical trials in which the patient's T cells are genetically modified to express a synthetic chimeric antigen receptor (CAR) specific for the CD19 B-cell lineage molecule that is expressed on B cell leukemias and lymphomas. This therapy induces complete remissions in >80% of patients with chemotherapy refractory B cell acute lymphocytic leukemia (ALL) and complete or partial responses in >70% of patients with non-Hodgkin's lymphoma. A complication of therapy is that the CAR-T cells also eliminate normal B cells that express the CD19 molecule, which if prolonged, results in a deficiency in antibody production. Paulina Paskiewicz, who successfully defended her PhD thesis in 2014, performed experiments demonstrating that co-expression of a cell surface molecule composed of a truncated version of the epidermal growth factor receptor (EGFRt) on CAR-T cells can provide a target for antibody-mediated elimination of transferred T cells by administering the clinical grade anti-EGFR antibody Cetuximab.

Clinical applications of T cell therapies utilizing Focus Group innovations

Advances in cell selection, genetic engineering, and synthetic biology have made it possible to generate human T cells that display desired specificities and enhanced functionalities. This has changed the prospects for the widespread use of adoptive T cell therapy for infections, cancer, and autoimmunity. Work by Focus Group investigators has defined fundamental properties of T cell subsets and provided a new class of cell purification reagents that has facilitated the first clinical trials of adoptive T cell therapy in the United States and Europe using cell products of defined composition and function. Studies in Seattle have focused on targeting B cell malignancies with CAR-T cells and will be expanded to common epithelial cancers in 2015. Studies in Germany are examining reconstitution of protective T cell immunity to pathogens after allogeneic stem cell transplantation using T_{CM}. Joint grant applications between groups in Germany, other European centers, and Seattle have been submitted to expand the applications of clinical cell therapy. This nascent field faces scientific and regulatory challenges, and surmounting these will require continued collaboration between academia and biotechnology – a hallmark of our Focus Group – to ensure that cellular therapies are established as a viable approach for common human diseases.

Selected Publications

[1] P. Graef, V. R. Buchholz, C. Stemberger, M. Flossdorf, L. Henkel, M. Schiemann, I. Drexler, T. Höfer, S. R. Riddell, and D. H. Busch, "Serial transfer of single-cell-derived immunocompetence reveals stemness of CD8+ central memory T cells," *Immunity*, vol. 41, no. 1, pp. 116–126, Jul. 2014.

[2] C. Stemberger, P. Graef, M. Odendahl, J. Albrecht, G. Dössinger, F. Anderl, V. R. Buchholz, G. Gasteiger, M. Schiemann, G. U. Grigoleit, F. R. Schuster, A. Borkhardt, B. Versluys, T. Tonn, E. Seifried, H. Einsele, L. Germeroth, D. H. Busch, and M. Neuenhahn, "Lowest numbers of primary CD8(+) T cells can reconstitute protective immunity upon adoptive immunotherapy," *Blood*, vol. 124, no. 4, pp. 628–37, Jul. 2014.

[3] C. Berger, D. Sommermeyer, M. Hudecek, M. Berger, A. Balakrishnan, P. J. Paszkiewicz, P. L. Kosasih, C. Rader, and S. R. Riddell, "Safety of targeting ROR1 in primates with chimeric antigen receptor-modified T cells," *Cancer Immunol. Res.*, vol. 3, no. 2, pp. 206–216, Feb. 2015. doi: 10.1158/2326-6066.CIR-14-0163 (2014).

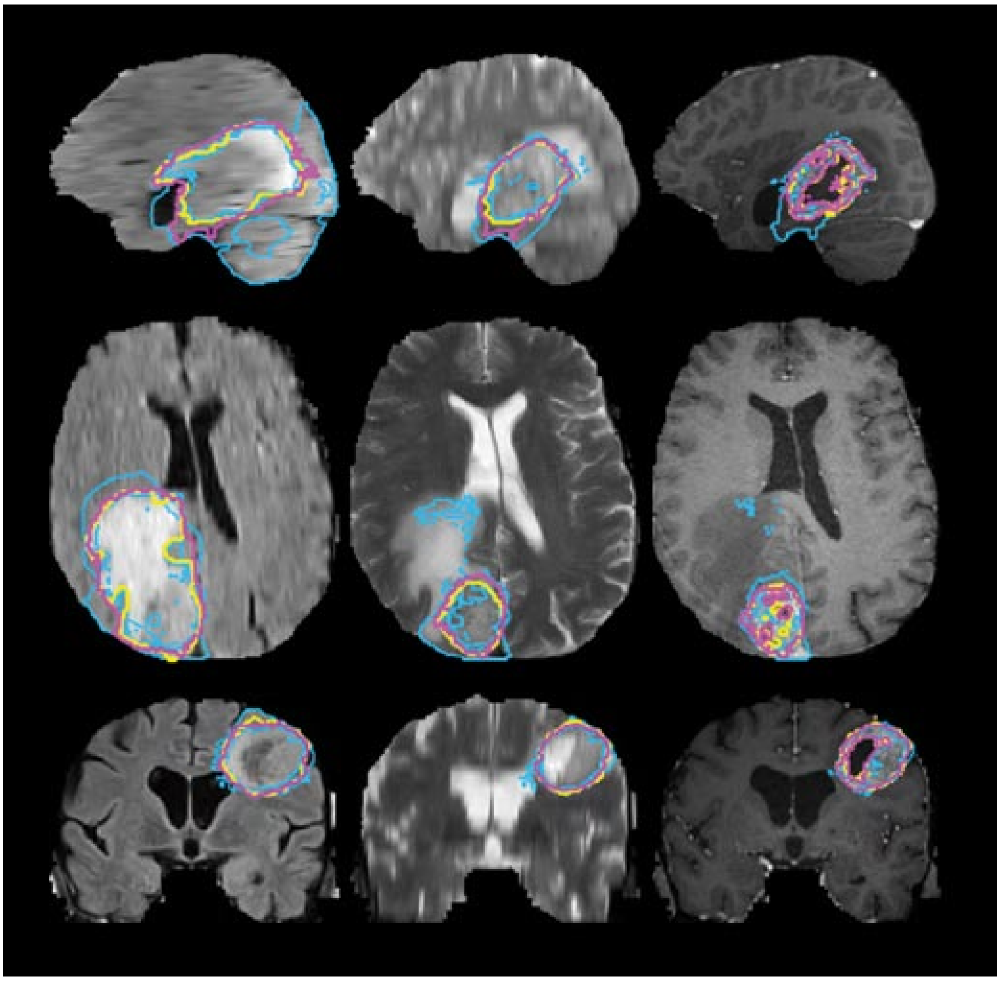
Publications by this Focus Group can also be found on page 149.

Focus Group **Image-based Biomedical Modeling**

Prof. Bjoern Menze (TUM) | Rudolf Mößbauer Tenure Track Professor
Dr. Vasileios Zografos | Postdoctoral Researcher
Esther Alberts | Doctoral Candidate
Image-based Biomedical Modeling, TUM

Bjoern Menze

The Focus Group Image-based Biomedical Modeling develops computational algorithms that analyze biomedical images using statistical, physiological, and biophysical models. The work strives towards 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 data bases 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.



1 | **Automated tumor image segmentation.** The images show the results of different algorithms for tumor image segmentation (blue), together with the expert annotation (yellow). Segmentations outlined in magenta represent results of an ensemble of 20 tumor segmentation algorithms that we evaluated in a collaborative effort of more than 60 participants as part of the "Multimodal Brain Tumor Image Segmentation Benchmark" (BRATS), co-organized by us in conjunction with the MICCAI 2014 conference in Boston. Shown are results for three patients (rows from top to bottom) and three different magnetic resonance imaging modalities (columns from left to right) each of which mapping different physiological features of the organ and of the tumor.

Clinical neuroimage analysis

The first direction is the modeling of processes underlying images acquired in common diseases of the brain. The focus is on the analysis of images acquired in glioma and stroke patients, including the development of algorithms for the longitudinal analysis of brain lesions using statistical and physiological lesion evolution models [1] (figure), and new computational techniques for extracting vascular networks from angiographic images in order to seek correlations between blood flow and local metabolic processes [2]. The main sources of information are multimodal and multi-parametric clinical image data featuring magnetic resonance (figure), position-emission-tomography, and computer tomography scans. We use these image data, for exampe, to personalize tumor models that are used to optimize the radiotherapy of glioma patients [3].

Disease progression models

The second direction deals with the task of optimal oncological staging. It includes the anatomical annotation of images with a large field of view, such as abdominal scans or whole body images, the detection of lesions across modalities and in repeated scans, and the analysis of individual lesions using pathophysiological models. Emphasis is placed on clinical applicability, and algorithms are supposed to scale well to large data sets enabling the development of population-wide disease progression models.

Selected Publications

[1] Y. Tarabalka, G. Charpiat, L. Brucker, and B. H. Menze, “Spatio-temporal video segmentation with shape growth or shrinkage constraint,” *IEEE Trans. Image Process.*, vol. 23, no. 9, pp. 3829–40, Sep. 2014.

[2] M. Rempfler, M. Schneider, G. D. Ielacqua, X. Xiao, S. R. Stock, J. Klohs, G. Székely, B. Andres, and B. H. Menze, “Extracting vascular networks under physiological constraints via integer programming,” *Med Image Comput Comput Assist Interv*, vol. 17, no. Pt 2, pp. 505–12, Jan. 2014.

[3] J. Unkelbach, B. H. Menze, E. Konukoglu, F. Dittmann, M. Le, N. Ayache, and H. A. Shih. „Radiotherapy planning for glioblastoma based on a tumor growth model: improving target volume delineation,” *Phys. Med. Biol.*, vol. 59, no. 3, pp.771–784, Feb. 2014.

Publications by this Focus Group can also be found on page 150.

Bjoern Menze received degrees in physics from Uppsala University (2002) and Heidelberg University (2007), where he also obtained his doctoral degree in mathematics and computer science in 2007, supervised by Fred Hamprecht. Following postdoctoral work at Harvard University in the Anthropology Department (Jason Ur) and Surgical Planning Laboratory (Ron Kikinis), he joined Polina Golland’s Computer Vision Group at the Massachusetts Institute of Technology in 2009. Before joining the Department of Informatics at TUM as the first Rudolf Mößbauer Tenure Track Professor in 2013, Bjoern Menze was senior researcher and lecturer in the Computer Vision Lab at ETH Zurich (Gabor Szekely), and a lab member of Nicolas Ayache’s Asclepios Project at INRIA Sophia Antipolis.

Focus Group **Intra-Operative Therapy**

Prof. Michael Friebe (IDTM GmbH & Univ. of Magdeburg) | Rudolf Diesel Industry Fellow
Philipp Matthies | Doctoral Candidate
Prof. Nassir Navab, Computer Aided Medical Procedures & Augmented Reality, TUM

Michael Friebe

Intraoperative radiation therapy

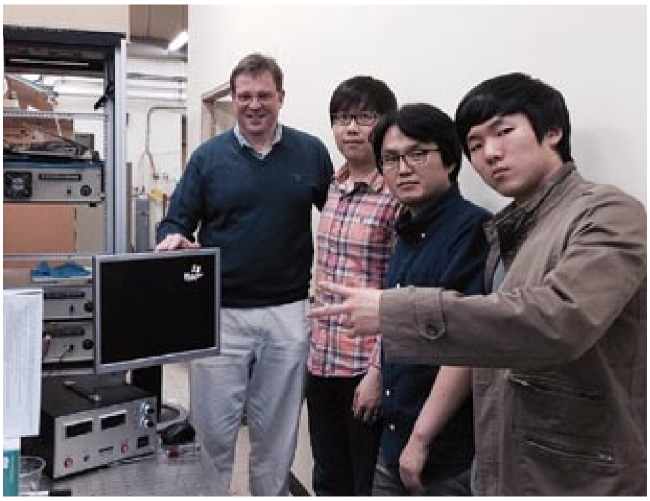
Minimally Invasive Image-Guided Tumor Therapy

The research goal of our Focus Group is the development of an environment that allows the use of a radiation source that can be delivered to a target site intraoperatively with the imaging support of a Magnetic Resonance Imaging (MRI), Ultrasound (US), handheld Single Photon Emission Computed Tomography (SPECT), or a combination of these (Hybrid Imaging).

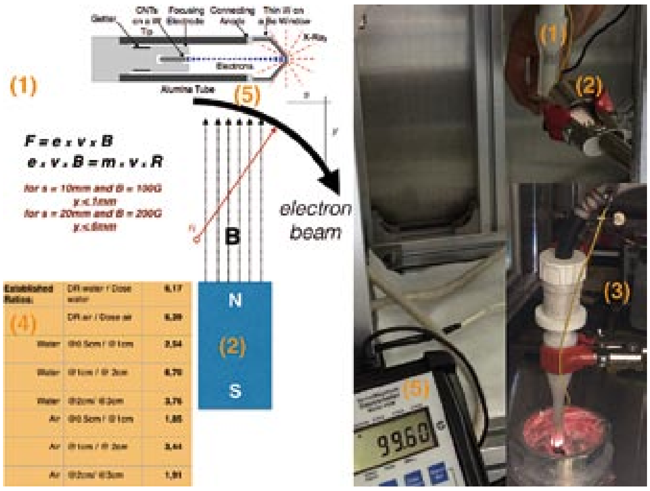
This requires a dedicated radiation source that is small enough to be placed at the tumor site or in a tumor bed accessible through a small incision, or utilizing the surgical path used for the tumor removal in case of tumor bed radiation. The radiation source obviously needs to be safe for patient use in terms of heat generated and radiation delivered. It also requires a software model for radiation dose calculation and visualization, tracking/navigation within a diagnostic imaging environment, and if used in MRI a compatible integration and safe use with the magnetic field.

Tumor cell killing occurs with a radiation dose delivered of around 15 to 20 Gy. The initial target tumor size (breast) for our intraoperative approach is less than 10 mm in diameter, and the radiation time as a boost (one time delivery) should not exceed 30 minutes, which translates to a dose rate delivered of about 0.75 Gy/min. We were able to achieve that for a distance of 5 mm (1.51 Gy/min) but are still off by a factor of 2 for a distance of 12-15 mm (0.41 Gy/min) from the tip of the radiation source. We believe that we can achieve higher values in the future by changing several of the delivery parameters (duty cycle, voltage, current). We did these tests and the research in close cooperation with our Korean development partners from the Quantum Beam Engineering lab under Prof. Sung Oh Cho, KAIST, Daejeong (see figure 1).

To use such a setup with an MRI system, the effects of the magnetic field on the performance of the radiation source need to be known. It does not seem feasible to use such a source directly inside the MRI magnet system (15,000G–30,000G). As we wanted to perform the radiation delivery within the MRI suite, compatibility of the radiation source to about 100G is needed, which is approximately 1.25 m from the end of the MRI magnet bore. The radiation source was exposed in a worst case laboratory setup (figure 2) to external B-fields of 50G to 500G and the delivered radiation dose compared to the theoretical values. We found very close correlation and proved that the source is compatible to and useable in magnetic fields of up to 200G without any major change in performance (1).



1 | With our cooperation and R&D partners from the Quantum Engineering Lab (Prof. Sung Oh Cho) of the KAIST in Daejeong.



2 | (1) Miniature X-ray source (10mm diameter) exposed to an external magnetic field (2) in worst-case setup perpendicular to the electron beam. Previous tests in water bath (3) helped establish ratios (4) for further testing in air. The B field of the magnet (5) causes a bending of the electron beam that limits the use of the radiation source in a MRI system to within the 100G fringe field, which is approximately 1.25m away from the 3T MRI magnet bore.

Initial software and the tracking/navigation were established and developed using an MRI biopsy device (2) and the SPECT environment that we worked on with our industrial partners from Surgiceye, Munich (3). Starting December 15, 2014, Michael Friebe became the chair of Catheter Technologies at the Otto von Guericke University in Magdeburg, Germany. Our group is looking forward to the cooperation between his new Medical Technology department and the Biomedical Computing program of Prof. Navab at TUM. We will continue on developing an integrated approach and improving the delivery parameters.

Selected Publications

[1] M. Friebe, P. Matthies, and S. O. Cho, "Low Energy Radiation Therapy - feasibility of using a field emission miniature X-ray tube for intraoperative treatments under MRI guidance," *Int. J. Comput. Assist. Radiol. Surg.*, vol. 9, pp. 65–70, Jun. 2014.

[2] M. Friebe, H.-W. Henke, G. Krombach, P. Matthies, and A. Katouzian, "MRI biopsy with semi–automated biopsy needle in Slicer 3D environment," in *IGIC*, 2014.

[3] J. Traub, M. Friebe, S. Wiesner, T. Wendler, M. Keicher, S. Paepke, and M. Horn, "Hybrid Interventional Imaging for non-surgical SNLB staging," in *SMIT 2014*, 2014.

Publications by this Focus Group can also be found on page 150.

Focus Group **Molecular Imaging**

Prof. Silvio Aime (Università di Torino) | Hans Fischer Senior Fellow
Giaime Rancan | Doctoral Candidate
Prof. Markus Schwaiger, Clinic for Nuclear Medicine, TUM

Silvio Aime

Advances in preclinical paraCEST

Chemical Exchange Saturation Transfer with paramagnetic contrast agents (paraCEST) is a complex contrast-generating technique used for functional and molecular imaging with nuclear magnetic resonance (NMR). The technique offers some unique advantages in the detection and analysis of the CEST signal, due to large chemical shifts in the exchanging proton pools. The lack of competing magnetization transfer (MT) contributions from endogenous molecules and the minor impact of direct water saturation help to reduce uncertainty in the measurement and allow the mapping of pH through ratiometric techniques [1]. Accurate pH mapping is especially interesting in the characterization of tumors, for which there is a high preclinical and clinical demand. The major limitations of the methodology are the bioavailability of the contrast agent in the tissue of interest, the characteristics of the chemical systems involved, and instrumental specifications of the MRI scanners.

Considering the complexity of the contrast agents involved, thorough studies on the effects of magnetic field strength (accepted paper) and the radiofrequency saturation pulses (awaiting final acceptance) have been conducted. Low field (<1.5T) applications are particularly interesting for clinical translation and the availability of suitable lanthanide ions. Conversely, high field (>=3T) paraCEST is optimal for preclinical imaging using a limited selection of paramagnetic ions.The RF pulse optimization has been extended to pulse trains in a proof-of-concept study on a clinical 3T Siemens Biograph, confirming the spectroscopical results *in vitro*.

With the agents and instrumentation available, a preclinical study is ongoing, with the goal of quantifying pH in rat tumor models. The results will be compared with other experimental imaging techniques such as hyperpolarized pyruvate metabolism mapping and hyperpolarized pH imaging. If successful, the multimodal approach is expected to confirm or disprove the reduction in tumor pH due to changes in metabolism (Warburg effect) and to detect tumor heterogeneities, as well as cross-validating the pH imaging modalities, for which no gold standard yet exists.

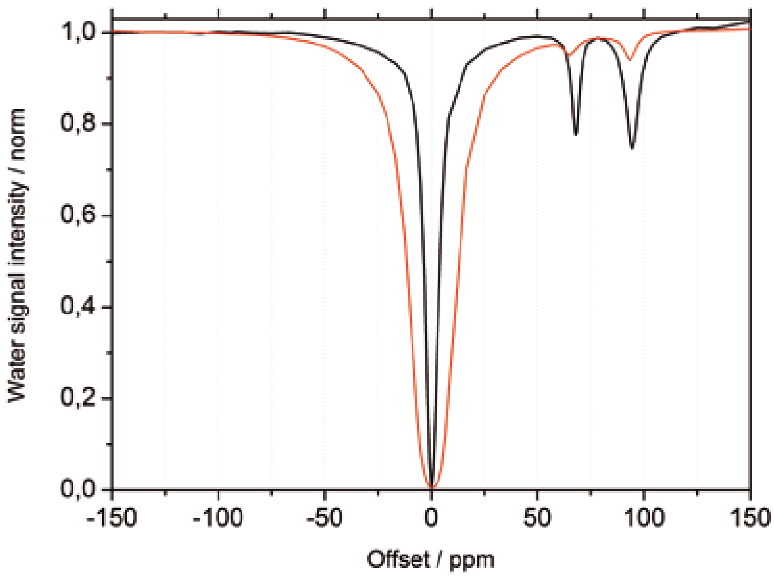
To improve the bioavailability of the paraCEST agents, liposomial drug delivery formulations have been investigated. In a liposomial formulation with a high loading, the inhomogeneous distribution of the paramagnetic agent causes a dramatic reduction in T2 that quenches the CEST signal (figure 1). At lower concentrations, a maximum saturation amplitude is defined by the liposomial membrane acting as the rate-determining step in the transfer of saturation. The pH within the liposome equilibrates with the external solution in the formulation used, allowing the ratiometric analysis to be performed.

Reference

[1] D. Delli Castelli, E. Terreno and S. Aime, “YbIII-HPDO3A: A dual pH and temperature responsive CEST agent,” *Angew. Chem. Int. Ed.*, vol. 50, no. 8, pp. 1798–1800, 2011.

Selected Publication

[2] G. Rancan, D. Delli Castelli, and S. Aime, “MRI CEST at 1T with large μeff Ln3+ complexes. Tm3+-HPDO3A: an efficient MRI pH reporter,” *Magn. Reson. Med*, accepted for publication.



1 | Z spectrum (water signal with changing saturation frequency) for a high-loading paraCEST liposome (red line), with a shortened T2/T2* due to the inhomogeneous distribution of the paramagnetic compound. After sonication, the contrast agent is homogeneously distributed in the solution and the quenching is lost (black line).

Focus Group **Neuroimaging**

Prof. Josef P. Rauschecker (Georgetown University) | Hans Fischer Senior Fellow
Dr. Valentin Riedl (Klinikum rechts der Isar)
Lukas Utz | Doctoral Candidate
Prof. Bernhard Hemmer, Neurological Clinic and Policlinic, TUM

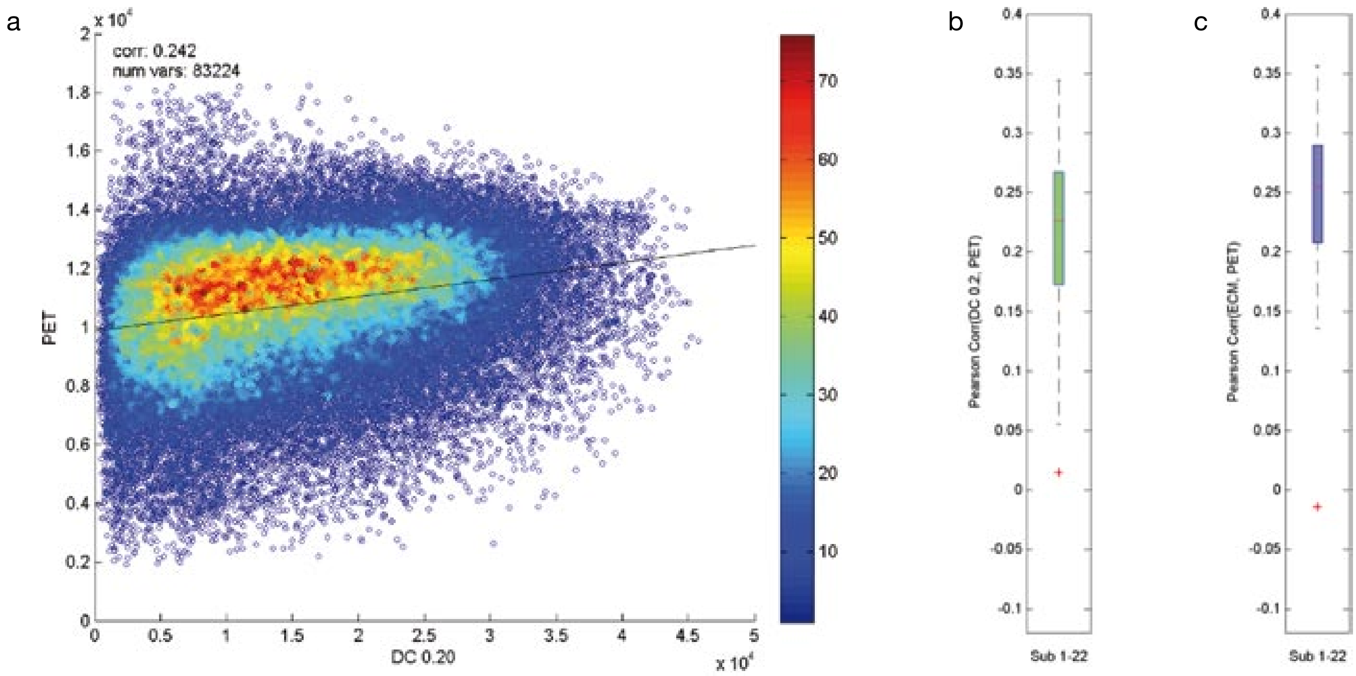
Josef P. Rauschecker

Energetic costs of global functional connectivity in the human brain

The human brain is a highly connected organ, and its basal components facilitate these connections. The brain with its $>10^{10}$ neurons and $>10^{14}$ synapses is known to consume a high amount of energy. The demand for metabolized glucose in the human brain is high in proportion to its size and is not only caused by cognitive performance; it accounts for about 25% of total body glucose consumption at rest (Clark & Sokoloff, 1999). However, only a small amount of energy is utilized for basic metabolism, leaving a significant fraction for the implementation of neuronal communication (Tomasi, Wang, & Volkow, 2013).

In this project, we are trying to answer the question: How is the relationship between neuronal communication and the local energetic cost represented in different regions of the human brain? There are several possible answers to this question. If this relationship is linear, it would imply that each connection, regardless of its distance or location, would cost a constant amount of energy. However, if the relationship is logarithmic or exponential, it would indicate an increase or decrease, respectively, in efficiency for highly connected regions in the human brain. To date, this relationship is unknown yet of great importance, as it would allow a predication of a region's energy consumption knowing only some characteristic properties such as spatial location and degree of connectivity.

We address this question by using the new integrated PET/MRI scanner (Positron Emission Tomography/Magnetic Resonance Imaging) at the Klinikum Rechts der Isar, which combines two imaging techniques and measures these two modalities simultaneously in the same subjects. Hereby we obtain direct information about the glucose consumption (local energy usage) in the neurons through PET and are able to calculate different global measures of functional connectivity between different brain regions (e.g., Degree Centrality [DC] and Eigenvector Centrality Mapping [ECM]) using functional MRI (fMRI). In this project, 22 healthy human subjects were simultaneously scanned with FDG-PET (fluoro-deoxy-glucose) and fMRI during conditions of "eyes closed" and "eyes open," and we established a multimodal analysis framework. In contrast to most other approaches investigating the relationship between global connectivity and local energy consumption, a great advantage of our approach is that it can be accomplished in single-subject space.



1 | (a) Whole-brain representation of measures of glucose consumption (PET) and global connectivity (DC, correlation threshold of r = 0.2) in a single subject. (b, c) Group results of correlation between glucose consumption (PET) and both measures of global connectivity (DC (b) and ECM (c)).

From the preprocessed MRI data, we calculated two connectivity measures, the Degree Centrality (REST V1.8) and the Eigenvector Centrality (Wink and van den Heuvel, 2012), respectively. In both DC and ECM calculation, the time series for each voxel is extracted and used to calculate the connectivity between all pairs of voxels. Thus, this approach captures the entire functional connectome, as it takes into account the relationship of each region in the brain to every other region.

The first results from this analysis, which are currently being prepared for publication, show a positive and linear relationship between energy consumption and global connectivity in the human brain. In figure 1a, this positive correlation between DC and glucose consumption is shown in a single subject. This result is present not only in this particular subject, but there is also a general increase in efficiency across all 22 subjects for both measures of connectivity (DC/ECM, figure 1b/1c).

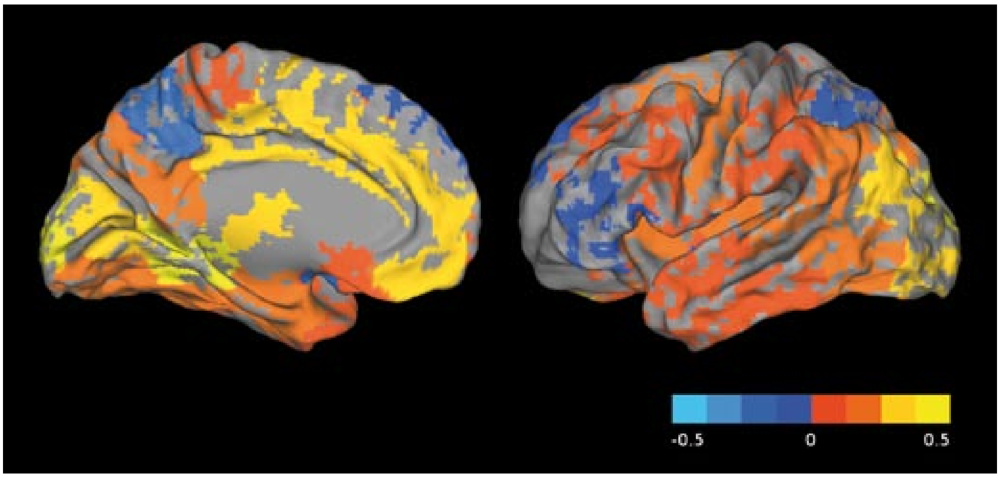
Josef P. Rauschecker received his PhD from the Max Planck Institute for Psychiatry in Munich in 1980 and his DSc in 1985 from Eberhard Karls University in Tübingen. After working as a staff scientist at the MPI of Biological Cybernetics from 1981–1989, he joined the National Institute of Mental Health (US) as a senior investigator in 1989. Since 1995, he has been a professor of physiology, biophysics, neurology, and neuroscience at Georgetown University. Josef P. Rauschecker's main research interests are in the functional specialization of the cerebral cortex and its organization into processing streams, plasticity of the cerebral cortex in early blindness, and the neural mechanisms of tinnitus.

Correlating glucose consumption with the connectivity measure Eigenvector Centrality Mapping (ECM) leads to a slightly higher and more robust correlation. This might be caused by two different factors. First, Degree Centrality is highly susceptible to the choice of threshold used to determine which correlation is considered a "true" connection between two regions. We chose a correlation threshold of r = 0.2, which is often used in the relevant literature and leads to the most normally distributed DC values across subjects. Second, ECM is a measure that emphasizes so-called "network hubs," thus emphasizing regions with a high number of connections, and might identify and indicate neuronal efficiency. Regions that are known to be central in the human functional connectome are the occipital cortex, the inferior parietal cortex, the medial orbitofrontal cortex, and the medial superior frontal cortex (van den Heuvel, 2013).

Considering these spatial differences in functional connectivity, we investigated the spatial correlation with glucose consumption across the brain. To enable this type of analysis, we used multiple different parcellations of the human brain based on structural similarities (AAL, Automated Anatomic Labeling), functional similarities (Shen, 2013), or independent component analysis (ICA) of our subjects' functional images. Figure 2 shows the mean correlation of Degree Centrality (r = 0.2) and FDG-PET across all 22 subjects in 44 regions of interest (ROI). This parcellation is based on the functional atlas provided by Shen et al. (2013). The spatial distribution reveals a decrease from occipito-parietal to frontal regions and reaches its maximum in early sensory and motor regions as well as in regions associated with the regulation of emotions.

For its projects, this Focus Group collaborates with Prof. Mark Mühlau, Prof. Markus Ploner, and Dr. Valentin Riedl at the Neurological Clinic as well as Dr. Sandro Krieg and Nico Sollmann at the Neurosurgical Clinic of the TUM Rechts der Isar Hospital. There are further collaborations with robotics experts at TUM: Prof. Martin Buss and Prof. Dongheui Lee (Focus Group Control and Robotics), Michaela Semmler (Automatic Control Engineering), Prof. Angelika Peer (Focus Group Cognitive Technology), and Prof. Gordon Cheng (Institute for Cognitive Systems).

2 | Mean spatial correlation of DC (r = 0.2) and FDG-PET across all subjects within 44 ROIs based on a functional parcellation (Shen et al., 2013) revealing a clear spatial distribution of glucose efficiency in the human brain.



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[3] M. P. van den Heuvel and O. Sporns, “Network hubs in the human brain,” *Trends Cogn. Sci.*, vol. 17, no. 12, pp. 683–96, Dec. 2013.

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Selected Publications

[6] J. P. Rauschecker, “Is there a tape recorder in your head? How the brain stores and retrieves musical melodies,” *Front. Syst. Neurosci.*, vol. 8, p. 149, Jan. 2014.

[7] C. I. Petkov, Y. Kikuchi, A. . Milne, M. Mishkin, J. P. Rauschecker, and N. K. Logothetis, “Different forms of effective connectivity in primate fronto-temporal pathways,” *Nat. Commun.*, accepted for publication.

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Publications by this Focus Group can also be found on page 151.

Focus Group **Phase Contrast Computed Tomography**

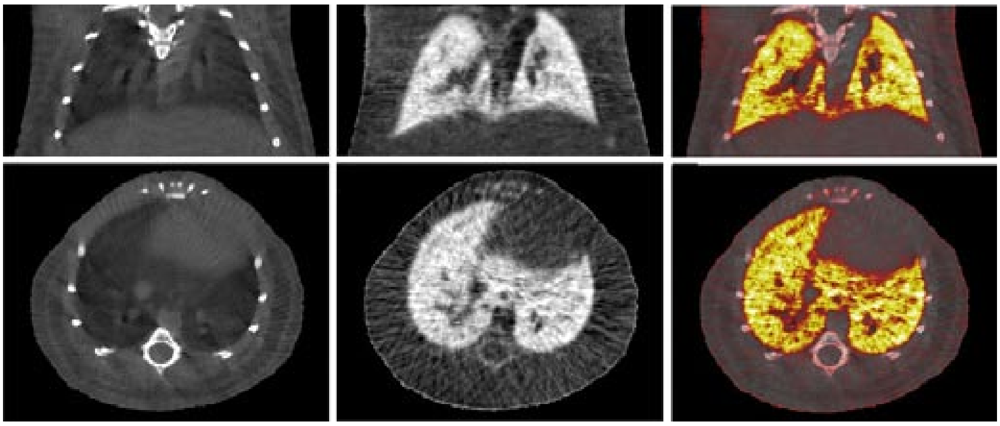
Dr. Thomas Koehler (Philips Research Laboratories) | Rudolf Diesel Industry Fellow
Prof. Franz Pfeiffer, Biomedical Physics, TUM
Prof. Ernst Rummeny, Radiology, TUM

Thomas Koehler

Exploring the translation of X-ray phase-contrast computed tomography from bench to bedside

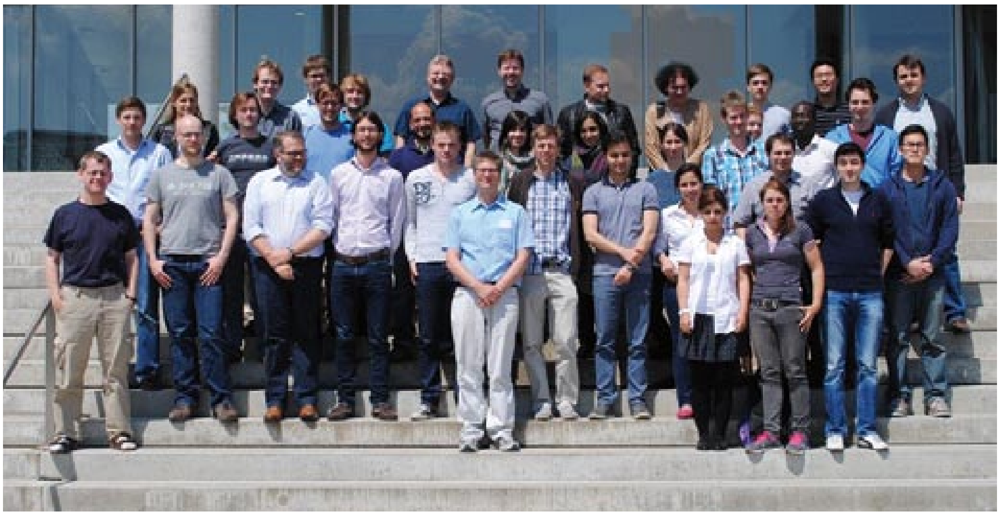
In conventional X-ray imaging, the image contrast is formed by X-ray attenuation, and reflects the physical interactions of photo-electric absorption and Compton scattering. Both of these interaction processes are modeled conveniently by interpreting X-rays as photonic particles. If instead X-rays are described as electromagnetic waves, other (wave-optical) interaction effects occur and yield to diffraction, refraction, phase-shift, and scattering. Several methods to exploit these wave-optical interactions of X-rays with matter have been investigated in recent years. Although some of them yield excellent results at highly brilliant synchrotron sources, none of them has so far found its way to routine medical CT applications, which require a large field of view of many centimeters, the efficient use of polychromatic and strongly diverging radiation, and a reasonably compact setup.

To make the advantages of phase- and/or dark-field contrast X-ray imaging available for routine X-ray medical diagnostics applications, we have started developing a grating-based approach to wave-optical X-ray imaging. So far, and as an intermediate achievement, we recently have been able to translate this methodology from the optical bench to a fully functional first pre-clinical phase- and dark-field-contrast CT scanner for small-animal (mouse) research. Example images of a mouse thorax are shown in figure 1.



1 | *In vivo* X-ray attenuation (left), dark-field (middle) and fused (right) CT images of a mouse thorax. The small-sized alveoli in the lung generate a large dark-field signal due to (small angle) scattering of the X-rays.

Andreas Fehringer, Max von Teuffenbach, and Wolfgang Noichl work with this Focus Group as doctoral candidates.



2 | A workshop with participants from five TUM groups dealing with medical image reconstruction was held during the summer.

Thomas Koehler studied physics at the Christian-Albrechts-University in Kiel from 1989 to 1994. After receiving his degree, he moved to Philips Research Laboratories in Hamburg and worked on the inverse problem of electro- and magnetocardiography, resulting in a PhD thesis. He has been working on several projects in the area of inverse problems for different applications, namely computed tomography (CT), diffuse optical tomography, transmission electron microscopy, and differential phase contrast imaging (DPCI). His primary focus in CT has been the development of methods to reduce the radiation dose by iterative reconstruction algorithms. The clinical evaluation of these algorithms is conducted together with the Department of Radiology at TUM. During the last few years, he developed an interest in the emerging field of DPCI, where he has worked on both projection imaging as well as on tomographic imaging.

Selected Publications

[1] F. M. Epple, S. Ehn, P. Thibault, T. Koehler, G. Potdevin, J. Herzen, D. Pennicard, H. Graafsma, P. B. Noel, and F. Pfeiffer, "Phase unwrapping in spectral x-ray differential phase-contrast imaging with an energy-resolving photon-counting pixel detector," *IEEE Trans. Med. Imaging*, Aug. 2014.

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[3] K. Burger, T. Koehler, M. Chabior, S. Allner, M. Marschner, A. Fehringer, M. S. Willner, F. Pfeiffer, and P. B. Noel, "Regularized iterative integration combined with non-linear diffusion filtering for phase-contrast x-ray computed tomography," *Opt. Express*, vol. 22, no. 26, p. 32107, Dec. 2014.

Publications by this Focus Group can also be found on page 151.

Focus Group **Regenerative Medicine**

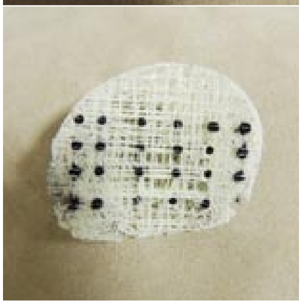
Prof. Dietmar W. Hutmacher (QUT) | Hans Fischer Senior Fellow
Dr. Elizabeth Rosado Balmayor | Postdoctoral researcher
Prof. Arndt F. Schilling, Clinic for Plastic Surgery and Hand Surgery, TUM

Dietmar W. Hutmacher

Three-dimensional printing has recently generated widespread news coverage and is on the verge of the peak of the consumer "hype cycle." However, it is still in its infancy in terms of the developmental "S-curve." The capabilities of 3D printing are increasingly leveraged in research and development in a wide range of fields, both in universities and in industry. The possible applications are endless and are only now starting to be truly explored. Additive manufacturing (AM) — the industrial version of 3D printing — is already used to make niche items such as filters or sculptures, and to produce plastic and metal prototypes for engineers and designers. While 3D printing for consumers and small business entrepreneurs has received a great deal of publicity, it is in manufacturing where the technology will have its most significant commercial impact. The rapid rise of additive manufacturing in recent years raises the intriguing possibilities of many new and highly innovative modalities of manufacturing. especially in the emerging field of additive biomanufacturing (ABM). The research program of this Focus Group aims to provide the technological breakthroughs required to establish an innovative ABM technology platform for biomedical applications, specifically for breast tissue engineering, and to change the current advanced manufacturing paradigms.

World-leading fundamental and translational biomedical research, together with advanced science and engineering, will be required to address the ABM design and fabrication challenge: through ground-breaking and highly innovative collaborative research; by building human capacity in a range of research areas; and by enhancing research performance and strategic development internationally. In recognition of the need for Bavaria to build capacity in key areas of economic importance, the topic of "Additive Biomanufacturing" is well aligned with national strategic priorities. Our research combines three topical areas: Fundamental and Translational Research; Education; and Intellectual Property and Commercialization.

In collaboration with PD Dr. Jan-Thorsten Schantz and Mohit Chhaya.



1 | Breast tissue engineering is an interdisciplinary field which combines expertise from engineering, cell biology, material science and plastic surgery primarily aiming to reconstruct breasts following a post-tumour mastectomy. The Focus Group has developed an integrated strategy whereby image is first taken of the breast region of a mastectomy patient using medical imaging techniques such as 3D laser scanning, CT or MRI scans. Software packages were then developed to process the captured images into a patient-specific 3D computer-aided design (CAD) model which is then sent to a bioprinter to be fabricated in the form of a scaffold suitable for breast tissue engineering.

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Selected Publications

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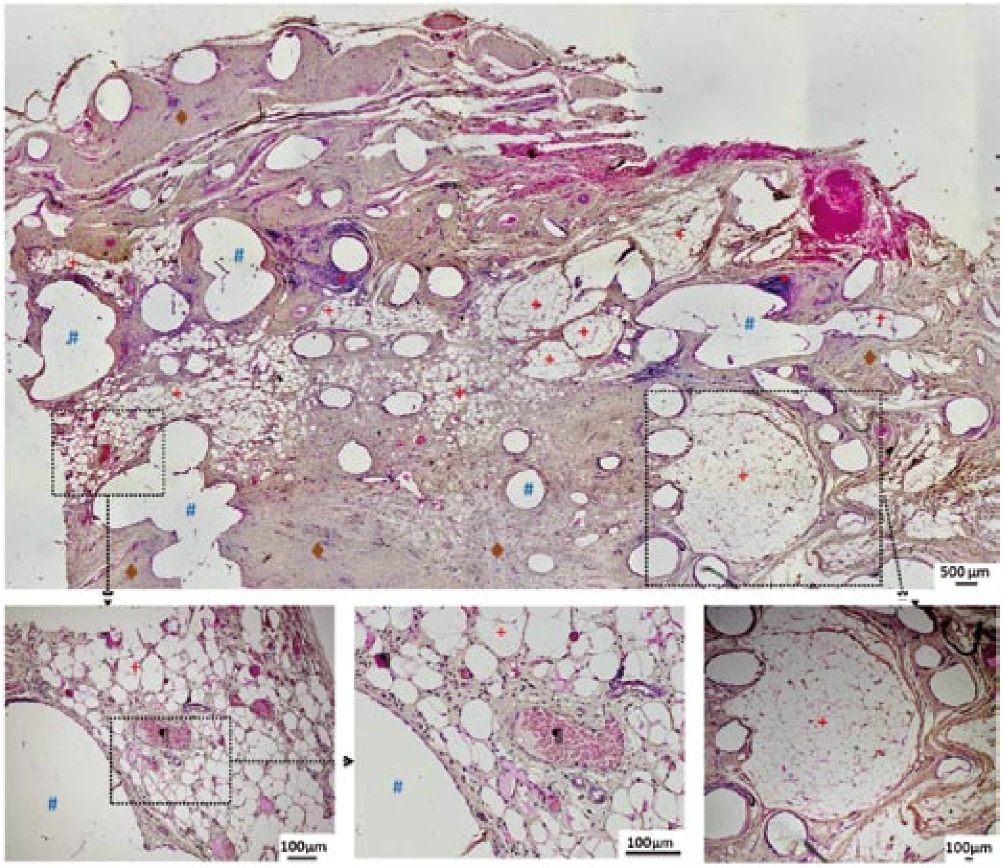
[3] E. Hadjipanayi and A. F. Schilling, "Regeneration through autologous hypoxia preconditioned plasma," *Organogenesis*, vol. 10, no. 2, pp. 164–169, 2014.

Publications by this Focus Group can also be found on page 151.

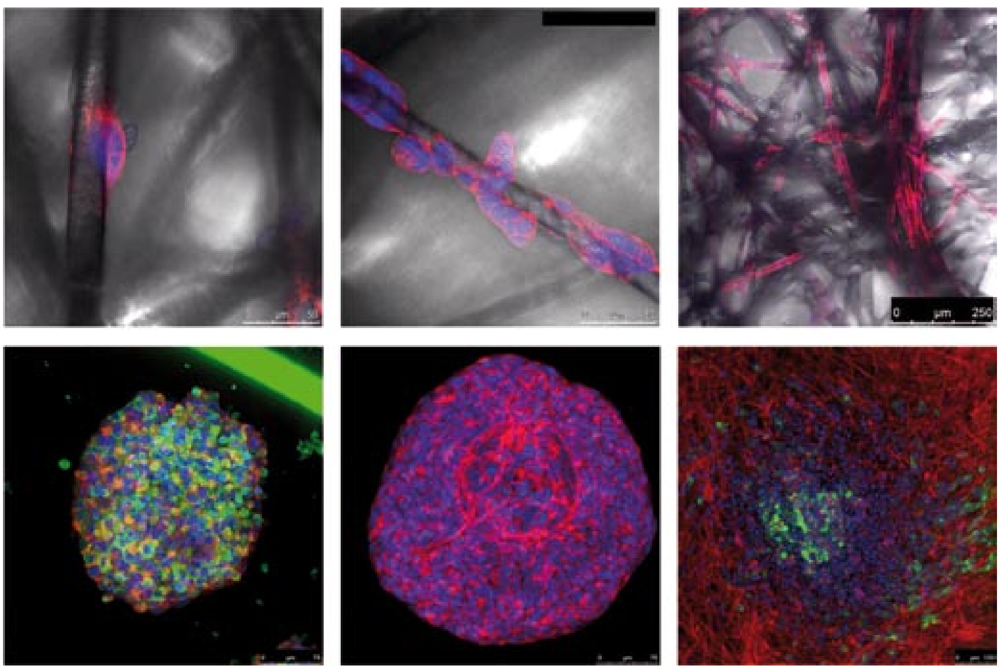
2 | H&E stained sections of prevascularisation + lipoaspirate group three months after implantantion. Adipose tissue area was the highest among all other groups. Adipose tissue regions seemed to be better connected to each other and formed interconnected structures.

Prevascularisation + Lipoaspirate group – Superficial layers



+ shows areas of fat tissue
¶ shows blood vessels
# shows scaffold strands
* shows areas of lymphatic structures
♦ shows connectives tissue

3 | Confocal laser microscopy of breast cancer cell cultured on breast scaffolds coated with a chemo drug.



Bio-related Natural Sciences

New in this Research Area

Focus Group **Biochemistry**

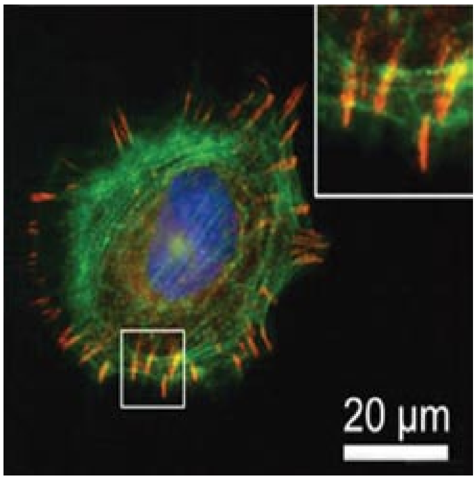
Prof. Horst Kessler (TUM) | Carl von Linde Senior Fellow
Chemistry, TUM

Horst Kessler

Interface immobilization chemistry of *c*RDG-based peptides regulates integrin mediated cell adhesion

The interaction of specific surface receptors of the integrin family with different extracellular matrix-based ligands is of utmost importance for the cellular adhesion process. To study this integrin-mediated cell adhesion on artificial substrates, the ligands consist of a specific integrin-binding group, such as a *c*(RGDfX) peptide, a spacer moiety that lifts the integrin-binding group from the surface and presents it to cells, and a thiol functionality as an anchoring group. These peptides are immobilized on gold nanoparticle (AuNP) structured surfaces via three chemically different types of spacers: the flexible aminohexanoic acid (Ahx) and PEG-based spacers, and the more rigid polyproline sequences.

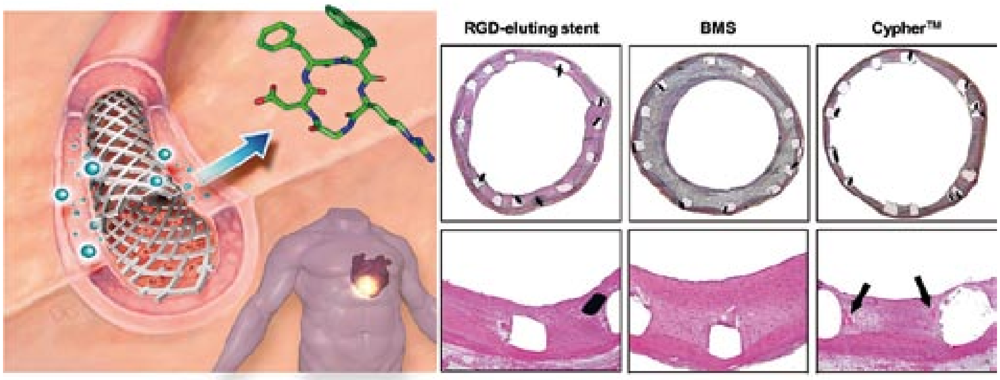
For immunohistochemical and dynamic analyses of cell spreading and focal adhesion (FA) assembly the integrin-binding moiety of all ligands was constant, but changes in the spacer chemistry and length of the distinct ligands reveal significant differences in cell adhesion activation and focal adhesion formation. Polyproline-based peptides demonstrate improved cell adhesion kinetics and focal adhesion formation compared with common Ahx or PEG spacers. Binding activity can additionally be improved by applying divalent ligands, inducing a multimeric effect.



1 | Fluorescent micrographs of REF52 cells on gold nanopattern functionalized with *c*RGD peptides. Cells were fixed and stained for paxillin (red), nuclei (blue), and actin (green).

The integrin ligand *c*(RGDf(*N*Me)Nal) reduces neointimal hyperplasia in a polymer-free drug-eluting stent system

In the interventional treatment of myocardial infarctions and coronary artery disease, the development of drug-eluting stents (DES) was a major breakthrough, as it significantly decreased the risk of restenosis, the most significant limitation of percutaneous coronary intervention using bare metal stents (BMS). The principle of DES is the deferred release of anti-proliferative drugs to avoid re-narrowing of the vessel (neointimal growth). However, the major drawback is the unspecific inhibition of endothelial cells, which are important for regulating thrombosis, inflammation, and vascular healing. Furthermore, most of the currently approved DES use permanent polymers to facilitate drug coating and modulate drug release kinetics. Unfortunately, the permanent presence of these polymers is associated with inflammatory and hypersensitivity reactions, which cause late stent thrombosis and restenotic events. Integrins, especially $\alpha v\beta 3$, $\alpha v\beta 5$ and $\alpha 5\beta 1$, are of crucial relevance for the interaction between vascular cells and the extracellular matrix (ECM) during the process of neointimal formation after coronary interventions. For this reason, our research has focused on the improvement of polymer-free or biodegradable DES systems based on highly active and subtype-selective integrin ligands as a promising alternative to the release of classical immunosuppressive drugs.



2 | Schematic presentation of a DES in a blood vessel (left). Histopathological evaluation of a RGD-coated stent, a bare metal stent (BMS) and the Cypher™ DES *in vivo* (right).

We developed the $\alpha v\beta 3$-selective integrin ligand *c*(RGDf(*N*Me)Nal) as a potent anti-proliferative molecule. Loaded onto a polymer-free BMS and evaluated in a rabbit iliac artery model, the peptide clearly showed decreased neointimal growth and improved vessel healing and re-endothelialization compared with the FDA-approved Cypher DES.

Selected Publications

[1] D. Pallarola, A. Bochen, H. Boehm, F. Rechenmacher, T. R. Sobahi, J. P. Spatz, and H. Kessler, “Interface immobilization chemistry of cRGD-based peptides regulates integrin mediated cell adhesion,” *Adv. Funct. Mater*, vol. 24, no. 7, pp. 943–956, Feb. 2014.

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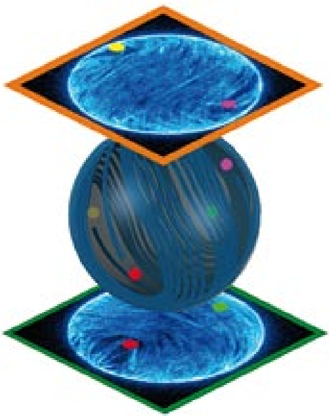
Publications by this Focus Group can also be found on page 152.

Focus Group **Biologically Inspired Material Science**

Prof. Zvonimir Dogic (Brandeis University) | Hans Fischer Senior Fellow
Felix Keber | Doctoral Candidate
Prof. Andreas Bausch, Molecular and Cellular Biophysics, TUM

"Bottom-up" assembly of active biomimetic materials

Zvonimir Dogic

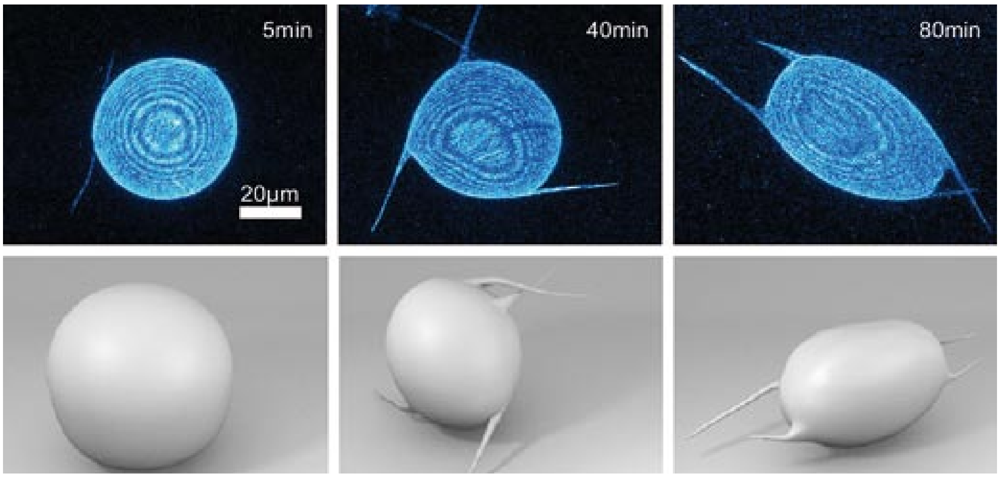


1 | Hemisphere projection of a 3D confocal stack of a microtubule-based active nematic vesicle. The positions of four +½ disclination defects are identified.

Our understanding of how complex materials assemble from simple inanimate molecules is remarkably advanced. Given the interaction between a pair of molecules, laws of fundamental physics predict with high accuracy the collective emergent behavior, such as a temperature at which a freely flowing liquid freezes into a solid crystal. The crystallization of molecules is intrinsically a property of a collective, for one cannot construct a crystal with one or a few molecules. Compared to these remarkable advances our ability to describe and predict collective behavior of animate energy-consuming ensembles of objects is still in its infancy. A particularly striking example of this is seen in the murmurations of a flock of starlings as they settle at dusk for a night's sleep [1]. Within such a flock, hundreds of thousands of birds form a seemingly continuous collective that exhibits rich dynamics consisting of endless turns, twists, and shape changes. It remains an open question if there are any fundamental laws that are able to predict the dynamics of such a social and inherently far-from-equilibrium collective.

The long-term goal of the collaboration between the groups of Andreas Bausch at TUM and Hans Fischer Senior Fellow Zvonimir Dogic is to experimentally establish fundamental principles that are able to predict the collective behavior of such far-from-equilibrium systems. The inspiration for this collaboration is the cellular cytoskeleton, a complex material that is assembled from diverse proteins, including ATP-consuming molecular motors that move along tracks provided by filamentous proteins such as microtubules or actin filaments [2]. Being released from constraints of equilibrium statistical mechanics, the cytoskeleton exhibits a number of remarkable properties such as dynamical shape changes, motility, and division. Just like a flock of birds, the cellular cytoskeleton is an example of far-from-equilibrium active matter. However, its biology is much too complex to enable detailed and quantitative comparison to relatively simple theoretical models of living matter. For this reason it remains an important challenge to assemble synthetic materials that are able to mimic the materials properties of the cellular cytoskeleton, yet at the same time can be described by highly simplified theoretical models.

During 2014, Andreas Bausch and Zvonimir Dogic through a highly collaborative effort have accomplished significant advances in this research area [3]. By encapsulating microtubule filaments and clusters of molecular-motor kinesin within a shape-changing lipid vesicle, they have demonstrated assembly of novel materials that exhibit a range of intriguing biomimetic properties reminiscent of those found in living cells. Once encapsulated within a vesicle, filamentous microtubules form a thin liquid crystalline layer of aligned rods that uniformly covers the inner surface of the lipid bilayer. However, fundamental mathematical laws (as well as everyday experience) demonstrate that it is not possible to cover a spherical surface with uniform lines without introducing topological singularities or defects. For example, covering the earth's surface with lines of longitude or latitude requires formation of two poles. In a similar way, covering the vesicle surface with a microtubule-based liquid crystal introduces the formation of four topological defects. The surprising finding was that, unlike the traditional case where these defects move to the corners of a tetrahedron in order to



2 | Vesicle shape changes driven by defect dynamics. Confocal images showing the z-projection of the vesicle shape, with corresponding volume representations of the 3D deformable vesicles structure. Starting from a spherical nematic vesicle with four +½ defects at t = 5 min, the vesicle slowly contracts, and four dynamic protrusions grow from the defect sites.

minimize the elastic free energy, defects in active vesicles powered by clusters of molecular motor kinesin acquire finite motility and stream around on the vesicle surface. Andreas Bausch and Zvonimir Dogic have demonstrated that these defects oscillate between two well defined configurations, and the frequency of such oscillations can be tuned by controlling ATP concentration. Thus active vesicles behave like tunable colloidal clocks that are able to keep time. A simple theoretical model developed by Mark Bowick and Cristina Marchetti from Syracuse University and Luca Giomi from SISSA is able to quantify these observations.

By suspending active liquid crystalline vesicles in a suspension of highly concentrated sugar, it is possible to deflate the vesicles, creating floppy surfaces. At this limit the stress induced by defects creates large filopodia-like protrusions that distort the entire structure, creating a deformable and motile material that resembles a living creature but is only assembled from five simple components. Fundamental laws of mathematics ensure that at any given time there are only four motile protrusions present in each structure. These results represent perhaps a first step towards making artificial protocells "from the bottom-up" using a well-defined set of biochemical components. The combined experimental and theoretical results also form the foundation for the field of topological active matter, while providing insight into a broad class of spatiotemporal pattern-forming systems and suggesting a pathway for development of a new class of materials endowed with properties that have hitherto been mostly confined to living organisms.

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Selected Publications

[3] F. C. Keber, E. Loiseau, T. Sanchez, S. J. DeCamp, L. Giomi, M. J. Bowick, M. C. Marchetti, Z. Dogic, and A. R. Bausch, "Topology and dynamics of active nematic vesicles," *Science*, vol. 345, no. 6201, pp. 1135–1139, Sep. 2014.

Publications by this Focus Group can also be found on page 153.

Zvonimir Dogic received his BA (1995) and PhD (2001) in physics from Brandeis University, USA, and spent his postdoctoral studies at the Research Center Jülich in Germany as a Humboldt Postdoctoral Fellow (2001–02), and at the University of Pennsylvania (2002–03). After an appointment at Harvard University as a Rowlatt Junior Fellow (2003–07), he returned to Brandeis University as an assistant professor. Since 2010, he has been an associate professor of physics. His research interests lie in elucidating rules that govern self-assembly of materials, with a particular emphasis being placed on the role the particle's shape and chirality play in these assembly processes.

Focus Group **Proteomics**

Dr. Peer-Hendrik Kuhn (TUM) | Carl von Linde Junior Fellow
Alperen Serdaroğlu | Doctoral Candidate
Prof. Stefan Lichtenthaler, Neuroproteomics, TUM

Peer-Hendrik Kuhn

Proteomic analysis of secretomes for deorphanization of proteases and identification of disease-related biomarkers

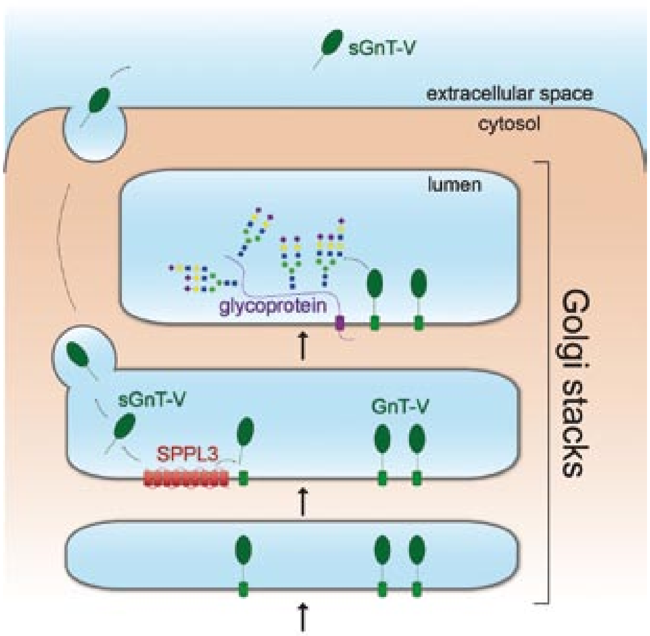
2014 has been a productive year for our Focus Group. We extended our work on proteases and started a new field of research on acute myeloid leukemia. The common denominator of our research is the analysis of the cellular secretome, which per definition is the entirety of all released factors of a given cell type including proteins released upon proteolysis. The secretome of a given cell type contributes to the composition of body fluids and thus is a source for disease- or therapy-related biomarkers and the identification of new drug targets. Our first field of research deals with the deorphanization of extracellular proteases, molecular scissors that are able to release membrane-tethered proteins from the membrane by cleavage. Recently, we published the SPECS method, which makes the secretome accessible to mass spectrometric analysis. Using this technology we identified the substrates of BACE1, an aspartyl protease that plays a pivotal role in the pathogenesis of Alzheimer's disease. Now, we are studying the physiological function of these substrates to better understand how BACE1 modulates their function and what side effects we may need to expect from a therapeutic BACE1 inhibition in patients. Recently, we extended our SPECS analyses to other proteases, such as MT5-MMP, SPPL3 and ADAM10, to better understand their physiological function and their therapeutic potential.

The metalloprotease ADAM10 is a counter player of BACE1 and seems to positively influence Alzheimer's disease pathogenesis. Therefore, ADAM10 activation is considered a viable approach to slow down the progression of Alzheimer's disease. However, only little is known about ADAM10 proteolytical function in the central nervous system, which would determine side effects in case of therapeutic ADAM10 activation as well. Hence, we are currently investigating the substrate spectrum of ADAM10 in the brain. Our data speak for a fundamental role of ADAM10 in brain development and synapse function. A manuscript is in preparation.

This year we published a seminal study on SPPL3 in a collaborative effort. We were able to show that SPPL3 proteolytic activity regulates protein glycosylation in the Golgi by cleaving, among others, the glycosylation enzyme MGAT5 (figure 1). Following up on this study, we have investigated the whole substrate spectrum of SPPL3 with SPECS. Our proteomic analysis reveals that SPPL3 cleaves numerous other glycosylation modifying enzymes besides MGAT5. This speaks in favor of a general regulatory function of SPPL3 in glycosylation which is a fundamental biological process and contributes, for example, to the interaction between the cells in our body and their environment.

A new emerging field in our focus group is the study of secretomes of hematopoetic disorders. Doctoral candidate Alperen Serdaroğlu moved forward on the secretome analyses of acute myeloid leukemia cell lines. In studying this, we aim to identify soluble biomarkers that might make diagnostic bone marrow punctures obsolete in the future. The second part of his project deals with studying the impact of receptor tyrosine kinase signaling on the secretome of AML cell lines.

Finally, our Focus Group host Stefan Lichtenthaler was awarded the Alzheimer research prize of the Hans and Ilse Breuer Foundation, which is the highest prize for neurodegeneration research in Germany.



1 | SPPL3 physiology (Voss et al. 2014)

Selected Publications

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Publications by this Focus Group can also be found on page 154.

Focus Group **Statistical and Quantitative Genomics**

Prof. Daniel Gianola (University of Wisconsin-Madison) | Hans Fischer Senior Fellow
Katrin Töpner | Doctoral Candidate
Prof. Chris-Carolin Schön, Plant Breeding, TUM

Enhancing accuracy in genome-assisted prediction and inference

Daniel Gianola

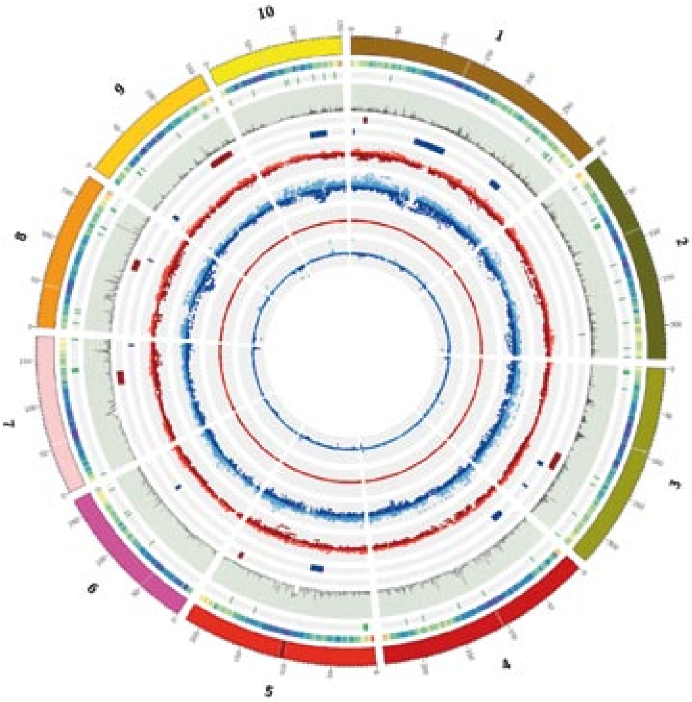
In human, animal and plant genetics, genome discovery has opened new avenues for addressing key theoretical and applied questions of quantitative genetics. Examples include unraveling the architecture of quantitative traits using massive genomic data and identifying genomic regions associated with the expression of complex traits. Additional issues include the evaluation of gene × gene and gene × environment interactions as well as the selection mechanisms that operate in natural and managed populations of animals and plants.

In agricultural genomics the multifactorial basis of many important traits has been corroborated using molecular markers, leading to the development of whole-genome based statistical methods from the perspective of prediction of unobserved or future phenotypes. The employed Bayesian models differ mainly in the prior probability distributions assigned to marker effects. We have shown that there are substantial differences in the sensitivity of these models with respect to the specification of prior distributions and in Bayesian learning ability [1]. We also demonstrated the requirements underlying successful variable selection in high-density genotyping and sequencing data [2]. A method that performs well over a wide range of traits and experimental settings is genomic best linear unbiased prediction (GBLUP). This is fortunate, because the method is easier to compute than procedures that require extensive use of Monte Carlo sampling. We have proposed a way of enhancing GBLUP by using a resampling method from machine learning: “bagging,” i.e., bootstrap aggregating sampling [3]. It was found that bagging improved the predictive performance of GBLUP when applied to experimental wheat data, and that it made it more robust against over-fitting. Bagging also enables calculation of an empirical prediction mean-squared error metric for each item being predicted.

In situations where the number of markers is much larger than the number of phenotypic observations ($n << p$), marker effects are severely shrunken in whole-genome regressions, and inferences on the genetic architecture of the analyzed traits are ambiguous. Thus, in identifying individual genomic regions contributing to trait expression, genome-wide association studies (GWAS) are performed. In GWAS, significant associations between single nucleotide polymorphisms (SNPs) and traits are inferred from linear regression of a phenotypic measurement on the number of copies of a reference allele at a given locus. Literature shows that GWAS often fail to return significant signals at causal genomic variants or produce a large number of false positive results. To overcome some of the limitations of this approach we are currently investigating specific properties of GWAS models theoretically. Successful GWAS also depend on correct specification of genetic or molecular similarity between individuals, and we are in the process of developing an efficient method for calculation of a massive number of inverse matrices needed for that purpose. We are also working on juxtaposing GWAS results from experimental populations and massive sequence scans of their ancestors, so as to refine the localization of genomic regions controlling the expression of complex traits. Merging results from GWAS and selection scans may alleviate some shortcomings and pitfalls of the single marker methods.

Our group also wrote an invited review on around a century of statistical developments in animal breeding, including an account of the transition from methods developed in the Victorian era to the Bayesian hierarchical models for whole-genome data employed at present, including applications and potential of machine learning procedures [4].

Our future efforts will also be devoted to the examination of dependencies between predictor variables in GWAS, known as linkage disequilibrium (LD) between markers, and the impact of LD on the performance of whole-genome based prediction models. One approach will be to model the structure of LD by multi-dimensional, specific probability distributions, and to examine parameters that reflect how LD is conserved over sub-population clusters such as plant populations or animal breeds. We will advance our analysis of experimental data by developing causal models based on structural equation modeling and Bayesian networks and by expanding analyses from using end-point phenotypes (such as economically important traits) as well as upstream phenotypes (e.g., transcription levels) to studying gene-gene and gene-phenotype networks.



1 | The Circos plot shows the ten maize chromosomes in the outer circle. From outside to inside the data tracks represent gene density, positions of genes involved in maize flowering time, cross-population composite likelihood ratio test results, published QTL information for flowering time in the two maize populations Dent (red) and Flint (blue), SNP effects obtained with GWAS and a Bayesian method (BayesCπ) for Dent and Flint, respectively.

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Publications by this Focus Group can also be found on page 154.

Focus Group **Structural Membrane Biochemistry**

Prof. Franz Hagn (TUM) | Rudolf Mößbauer Tenure Track Professor
Joka Pipercevic | Doctoral Candidate
Structural Membrane Biochemistry, TUM

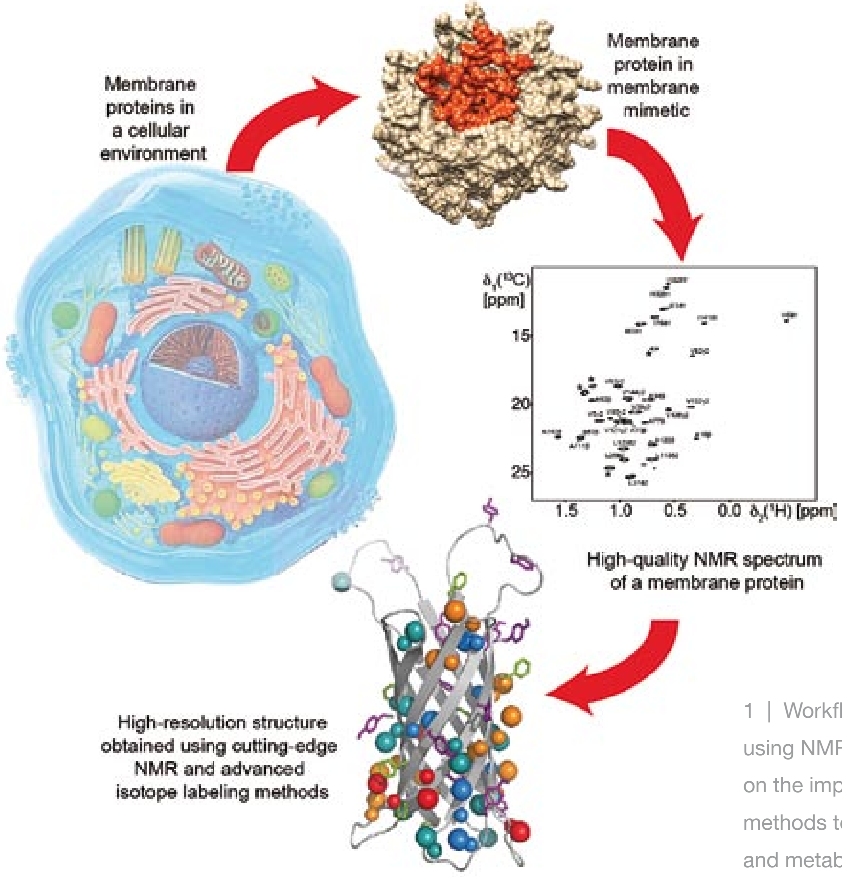
Franz Hagn

The research of the newly established Focus Group Structural Membrane Biochemistry is concentrated on the structure and function of membrane proteins and their partner proteins, using mainly nuclear magnetic resonance (NMR) spectroscopy among a variety of other biophysical and biochemical methods. We are interested in the mechanism and the mode of action of membrane protein systems connected to cancer, neurological disorders, and metabolic diseases. For these pharmaceutically relevant proteins, and in particular membrane proteins, molecular and structural details are often sparse or absent. Therefore, there is an urgent need for an in-depth structural characterization of this important protein class to facilitate targeting by tailored small molecule drugs in a rational, structure-based manner.

In order to obtain high-quality structural data, we are employing cutting-edge biochemical methods for membrane protein sample preparation using various membrane mimetics, such as detergent micelles, detergent-lipid bicelles, and phospholipid nanodiscs, a detergent-free native-like membrane system. This system has recently been optimized in the lab to enable structure determination by NMR [1]. More recently, we have established a protocol for high-resolution structure determination of membrane proteins in nanodiscs. A combination of specific isotope labeling and suitable NMR methods yielded the first protein side chain-based structure of a membrane protein in nanodiscs [2].

To produce all kinds of eukaryotic membrane proteins, we are using not only cell-based expression, but also cell-free protein production systems. We recently adapted cell-free protein expression methods for the production of selectively labeled membrane proteins that could not be obtained in living cells and were able to record high-resolution NMR data [3].

This groundwork is now being applied to the structural and dynamical characterization of membrane proteins, including G-protein coupled receptors (GPCRs) and the mitochondrial voltage-dependent anion channel (VDAC). Even though structural information is available for most of these systems, their complexes with partner proteins are less well understood. In addition, dynamics linked to protein function cannot be obtained by any other high-resolution structural method except NMR spectroscopy. We are going to explore these possibilities and are hoping to gain biological insights on an atomic level.



1 | Workflow for the structure determination of membrane proteins using NMR spectroscopy. In the lab, we are continuously working on the improvement of this cycle and the application of these methods to proteins involved in cancer, neurological disorders, and metabolic diseases.

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Publications by this Focus Group can also be found on page 154.

Franz Hagn studied biochemistry at the Universities of Bayreuth and Stockholm and moved to TUM to complete a doctorate involving structural and functional studies of molecular chaperones, tumor suppressor proteins and spider silk proteins. After a short period as a postdoctoral researcher at TUM he joined Harvard Medical School where he worked on the development of native membrane mimics for the structure determination of membrane proteins using NMR. In the fall of 2014, he accepted a Rudolf Mößbauer Tenure Track Assistant professorship of Structural Membrane Biochemistry at TUM-IAS.

Focus Group **Synthetic Biochemistry**

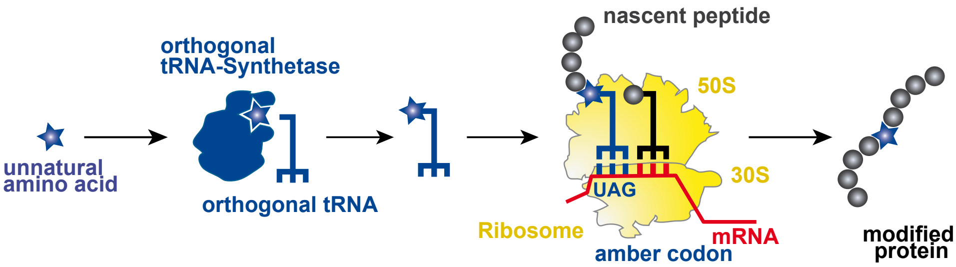
Prof. Kathrin Lang (TUM) | Rudolf Mößbauer Tenure Track Professor
Susanne Mayer | Doctoral Candidate
Synthetic Biochemistry, TUM

Applications of an expanded genetic code – novel methods for labeling proteins

Kathrin Lang

The Focus Group Synthetic Biochemistry was established in April 2014 and conducts research in the interdisciplinary area of chemical biology, applying concepts from organic chemistry to develop new tools to study and manipulate complex biological systems.

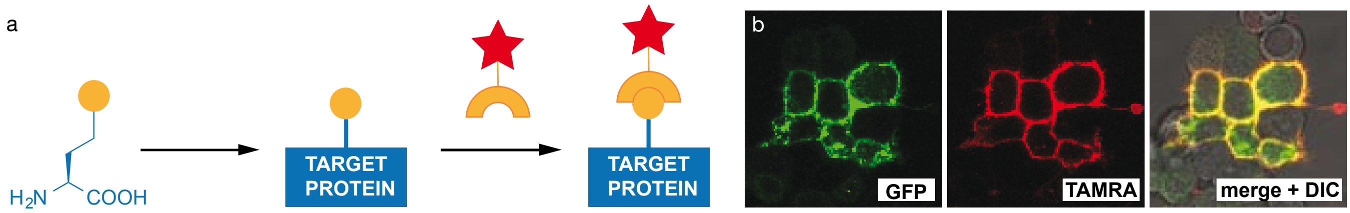
In particular, we develop and apply approaches to allow the site-specific incorporation of unnatural amino acids with tailored physical and chemical characteristics into proteins in diverse cells and organisms by genetic code expansion. This can be achieved by using an expanded machinery of translation, consisting of an “orthogonal” aminoacyl-tRNA synthetase/tRNA pair that directs the incorporation of an unnatural amino acid in response to an amber stop codon (UAG) placed in a gene of interest (amber suppression, figure 1) [1].



1 | Site-specific incorporation of unnatural amino acids via amber suppression

By extending this technology we have developed a new approach to site-specifically incorporate custom-synthesized unnatural amino acids bearing a bioorthogonal functional group into proteins in bacteria and mammalian cells *in vivo*. These modified proteins can react in a rapid and highly specific manner with a chemical reporter with tailored properties under physiological conditions in live bacteria and mammalian cells (figure 2a). This makes it possible to label any specific protein at a single position within the polypeptide with any desired small molecule fluorophore and thereby provides the ultimate labeling method for sophisticated *in vivo* imaging techniques such as super-resolution microscopy, FRET and single-molecule imaging (figure 2b) [2–4]. We envision that this labeling approach will have an impact on addressing important biological questions, since it allows the non-invasive, site-specific, efficient and rapid labeling of target proteins using chemical probes with tailored physical and biological properties.

Future aims of our research consist in gaining insights into mechanisms of complex biological processes through application of synthetic molecules with tailored functions and properties. Research will focus on the targeted chemical synthesis of new artificial biomolecules (amino acids, proteins, nucleotides, oligonucleotides) designed to investigate and manipulate complex cellular processes in *in vitro* and *in vivo* biological systems. In particular, we plan to extend and apply approaches of site-specifically modifying and engineering proteins, thereby endowing them with



2 | a) Bioorthogonal chemical reactions allow labeling of an incorporated unnatural amino acid bearing a bioorthogonal functional group (yellow circle) with a chemical reporter (red star). b) Fluorescent labeling of a GFP (green fluorescent protein)-fused cell-membrane protein with a red fluorophore (TAMRA) in live mammalian cells.

new function, by using and developing extended, engineered orthogonal translation machineries *in vivo*. The chemical focus will lie on the synthetic development of new, genetically encodable bioorthogonal reactions, including photo-inducible reactions, that enable the *in vivo* site-specific modification of target proteins with modified ligands, oligonucleotides and biophysical probes. Such approaches which will be interesting not only for the study of important protein interactions and imaging of proteins *in vivo*, but also with respect to drug design and new biomaterials. Furthermore, genetically encodable bioorthogonal reactions will be implemented for the reversible photo-control of enzyme activity *in vivo* to dissect and study biological pathways, thereby enabling the control of biological processes in a reversible fashion by light. In general, our Focus Group pursues efforts to develop and extend toolkits and approaches, with the rational approach of a synthetic organic chemist, to contribute to the exploration of the questions arising on the fascinating interdisciplinary boundary of chemistry and biology. The ability to precisely design novel protein functions with new chemistries will open up many possibilities for synthetic biology, drug design, and gene therapy.

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Publications by this Focus Group can also be found on page 154.

Kathrin Lang studied chemistry at the University of Innsbruck, where she obtained a PhD in bio-organic chemistry under the supervision of Ronald Micura in 2008. She subsequently worked as a postdoctoral and investigator scientist at the Medical Research Council – Laboratory of Molecular Biology in Cambridge, UK, in the research groups of Venki Ramakrishnan (ribosome crystallography) and Jason Chin (chemical and synthetic biology). She now heads the synthetic biochemistry research group in the Chemistry Department.

Focus Group **Theory of Soft Matter**

Prof. Alessio Zaccone (TUM) | Rudolf Mößbauer Tenure Track Professor
Johannes Kraußer | Doctoral Candidate
Theory of Soft Matter, TUM

Alessio Zaccone

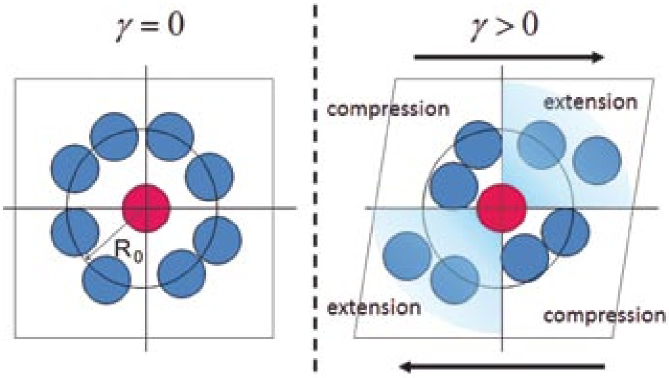
An unsolved mystery in condensed matter physics: why are things rigid?

Isn't it remarkable that just by pushing a few atoms on a localized spot of a chair, you can move the remaining ~10^{23} atoms that constitute the chair, as a whole? Well, this is the magic effect of rigidity. One of the many successes of quantum field theory is the explanation of the mechanism by which particles gain mass, with spontaneous symmetry breaking and the Higgs mechanism playing a crucial role. Essentially the same basic mechanism of spontaneous symmetry breaking fails spectacularly when it comes to explaining why certain condensed matter systems are rigid (thus being able to sustain an applied deformation without falling apart), whereas others are not.

The spontaneous symmetry breaking and Goldstone theorem explain that a system of many particles becomes rigid when its ground state violates (breaks) a continuous symmetry of the Hamiltonian (i.e., the sum of kinetic and potential energy of the atoms in the body). The prediction is quite successful for crystals: At the freezing transition, a liquid, which is not rigid, crystallizes into a regular array (a crystal lattice) that breaks both translation and rotational invariance. That is, not all translations or rotations bring the crystal lattice back to the original atomic configuration! The breaking of translation-rotation invariance, according to the Goldstone theorem, generates long-wavelength transverse phonons and makes the crystal rigid, with a finite stiffness given by the shear modulus $G>0$. So far, so good.

Take, now, any other form of condensed matter that is rigid but not crystalline. Nearly any other form of matter around us falls into this broad category: glasses, biological cells and tissues, construction materials, sand castles, etc. Disordered materials can be depicted at the atomic level as disordered arrays or random lattices that lack both translational and orientational order, just like liquids. According to field theory and the Goldstone theorem, we therefore expect glasses to lack rigidity, which is totally at odds with evidence. What is then the microscopic mechanism that grants rigidity to glasses, gels, cells, tissues, and our own human body, in the last instance? This is one of the deepest unsolved mystery in condensed matter physics.

We are investigating this problem using a theoretical tool called nonaffine response theory [1], which allows us to build an atomic theory of elasticity for disordered lattices. In collaboration with experimental physicists at the van der Waals-Zeeman Institute, University of Amsterdam, we recently studied the deformation of glasses as a function of the deformation amplitude (the applied strain). We discovered a remarkably sharp symmetry change right at the critical strain where the rigidity of the glass vanishes all at once, and the system turns into a liquid. The remarkable rotational symmetry detected in the strained glass before it loses rigidity vanishes abruptly (as in first-order phase transitions) at the yielding point. This rotational symmetry is not the result of a spontaneous symmetry-breaking process, but rather of a field-induced symmetry breaking. While the Goldstone theorem holds also for certain field-induced symmetry-breaking processes, further investigations are under way in our lab to reach a conclusive mechanistic clarification of this phenomenon in the frame of field theory.



1 | Schematic illustration of local atomic displacements in a disordered material (e.g., glass) under an externally applied shear deformation.

We are also working on technological applications such as metallic glasses, which are now among the most intensively investigated advanced materials in view of their impressive toughness. In this area, we applied our atomic theory of elasticity of disordered lattices to successfully describe the nonlinear deformation behavior and mechanical failure of complex metallic alloys, with a distinctive stress-strain overshoot we can trace back to the atomic-level structural disorder. These results were published in October 2014 as a Rapid Communication in the Physical Review [4].

Other activities in our theory and simulations lab are concerned with outstanding problems in condensed matter physics that overlap with biophysics and physical chemistry. For example, we are working to elucidate the anomalous vibrational spectrum and thermal properties of disordered systems, using the tools of modern random matrix theory. The big unsolved question here is about the origin of a strong peak in the acoustic phonon spectrum of glasses, an issue probably related to the breakdown of continuum elasticity at the atomic scale. This anomaly, in turn, is thought to be responsible for the anomalous specific heat of glasses at low temperatures, which vanishes with a linear ~T law upon reaching T=0, instead of the $\sim T^3$ law predicted by continuum theories (such as Debye's theory). We expect to show new intriguing developments on this topic in 2015.

In other projects, we are developing a unifying framework to achieve a bottom-up description of (bio) molecular and nanoparticle self-assembly processes, to link the level of intermolecular and solvent-solute interactions to the morphology of large-scale structures (typically clusters or aggregates that may reach macroscopic sizes or even form a three-dimensional network [3]). A key project, in collaboration with experimental groups at the University of Cambridge and the University of Copenhagen, is focused on amyloid protein aggregation [2] and the role of co-solvents (e.g., alcohols in water) to change the aggregation propensity in the context of finding new therapies for neurodegenerative diseases (e.g., Alzheimer's disease).

In yet another another project, we are providing theoretical and modelling support to the Chair of Soft Matter and Functional Materials in the Physics Department of TUM, where the self-assembly of smart polymers such as PNIPAM (which start to aggregate in water only above a critical temperature) is investigated experimentally using neutron scattering techniques at the nearby Maier-Leibnitz reactor. These smart self-assembling systems could have broad applications in drug delivery, defense, and new materials for sustainable energy.

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Publications by this Focus Group can also be found on page 154.

Alessio Zaccone (b. 1981) studied at Politecnico di Torino and completed his MSc thesis at Technische Universität Berlin. After obtaining a PhD in chemical physics at ETH Zurich (Department of Chemistry and Applied Biosciences), he worked as a postdoctoral researcher and as an Oppenheimer Research Fellow in physics at the Cavendish Laboratory, University of Cambridge. Since 2014, Alessio Zaccone has been a Rudolf Mößbauer Tenure Track Professor at TUM.

Communication and Information

Fiber-Optic Communication and Information Theory

Dr. René-Jean Essiambre | Bell Laboratories Alcatel-Lucent, USA
Prof. Frank Kschischang | University of Toronto, Canada
Prof. Gerhard Kramer | Communications Engineering, TUM

See the interview on page 54

New in this Research Area

Exploiting Antenna Arrays for Next Generation Wireless Communications Systems

Prof. A. Lee Swindlehurst | University of California, Irvine, USA
Prof. Josef A. Nossek | Circuit Theory and Signal Processing, TUM,
Prof. Wolfgang Utschick | Signal Processing Methods, TUM

Information, Interaction and Mechanism Design

Prof. Dirk Bergemann | Yale University, USA
Prof. Martin Bichler, Prof. Felix Brandt | Decision Sciences and Systems, TUM

Control Theory, Systems Engineering and Robotics

New in this Research Area

Networked Cyber-Physical Systems
Prof. John S. Baras | University of Maryland, USA
◎ Prof. Sandra Hirche | Information-Oriented Control, TUM

Prof. Angelika Peer (University of the West of England) | Carl von Linde Junior Fellow
Prof. Martin Buss, Automatic Control Engineering, TUM

Angelika Peer

Haptic interaction and collaboration in human-human and human-robot dyads

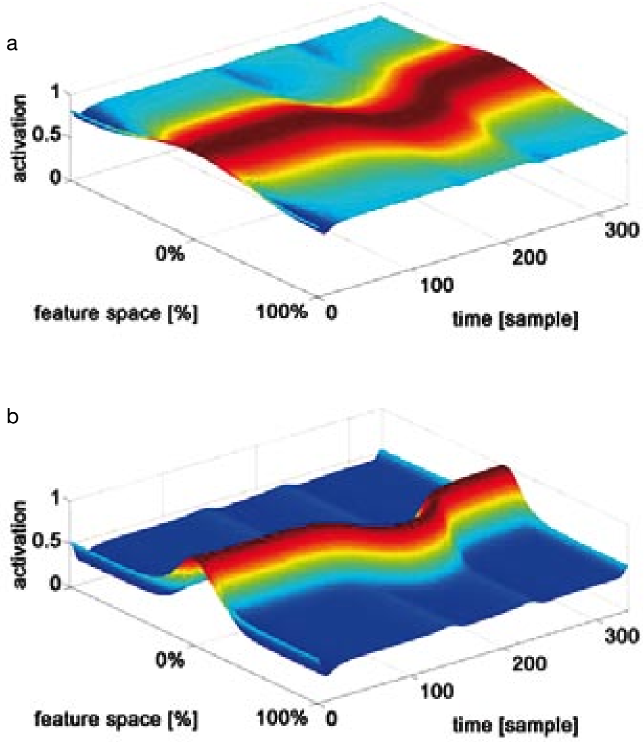
Touch is an indispensable component of interaction in real and virtual collaborative environments. Compared to other fields of interaction research such as communication via speech and gestures, haptic interaction is still largely underrepresented. Doubtlessly, however, haptic interaction is an essential component for future robotic systems that are supposed to collaborate closely with humans in performing physical tasks as required, for example when assisting elderly persons in standing up, walking and sitting down, or when enhancing motor training and rehabilitation.

In such situations, people are not only expected to interact, but to collaborate, which means that both partners try to accomplish a common goal and therefore share intentions and action plans. Thus, haptic collaboration not only implies the physical coupling of two bodies either directly or via an intermediate object, but also involves higher-level cognitive processes. The underlying principles of these processes, however, are largely unknown, which makes their implementation on a robotic platform challenging.

To gain better insight into processes involved in intention recognition and decision making, we have made a series of recordings of human-human dyads. This involved the recording of pairs of healthy subjects in typical decision-making situations, as well as the recording of more complicated situations capturing the interaction of a caregiver and an elderly person in situations such as standing up, walking and sitting down. We also undertook first attempts at modelling decision-making processes by investigating the Win-Stay-Lose Switch Rule and the Drift-Diffusion model first introduced in cognitive science. Both models were analyzed for their capability of modeling haptic interaction in human-human dyads and finally were also implemented on a robotic platform to mimic human-like haptic assistance behaviour [1].

Alumni Members

Prof. Kolja Kühnlenz (Coburg University of Applied Sciences and Arts) | Carl von Linde Junior Fellow
Dr. Georg von Wichert (Siemens AG) | Rudolf Diesel Industry Fellow
Prof. Dirk Wollherr (TUM) | Carl von Linde Junior Fellow
Dr. Ziyuan Liu | Doctoral Candidate



1 | Example preshape adapted with a kernel having a) almost no confidence and b) some confidence

While these first models can capture basic human intention-recognition and decision-making rules, over the last year we developed a more complex cognitive decision-making framework formulated as dynamical model that enforces concepts of embodied embedded cognition – where intelligent behavior is a product of interaction between the agent's body and cognitive abilities and the environment that he is situated in – to realize human action recognition. Our future work will concentrate on extending this framework to recognition of plans and intentions, and combining these efforts with human motor control models for internal simulation of human movements as well as the testing of the overall framework in human-robot collaboration scenarios.

Doctoral candidates Mohammad Abu-Alqumsan, Ken Friedl, Milad Geravand and Salih Özgür Ögüz also work in this Focus Group.

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Publications by this Focus Group can also be found on page 155.

Focus Group **Control and Robotics**

Prof. Dongheui Lee (TUM) | Carl von Linde Junior Fellow
Prof. Martin Buss (TUM) | Carl von Linde Senior Fellow
Sang-Ik An | Doctoral Candidate
Automatic Control Engineering, TUM

Control strategies for multiple tasks with priority

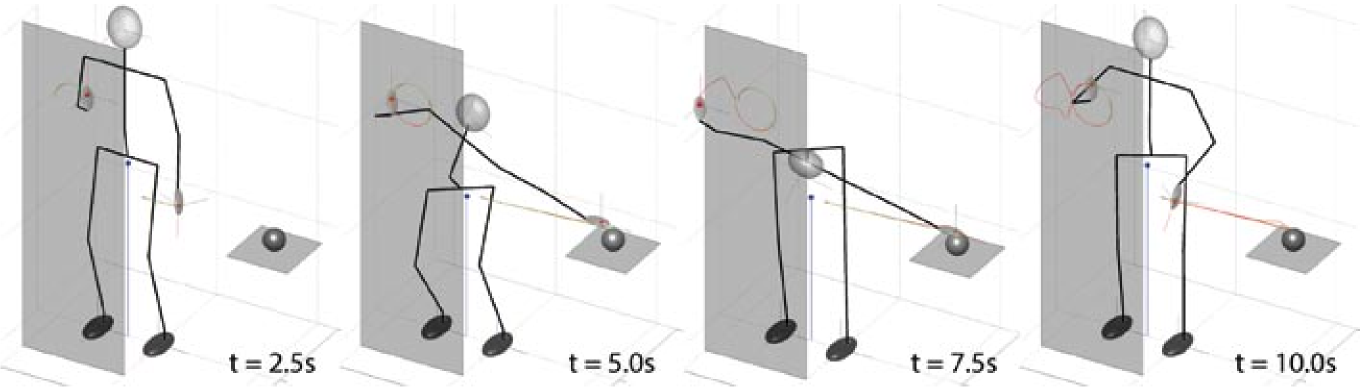
Dongheui Lee

Martin Buss

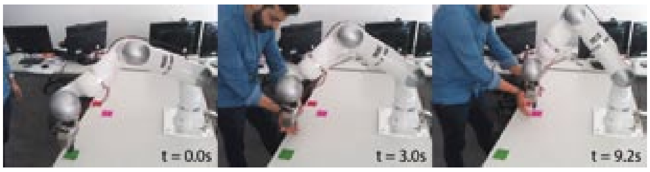
Roboticists have tried to achieve the expectation that robots should be as versatile as, or even more capable than, living creatures. In the last thirty years, many achievements have been made focused on limited areas such as industry, and there are persistent attempts to build general-purpose robots that can be used in more practical cases in daily life. Nowadays, researchers are pushed to think of how living creatures move and learn to move in the natural environment, and to construct computational methods to endow robots with similar control strategies to those observed in life. An important feature of the skills animals, including humans, possess is the ability to perform multiple tasks simultaneously, allowing for efficient and reliable movements in unstructured and unpredictable environments. Consider, for example, how a human can walk up stairs stably while holding a full cup of coffee. In the history of robotics, there have been intensive research activities to develop control methods for multiple tasks with priority; in 2014, we proposed prioritized inverse kinematics algorithms based on QR (quick response) codes and Cholesky decompositions [1]. We are now trying to extend our study to include another important property: that is, the ability to change tasks during operation [2][3]. This sophisticated skill increases the availability of the physical body and also provides the potential ability to learn intelligent behavior.

The motion of a robot is typically generated by tasks that are defined by human operators on the basis of a scenario. Specifically, a task is defined with the task motion that is needed to execute it, and with the forward mapping function that maps robot motions to task motions. If the scenario is complex and contains uncertainty, then the definition of tasks may need to be changed during operation. A typical source of complexity and uncertainty is interaction with a human. The robot has to change currently operating tasks when the human orders something different. Also, the robot must place greater importance on a task for safety when there is higher possibility of physical contact that could harm humans, the environment, or the robot itself; this results in changing priority between tasks during operation. One of the fundamental technologies needed to realize this skill is to find the smooth inverse mapping function that maps multiple definitions of multiple tasks with priority to robot motions: i.e., the robot has to move smoothly with discrete transitions of the definition of prioritized tasks. Several conventional approaches that interpolate task trajectories to generate smooth robot motions suffered from inherited weaknesses in complexity, stability, and generalization.

To tackle this problem, we first introduced a mathematical description of multiple task definitions that provides an efficient and definite way to show unprioritized and prioritized accumulations of tasks. Then we proposed a method called task transition control for the smooth, arbitrary, and consecutive transitions between all task definitions. The basic idea is to interpolate joint trajectories instead of task trajectories using the barycentric coordinates and the linear dynamic system. The proposed method is simple, direct, and general and also assures the boundedness of the robot's motions. Furthermore, we showed that the joint space representations of the conventional methods are special forms of our proposal. The effectiveness of the proposed method has been successfully tested by kinematic simulation with the 32-degrees-of-freedom (DOF) humanoid robot and a real experiment with the 7-DOF manipulator, KUKA LWR.



1 | The humanoid robot executes multiple prioritized tasks: 1) maintaining balance, 2) drawing a circle on the wall with the right hand, and 3) taking an object on the table with the left hand. At 5.0 second, the left hand cannot move further to the object because of higher-priority tasks, so priority of the left hand is switched with the right hand; then the left hand can reach the object while the right hand leaves the original task trajectory. Later on, the robot recovers the lost DOFs when the left hand moves to the initial location and the right hand can come back to the original trajectory.



2 | Initially, the manipulator is following the original end-effector trajectory that moves from the green marker to the red marker. From 3.0 second, the human operator pushes the end-effector to modify the destination of the original trajectory to the magenta marker; then the task for the physical human interaction is inserted as the higher-priority task over the end-effector control and the robot changes the original trajectory as intended.

Introduction to the new Focus Group "Control and Robotics"

Having been a member of the Focus Group Cognitive Technology, which is now an Alumni Focus Group, Prof. Dongheui Lee joined newly appointed Carl von Linde Senior Fellow Prof. Martin Buss in the new Focus Group "Control and Robotics" in 2014. The research team of the ERC Advanced Grant "Seamless Human-Robot Interaction in Dynamically Changing Environments" (SHRINE) also joined the Focus Group. Its main research interests are control in human-machine systems, automation, and advanced robotics for the benefit of academia, industry, and society.

Selected Publications

[1] S. An and D. Lee, "Prioritized inverse kinematics using QR and Cholesky decompositions," in *2014 IEEE International Conference on Robotics and Automation (ICRA)*, 2014, pp. 5062–5069.

[2] S. An and D. Lee, "Prioritized inverse kinematics with multiple task definitions," in *IEEE International Conference on Robotics and Automation (ICRA)*, 2015, accepted.

[3] M. Saveriano, S. An, and D. Lee, "Incremental kinesthetic teaching of end-effector and null-space motion primitives," *IEEE International Conference on Robotics and Automation, 2015*, accepted.

Publications by this Focus Group can also be found on page 155.

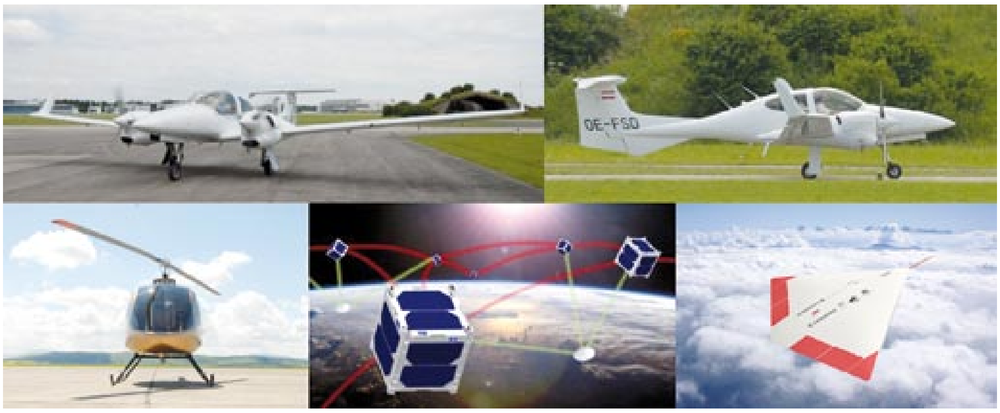
Martin Buss studied electrical engineering at TH Darmstadt and was awarded a doctorate at the University of Tokyo (1994). In 2000, he completed his lecturer qualification at TUM and was appointed to the Chair of Control Systems at TU Berlin. He has been a professor at TUM in the Chair of Automatic Control Engineering full professor of control technology at TUM since 2003. In 2014, he became a fellow of the Institute of Electrical and Electronics Engineers (IEEE). Martin Buss researches methods in control and system theory, in particular hybrid (discrete/continuous), switching, nonlinear dynamic systems for use in mechatronics, robotics, medical technology, communication technology, telepresence systems, teleaction systems and man-machine systems.

Focus Group **Safe Adaptive Dependable Aerospace Systems (SADAS)**

Dr. Matthias Heller (Airbus Defence and Space) | Rudolf Diesel Industry Fellow
Prof. Naira Hovakimyan (University of Illinois) | A. v. Humboldt Research Awardee
Prof. Klaus Schilling (University of Würzburg) | Visiting Fellow

The Focus Group Safe Adaptive Dependable Aerospace Systems (SADAS) was established in August 2014 to advance results from the former Focus Groups Aircraft Stability and Control and Diesel Reloaded, and to expand them towards the new topic of multi-vehicle systems (brought in by an ERC Grant). The dedicated project is supported by a research collaboration between TUM, AIRBUS DS, Siemens, Universität Würzburg, and the University of Illinois.

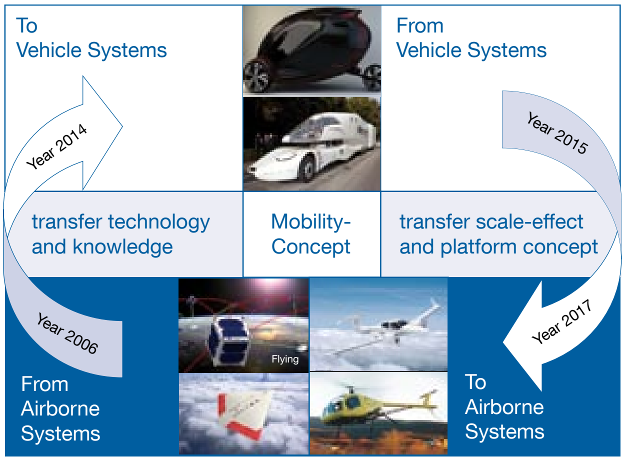
The mission of SADAS is to provide safe, highly reliable and affordable automation for aerospace systems. In aerospace applications, specific challenges relate to extreme systems dynamics and to the highest safety requirements. A key research topic therefore concerns innovative methods enabling adaptive as well as real-time capabilities in order to achieve progress, e.g., with respect to networked formations of vehicles. Within this Focus Group, automation approaches addressing robust, reliable, and affordable solutions at all modular integration levels will be emphasized – ranging from human assistance for a single vehicle to highly automated control of distributed, decentralized, networked, self-organizing multi-vehicle systems. This comprises adaptive control and envelope protection as well as coordinated mission planning strategies. Given the expertise in the team, the application range extends from automobiles to aircraft to space systems. A wide variety of interesting hardware demonstrators are available to assess and exhibit the achieved performance (figure 1).



1 | Available demonstrators of the Focus Group – Flying Testbed DA-42 NG MPP (TUM-FSD); Experimental Rotary Wing Testbed; NetSat: distributed, networked pico-satellites (ERC Advanced Grant); SAGITTA – flying wing UAS (TUM-IAS/FSD)

Progress in vehicle automation has led to application visions, from Google's self-driving cars to Amazon's air vehicle-based fast delivery services. Despite the fact that the first demonstrators are available, there is still significant research to be performed to achieve safe, highly reliable and affordable systems satisfying the rigid requirements that are mandatory in transportation, and particularly in the aerospace business. Techniques for distributed, decentralized and networked control have been applied to different land, water, aerial, and space vehicles to achieve survivable, robust, modular and reconfigurable (multi-)vehicle systems in several precursor research projects (e.g., the SAGITTA demonstrator, figure 3). This Focus Group integrates the different complementary fields of competence in mechanical engineering, aerodynamics, flight system dynamics, control, and embedded computers to achieve innovative results at the aerospace system level in order to bridge the gap between theory and real flight applications.

Prof. Gernot Spiegelberg (Siemens AG) | Rudolf Diesel Industry Fellow
Markus Geiser | Doctoral Candidate
Prof. Florian Holzapfel, Flight System Dynamics, TUM



2 | Research concept: "From Aerospace systems to vehicle systems – and back."

3 | Klaus Schilling (left), Florian Holzapfel (center) and Matthias Heller (right) in front of the SAGITTA demonstrator wind tunnel model at the TUM-IAS General Assembly, April 2014, with guests Steffen Glaser (Organic Chemistry, TUM) and Hauke Stähle (Alumni Focus Group Diesel Reloaded).

Scientific Emphasis and Research Topics

The complementary experiences of the cooperating Focus Group members will enable promising approaches in the dedicated key research topics in order to realize our vision "From aerospace systems to vehicle systems – and back" (figure 2).
Accordingly, the associated research focal points are: stability and performance guarantees for complex coupled highly nonlinear dynamic systems (adaptively stabilizing systems, flight envelope protection, enhanced safety); networked control of distributed vehicle formations; and self-organizing control of the cooperating vehicles. Furthermore, vehicle system topology optimization regarding to communication and data acquisition tasks (e.g., ad hoc networks, measurement coordination, 4D-observations) represents an allied emerging field of research, which the Focus Group SADAS will work and provide contributions.

Selected Publications

[1] S. Braun, M. Geiser, M. Heller, and F. Holzapfel, "Configuration assessment and preliminary control law design for a novel diamond-shaped UAV," in *2014 International Conference on Unmanned Aircraft Systems (ICUAS)*, 2014, pp. 1009–1020.

[2] N. Tekles, F. Holzapfel, E. Xargay, R. Choe, N. Hovakimyan, and I. M. Gregory, "Flight envelope protection for NASA's transport class model," in *AIAA Guidance, Navigation, and Control Conference*, 2014.

[3] C. Wang, L. Drees, and F. Holzapfel, "Incident prediction using subset simulatio," in *29th Congress of the International Council of the Aeronautical Sciences*, 2014.

Publications by this Focus Group can also be found on page 156.

Dr. Matthias Heller is Expert Advisor for Flight Mechanics with Airbus Defence and Space. As a Rudolf Diesel Industry Fellow in the Focus Group Aircraft Stability and Control (2010 – 2013), he investigated new techniques in the field of dynamics, performance, stability and control of innovative unmanned aircraft systems.
Prof. Klaus Schilling, professor for Robotics and Telematics at the University of Würzburg, is a Visiting Fellow and holds an ERC Advanced Grant.
Prof. Gernot Spiegelberg works with Siemens Corporate Technology. As a Rudolf Diesel Industry Fellow, he developed the Diesel Reloaded Innotruck concept with drive-by-wire capability within the associated Focus Group (2010–2013).
Prof. Florian Holzapfel, TUM Flight System Dynamics, hosted the Focus Group Aircraft Stability and Control (2010–2013); now he is hosting the Focus Group Safe Adaptive Dependable Aerospace Systems.
Prof. Naira Hovakimyan is a professor of Mechanical Science and Engineering and an affiliate of Electrical and Computer Engineering as well as Aerospace at the University of Illinois. In 2014, she was selected as Alexander von Humboldt Research Awardee and thus is a Honorary Hans Fischer Senior Fellow of TUM-IAS.

Environmental and Earth Sciences, Building Technology

New in this Research Area

Advanced Construction Chemicals and Materials
Dr. Norman Blank | Sika AG, Switzerland
Prof. Johann Plank | Construction Chemicals, TUM

Environmental Sensing and Modeling
Prof. Jia Chen | Environmental Sensing and Modeling, TUM

Sustainable Water Cycles for Cities of the Future
Prof. Stuart Khan | University of Western Australia
Prof. Jörg Drewes | Urban Water Systems Engineering, TUM

Focus Group **Cradle to Cradle**

Prof. Michael Braungart | EPEA Internationale Umweltforschung GmbH
Martin Korndoerfer, Michiel Kulik | Research Members
Prof. Werner Lang, Energy-Efficient and Sustainable Design and Building, TUM

Michael Braungart

Registry for Cradle to Cradle®-inspired elements in buildings Creating buildings with positive footprints

The Cradle to Cradle® (C2C) workgroup at TUM is currently developing an online platform dedicated to "C2C in the Built Environment: The Registry for Cradle to Cradle-Inspired Elements for Building Developments."

What is Cradle to Cradle®?
In an ideal Cradle to Cradle® world, as in nature, there is no such thing as waste. Industrial systems are using biological and technological nutrient cycles in such a way that the right materials are brought to the right place at the right time.

The aim of the Cradle to Cradle® design concept is to improve the quality of products so that they:

- have an improved consumer quality for the user
- pose no health risk for anyone who comes into contact with them
- are of both economic and ecological benefit.

The Cradle to Cradle® method of production is conceptualized in direct contrast to the "Cradle to Grave" model in which material flows are formed without any conscious consideration of what happens to the resources after their active use period. Rather than attempt to reduce the linear material flows and optimize present-day methods of production, the Cradle to Cradle® design concept envisages their redesign into circular nutrient cycles in which value, once created, remains of worth to both mankind and nature.

Several successful Cradle to Cradle inspired buildings have already been realized, for example the Venlo City Hall and the Netherlands Institute of Ecology (NIOO-KNAW) head office in Wageningen.

Due to the success of Cradle to Cradle®, there are growing demands for a universally accessible and affordable mechanism to celebrate beneficial elements in building developments. Green building standards such as BREEAM, LEED, and DGNB are important but tend to focus more on minimizing negative impacts than on supporting beneficial impacts that add value. The number of buildings awarded those certifications over the past decades has been limited by the associated costs.

The Registry is designed for owners, architects, and other building stakeholders everywhere who would like to have the outstanding positive elements in their buildings recognized in an affordable international forum. The Registry provides stakeholders with a claim to be recognized for beneficial innovation and quality in the marketplace based on quick, easy, and affordable – but also peer-reviewed – evaluation. Stakeholders who are recognized in the program will benefit from more than just an award; they will be participating in the acceleration of best practices for C2C Elements.

http://www.stefanoboeriarchitetti.net

The Registry is an open-source, wiki-style platform for celebrating and continuously improving healthy positive elements of buildings. For example, in the common green building rating methods, a green roof is analyzed meticulously on material usage. The Registry first of all simply discourages or even bans the use of bad materials and focuses on the roof's positive impact to local biodiversity, air purification potential, and water management capacities. The goal is to share great ideas and inspire designers.

Buildings like trees, cities like forests.

Beneficial footprints represent a new approach requiring new rating mechanisms. An independent, university-based but practical review system will evaluate Registry applications. For this the Technische Universität München cooperates with the Dutch universities Rotterdam School of Management, TU Delft, and TU Twente. A qualified jury and a wiki-type peer review will keep claimants honest and ensure a speedy and affordable process.

The main points of an evaluation are based on the three basic Cradle to Cradle® principles:

Everything is a nutrient for something else (waste = food)

- Use healthy materials
- Integrate biological nutrients
- Enhance air quality and indoor climate
- Enhance water quality

Use current solar income

- Integrate renewable energy

Celebrate diversity

- Actively support biodiversity
- Celebrate conceptual diversity with innovation
- Celebrate cultural diversity

Selected Publications

[1] Cradle to Cradle Criteria for the Built Environment – Douglas Mulhall & Michael Braungart, CEO Media 2010. ISBN 978-94-91083-01-3, 2nd Edition revised in Dutch and Swedish in 2012.
[2] Creating Buildings with Positive Impacts – Douglas Mulhall, Michael Braungart & Katja Hansen, TUM 2014. ISBN 978-3-941370-34-0
[3] The Registry of Cradle to Cradle Inspired Elements for Building Developments – Douglas Mulhall, Michael Braungart & Katja Hansen, RSM 2012–2013.

Focus Group **Global Change**

Prof. Annette Menzel (TUM) | Carl von Linde Senior Fellow
Dr. Susanne Jochner | Postdoctoral Researcher
Julia Laube | Doctoral Candidate
Ecoclimatology, TUM

Footprints of global change on plants and human health

Annette Menzel

After roughly a decade of "standstill" in global warming, the year 2014 turned out to be the warmest on record. Global land-surface temperatures from January to December were 1,0°C higher than the 20th century average. In Germany, an overly warm winter (+3.1°C) was followed by a warm spring (+2.4°C), summer (+0.9°C) and autumn (+2.3°C). As in many other parts of Europe, measured temperature anomalies approached the important political benchmark of +2°C. Unsurprisingly, spring phenology significantly advanced in Central Europe from 1982-2011; however, for the last decade of this period in situ observations indicated a less pronounced but still advancing trend for leaf unfolding, whereas remote sensing NDVI series showed a delay [3]. Given the high uncertainties in climate change impacts on the biosphere, the Focus Group Global Change worked on observed as well as on expected responses of plants to several facets of climate change.

With a long-term data set (27 years) from the Island of Guernsey, Anna Bock studied climate change impacts on the first flowering dates of 232 plant species [1]. The study clearly demonstrated advances in first flowering dates that were strongly influenced by increasing temperatures. Moreover, the data set closed knowledge gaps with respect to flowering duration. Unexpectedly, a clear overall shortening of the flowering duration was detected, which seems to be affected by complex interplays of temperature and other climatic drivers. The data set was also used for a detailed analysis of flowering patterns in the Genus Narcissus (daffodils), an important horticultural crop, for which data on 26 differing cultivars were available [2]. Again a strong temperature influence on the overall flowering pattern was identified, however with cultivar-specific differences. In January 2014, Anna Bock successfully completed her doctoral thesis on novel unexploited long-term data sets. Her research resulted in highly valuable insights on climate change impacts on both agricultural and wild plant species.

In a greenhouse experiment in TUM Dürnast greenhouse facilities, Julia Laube tested the responses of three closely related native-invasive species pairs to extreme climatic events, such as frost, drought, and flooding [4]. Despite the overall concern that invasive species might profit from climate change, we showed that the reaction to climatic stresses was highly comparable for both groups of species. However, the results stressed the need to include several developmental stages and levels of competition in experimental settings, since they strongly influenced the absolute stress tolerance.

Susanne Jochner received the German Forestry Award 2014, which is endowed by the Eva Mayr-Stihl-Stiftung every second year, for outstanding research in forest science. Her doctoral thesis comprised the examination of phenological onset dates and pollen properties of silver birch in relation to global (climate) change and air pollution. Susanne Jochner based her studies on urban ecosystems, which are of special interest for forest science and other disciplines since cities that are currently characterized by higher temperatures and stronger air pollution may serve as a proxy for future scenarios.

Alumni Members

Prof. Tim Sparks (Coventry University) | Hans Fischer Senior Fellow
Dr. Nicole Estrella (TUM), Dr. Christian Zang (TUM) | Postdoctoral Researchers
Dr. Anna Bock (State Institute of Bavaria for Forestry and Silviculture / LWF) | Doctoral Candidate

1 | The "Forest Oscar" goes to Dr. Susanne Jochner. Award of the German Forestry Prize 2014 in Dresden.

Ongoing research concentrates on pollen sampling in Munich and in the pre-alpine area around the Environmental Research Station Schneefernerhaus (UFS), and also in Austin, Texas, where allergenic mountain cedar pollen constitutes an enormous health issue in winter months.

In 2015, the Focus Group will continue to study climate change impacts on the biosphere and link activities related to the Carl von Linde Senior Fellowship to current research in the ERC Starting Grant E3 (Extreme Event Ecology). Based on our expertise [6], and given the high interest of the scientific community in our novel approaches in phenological research (e.g., [5] is an ISI highly cited paper, top 1% in environment/ecology), we will continue to study the spring development of trees via climate chamber experiments. Moreover, the Focus Group digitized the largest long-term phenological data set worldwide collected by a single observer, which includes more than 7,000 phenological phases from over 1,000 species for 57 years. We will use these data to contrast species' responses with respect to taxonomic relatedness and species' traits, and to assess ecosystem synchrony and expected mismatch with climate change.

Selected Publications

[1] A. Bock, T. H. Sparks, N. Estrella, N. Jee, A. Casebow, C. Schunk, M. Leuchner, and A. Menzel, "Changes in first flowering dates and flowering duration of 232 plant species on the island of Guernsey," *Glob. Chang. Biol.*, vol. 20, no. 11, pp. 3508–19, Nov. 2014.

[2] A. Bock, T. H. Sparks, N. Estrella, N. Jee, A. Casebow, M. Leuchner, and A. Menzel, "Climate sensitivity and variation in first flowering of 26 Narcissus cultivars," *Int. J. Biometeorol.*, Aug. 2014. doi:10.1007/s00484-014-0885-6.

[3] Y. H. Fu, S. Piao, M. Op de Beeck, N. Cong, H. Zhao, Y. Zhang, A. Menzel, and I. A. Janssens, "Recent spring phenology shifts in western Central Europe based on multiscale observations," *Glob. Ecol. Biogeogr.*, vol. 23, no. 11, pp. 1255–1263, Nov. 2014.

[4] J. Laube, K. Ziegler, T. H. Sparks, N. Estrella, and A. Menzel, "Tolerance of alien plant species to extreme events is comparable to that of their native relatives," Preslia, vol. 87, no. 1, pp. 31-53, Jan. 2015

[5] J. Laube, T. H. Sparks, N. Estrella, J. Höfler, D. P. Ankerst, and A. Menzel, "Chilling outweighs photoperiod in preventing precocious spring development," *Glob. Chang. Biol.*, vol. 20, no. 1, pp. 170–82, Jan. 2014.

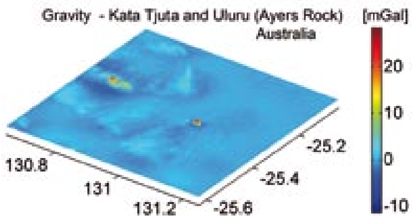
[6] A. Menzel, M. Matiu, and T. H. Sparks, "Twenty years of successful papers in Global Change Biology," *Glob. Chang. Biol.*, vol. 20, no. 12, pp. 3587–90, Dec. 2014.

Publications by this Focus Group can also be found on page 158.

Focus Group **High-Resolution Gravity Modeling**

Dr. Christian Hirt (Curtin University) | Hans Fischer Fellow
Moritz Rexer | Doctoral Candidate
Roland Pail, Institute for Astronomical and Physical Geodesy, TUM

Christian Hirt



1 | ERTM2160 gravity effects over Central Australia (Uluru and Kata Tjuta). The figure shows gravity signals of 10-20 mGal (1 mGal = 10^{-5} m/s^2) associated with the famous Australian monoliths.

High-resolution gravity modeling - Activities 2014

The Focus Group High-Resolution Gravity Modeling, founded in 2013, is concerned with accurate modeling of the Earth's gravity field to ultrahigh resolution. The research goal is the creation of a gravity field model to highest resolution of about 100 to 200 m over land areas of our planet. Accurate information on the gravity field is important for several geoscience and engineering applications. For instance, gravity is a fundamental quantity for precision heighting and topographic mapping with satellite systems. In geophysics, gravity is crucial for making inferences on the location and size of mass-density anomalies, e.g., salt domes or iron-ore bodies. In metrology, gravity is required for the calibration of precision scales.

The research focus is on a) assessment and improvement of modeling methods, b) assessment and combination of data sets (observations of the gravity field and auxiliary data such as topography models carrying information on the gravity field), and c) application of methods and data to create products describing the gravity field to ultrahigh resolution.

In 2014, group activities partially focused on the compilation and evaluation of the newest data sets to describe masses of the visible topography, major water bodies (oceans and lakes), and ice sheets over Antarctica and Greenland. This is necessary in order to have a reliable mass model ready for computing Earth's short-scale gravitational attraction due to the topographic masses. As a highlight, we were able to provide independent evidence that new ice-sheet data provides substantially improved knowledge of Antarctica's bedrock (rock below ice) geometry [1]. The evidence was gained from comparisons between gravity inferred from the new ice-sheet data and gravity observed aboard the GOCE gravimetry satellite. (GOCE was a European Space Agency mission with significant involvement of Focus Group host Roland Pail and Alumnus Carl von Linde Senior Fellow Reiner Rummel.) Given the global scope of the Focus Group High-Resolution Gravity Modeling, the results are immediately relevant for modeling of the gravity field over Antarctica in our future ultrahigh resolution gravity models.

As a second highlight, the group released the first ultrahigh resolution model of the Earth's short-scale gravity field to the public [2]. The model, named ERTM2160, is available via http://geodesy.curtin.edu.au/research/models/ERTM2160/. It describes the high-frequency constituents of Earth's gravity field based on the global SRTM (Shuttle Radar Topography Mission) elevation data set at ~3 billion points across Earth's surface. The spectral bandwidth of ERTM2160 is about 10 to 250 km. Thus it represents many gravity-field signatures associated with hills, valleys, mountains, and other such short-scale topographic features.

Derivation of the ERTM2160 model was based on assumptions of the mass-density of the topographic masses. ERTM2160 can be used to enhance presently available 10km-resolution models of Earth's gravity field at very short spatial scales.

This enhancement effectively increases the resolution by a factor of ~50. Examples of the ERTM2160 gravity field are shown in figure 1 and figure 2. Figure 1 shows the gravitational attraction of the SRTM topographic masses over central Australia (the famous Uluru area), and figure 2 displays the effect on the geoid (i.e., an equipotential surface of the gravity field) over the Mount Everest region (Himalaya Mountains). The ERTM2160 gravity signals (figure 1 and 2) reflect the main features of the topography and can be used to approximate as much as 70-80 % of real gravity signals.

The Focus Group has done further practical work (e.g., compilation of high-resolution topography data, and quality assessment of such data [3]) and theoretical work (e.g., advanced modeling techniques which take into account the ellipsoidal shape of planet Earth, and refinement of spectral approaches [4]). Dr. Sten Claessens (Curtin University, Perth) visited the group in June/July 2014 and contributed to the group's research activities with his expertise in gravity modeling.

Selected Publications

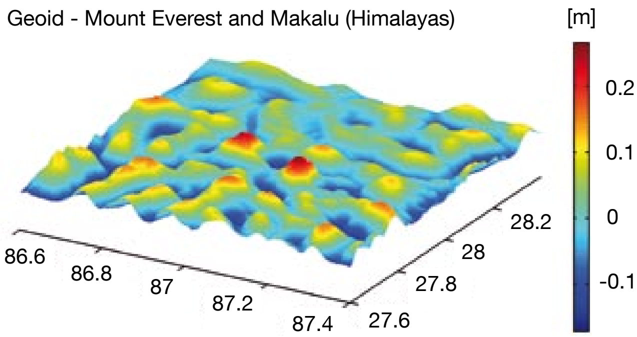
[1] C. Hirt, "GOCE's view below the ice of Antarctica: Satellite gravimetry confirms improvements in Bedmap2 bedrock knowledge," *Geophys. Res. Lett.*, vol. 41, no. 14, pp. 5021–5028, Jul. 2014.

[2] C. Hirt, M. Kuhn, S. Claessens, R. Pail, K. Seitz, and T. Gruber, "Study of the Earth' s short-scale gravity field using the ERTM2160 gravity model," *Comput. Geosci.*, vol. 73, pp. 71–80, Dec. 2014.

[3] M. Rexer and C. Hirt, "Comparison of free high resolution digital elevation data sets (ASTER GDEM2, SRTM v2.1/v4.1) and validation against accurate heights from the Australian National Gravity Database," *Aust. J. Earth Sci.*, vol. 61, no. 2, pp. 213–226, Feb. 2014.

[4] C. Hirt and M. Kuhn, "Band-limited topographic mass distribution generates full-spectrum gravity field: Gravity forward modeling in the spectral and spatial domains revisited," *J. Geophys. Res. Solid Earth*, vol. 119, no. 4, pp. 3646–3661, Apr. 2014.

Publications by this Focus Group can also be found on page 159.



2 | ERTM2160 geoid effects over the Mount Everest region. The short-scale effect on the geoid (as the equipotential surface at mean sea level) is 0.2-0.3 m. If a lake was covering the whole area, the lake's surface would exhibit a 0.2-0.3 m peak over the Mount Everest area, reflecting the gravitational attraction of Earth's tallest mountain.

Christian Hirt is a senior research fellow at Curtin University, Australia, and holds a German Dipl.-Ing. and a Dr.-Ing. degree in Geodesy. His professional appointments include stays at the University of Hanover and HafenCity University Hamburg (as an associate professor). He is responsible for the successful development of a Digital Zenith Camera System, and the development of high-resolution gravity field models for Earth, the Moon, and Mars. He has been involved in the development of regional geoid models for Australia, and New Zealand. Christian Hirt has more than 80 scientific publications in his name (50 of which were peer-reviewed), in most cases as a senior author. Together with others, he is responsible for or made essential contributions in attracting 1.25M AUD worth of research funding. He is chief investigator of a 450,000 AUD Australian Research Council (ARC) Discovery Project on the use of GOCE satellite gravimetry over the Australian region, and recipient of a prestigious ARC Discovery Outstanding Researcher Award (DORA).

Focus Group **Soil Architecture**

Prof. Ingrid Kögel-Knabner (TUM) | Carl von Linde Senior Fellow
Dr. Geertje Pronk | Postdoctoral Researcher
Soil Science, TUM

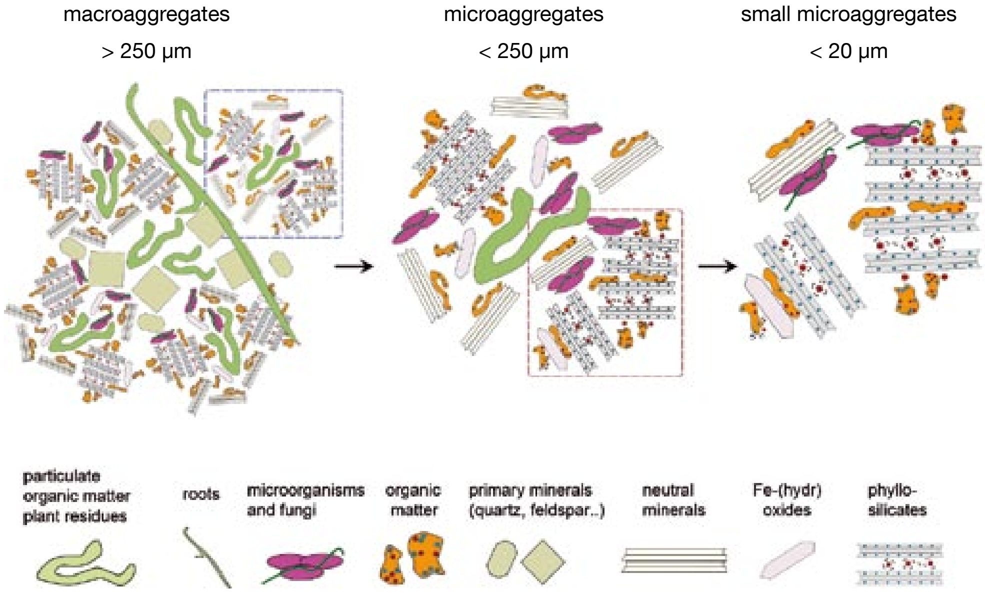
Ingrid Kögel-Knabner

Hierarchically organized aggregate structures produced in artificial soil materials

Aggregates in soils are formed by interactions between, e.g., particulate organic matter, plant residues, roots, microbes and fungi, primary minerals, neutral minerals, metal (Fe, Al, Mn)-(hydr)oxides and phyllosilicates. The number and heterogeneity of different components involved add to the complexity of soils. It is therefore exceedingly difficult to understand the effect of the presence of a particular component within this system, and even more so to gain a mechanistic understanding of the entire soil system. Observations of matured soils and the study of chronosequences in the field provide many valuable insights into soil formation and development over long time scales. However, these studies are limited by the availability of suitable field sites, natural heterogeneity in, e.g., parent material and environmental conditions and uncertainties in the development history. A novel approach is therefore to perform carefully designed laboratory studies with the goal of understanding a specific process under simplified conditions.

The use of model systems has thus been developed by our group as valuable alternatives, as they can be composed from clearly defined materials and can be fitted specifically to answer the respective hypotheses of the studies. We designed a large artificial soil incubation experiment and used extensive interdisciplinary characterization, covering both soil physical and chemical properties and the establishment and functionality of a microbial community, to elucidate the effect of mineral composition and charcoal presence on the formation of biogeochemical interfaces in a soil-like system. We assumed that the three essential ingredients for the formation of a soil-like material are (1) the mineral phase consisting of clay-sized phyllosilicates and/or iron oxides, (2) an organic C source, and (3) a microbial community. With this experiment, we aimed to test if we could simulate the formation of a soil-like material by combining these three components, and if it would lead to the formation of biogeochemical processes and interactions in a way that helps us understand processes in natural soils. Recent studies have shown that iron oxides, phyllosilicates, and charcoal play an important role in soil development and organic matter stabilization due to their large and reactive surface area. The main hypothesis of this experiment was that the development of the artificial soils would be controlled by their mineral composition and by the charcoal present. The artificial soils were composed so that their texture and organic matter content were the same, but they contained different mineral and charcoal surfaces.

For all artificial soil compositions, the percentage of aggregates > 2 mm increased within the first 6 months to 50-70% of total soil mass and remained more or less stable later, except for the soil containing only quartz and ferrihydrite. For this composition, the amount of macroaggregates increased only to 30% of total soil mass after six months. Obviously, the presence of clay minerals is important for the formation of an aggregate hierarchy structure, as in the absence of phyllosilicate clay minerals only low amounts of macroaggregates were formed. Iron oxides seem to play a role in the formation of microaggregates, but the formation of the aggregate hierarchy structure in soils seems to require the presence of both iron oxides and clay minerals.



1 | Understanding soil architecture: illustration of the aggregate hierarchy concept for structured soils.

Consequently, a lack of clay minerals leads to delayed aggregation and organo-mineral formation. Charcoal did not have an additional effect on aggregate formation. All particle size fractions <20 µm exhibited significant differences from their respective bulk soils by an increased ratio of alkyl C to O/N alkyl C as recorded with solid-state ^{13}C NMR spectroscopy. Accordingly, as expected, the organic material in the smaller particle size fractions was more decomposed.

We thus could confirm our hypothesis that the components and types of surfaces present were decisive for the establishment of microbial communities, although they had only small effect on the soil bulk organic matter and structural properties. The overall functionality with respect to CO_2 respiration was similar for all compositions, even though different communities developed depending on the components present. This obviously points to a functional redundancy of the different microbial communities that were observed in the artificial soils with different mineral compositions and has strong implications for understanding the microbial habitat development in soils with respect to biodiversity.

Selected Publications

[1] D. Babin, C. Vogel, S. Zühlke, M. Schloter, G. J. Pronk, K. Heister, M. Spiteller, I. Kögel-Knabner, and K. Smalla, “Soil mineral composition matters: response of microbial communities to phenanthrene and plant litter addition in long-term matured artificial soils,” *PLoS One*, vol. 9, no. 9, p. e106865, Jan. 2014.

[2] S. Filimonova, A. Hilscher, and I. Kögel-Knabner, “Nano-structural and chemical characterization of charred organic matter in a fire-affected Arenosol,” *Geoderma*, vol. 232–234, pp. 538–546, Nov. 2014.

[3] C. Vogel, D. Babin, G. J. Pronk, K. Heister, K. Smalla, and I. Kögel-Knabner, “Establishment of macro-aggregates and organic matter turnover by microbial communities in long-term incubated artificial soils,” *Soil Biol. Biochem.*, vol. 79, pp. 57–67, Dec. 2014.

Publications by this Focus Group can also be found on page 159.

Fundamental Physics

New in this Research Area

Focus Group **Flavour Physics**

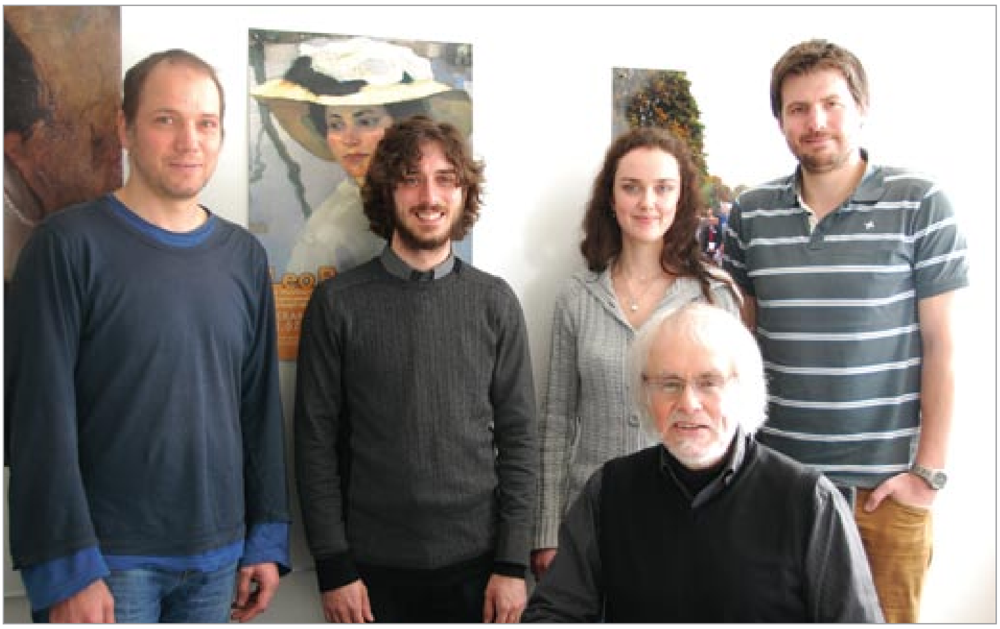
Prof. Andrzej Buras (TUM) | ERC Advanced Grant Awardee
Dr. Christoph Bobeth, Dr. Dario Buttazzo, Dr. Jennifer Girrbach-Noe,
Dr. Robert Knegjens | Postdoctoral Researchers
Institute for Advanced Study, TUM

Flavour physics preparing for the precision era

Elementary particle physics in the rest of this decade and in the next decade is expected to provide a very deep understanding of the fundamental laws of nature. Through the recent discovery of the Higgs particle at the Large Hadron Collider (LHC), the Standard Model (SM) of strong and electroweak interactions is now complete, with the masses of all its particles being below 200 GeV, corresponding to scales above one Attometer (10^{-18} m). According to the SM, in addition to the Higgs particle, six quarks and six leptons form the fundamental building blocks of matter. Aside from gravity, three types of interactions (forces) among the fundamental buildings blocks are present: electromagnetic interactions mediated by the photon, strong interactions mediated by gluons and weak interactions mediated by W and Z.
The discovery of the Higgs particle itself did not provide answers to several outstanding questions, in particular regarding the origin of the matter-antimatter asymmetry observed in the universe, which is essential for our existence. Similarly the observed vast hierarchies in the masses of elementary particles, quarks, and leptons and the hierarchies in their mutual interactions are not explained by this discovery. In order to address such questions, the SM has to be generalized to a more fundamental theory that contains new heavy particles, beyond the known quarks and leptons, and/or new forces beyond the electroweak and strong interactions present in the SM. Unfortunately, until now no convincing signs of new heavy particles and new forces have been seen in high-energy collisions at the LHC, even though this collider already explores distance scales as short as 10^{-19} m. The second run of the LHC, which will begin in 2015, can increase this resolution down to $5*10^{-20}$ m and in this manner will allow us to probe directly the existence of new heavy particles present in nature with masses up to a few TeV, which are expected in many models that aim to solve the outstanding problems of the SM. Yet we cannot exclude the possibility that the lightest new particle in nature is out of the direct reach of the LHC.

Fortunately there exists another route to short distance scales that allows us to search for very heavy particles existing at distance scales beyond the reach of the LHC. It is based on quantum fluctuations that cause very rare phenomena such as very rare decays of mesons and leptons. This approach is not limited by the available energy but only by the precision of both experiment and theory. The coming era of such precision experiments could allow us to get an insight into the dynamics at very short distance scales, possibly reaching the Zeptouniverse (10^{-21} m) corresponding to the energy scales of 200 TeV. This could allow us to construct a new SM, which could be tested by new LHC data. It would also give us an idea about the energy scale required for the next high-energy collider.

In this context our Focus Group has in the last three years performed detailed analyses of various extensions of the SM, identifying patterns of flavour violation and correlations between various observables; these should allow us, with the help of very precise measurements to be performed in the rest of this decade (flavour precision era), to uncover the presence of new forces and new particles with masses as high as 200 Tev or, equivalently, to resolve scales as short as 10^{-21} m.



Group members Christoph Bobeth, Dario Buttazzo, Jennifer Girrbach-Noe, Rob Knegjens, and Andrzej Buras.

In 2011 these activities received strong support from the European Research Council, which for the period 2011–2016 awarded the Advanced Grant (€1.6M) to Andrzej Buras, the leader of the Focus Group. In this context the project "Towards the Construction of the Fundamental Theory of Flavour" is presently executed with participation of first class researchers, in particular Alumni Hans Fischer Senior Fellows Gino Isidori (University of Zurich) and Stefan Pokorski (University of Warsaw), and a number of excellent postdoctoral researchers.

The highlights of our research in 2014 can be summarized as follows:

The second discovery at CERN was the measurement by the LHCb and CMS experiments of the rate for the decay of the B_s meson into a pair of leptons (muons). In 1993 Gerhard Buchalla and Andrzej Buras predicted that this decay would be significantly suppressed within the SM: only one in every 300 million B_s mesons produced by these experiments was expected to decay to a pair of muons. This result has been confirmed by both experiments, which find the probability (1 corresponding to 100%) for this decay to be (2.8+-0.7) 10^{-9}. In spite of this agreement some departures from SM predictions are still possible. Therefore in [1,2] a new more accurate prediction for this decay within the SM has been performed reaching the result (3.6+-0.2)10^{-9}. This is still consistent with the present experiment but could indicate the presence of new heavy particles, which through quantum fluctuations suppress this decay even more strongly than predicted within the SM. It has been shown in [3–4] that there are new physics models that can provide this suppression. Another highlight from CERN was the observation of departures from the SM in the transitions $B \rightarrow K'\mu^+\mu^-$. These departures have been analyzed in various extensions of the SM in [3–5].

The implications of the LHC on flavour physics and flavour symmetry has been analyzed in detail in [6]. On the other hand, in [7] it has been demonstrated that indeed rare B meson and K meson decays could in the future give us an insight into the dynamics at short distance scales corresponding to hundreds of TeV, well beyond the reach of the LHC. Such aspects have also been discussed in a long review [8], which outlined a 12-step program for searching for new particles and forces in the second half of this decade when the flavour precision era will be more advanced.

Twenty-eight years ago Andrzej Buras, in collaboration with William Bardeen (Fermilab, USA) and Jean-Marc Gerard (Leuven, Belgium) explained analytically the so-called $\Delta I = 1/2$ rule (a puzzle since 1955), using a large N approach to quantum chromodynamics (QCD), the theory of strong interactions (N refers to the number of colors in QCD). They calculated with this method various parameters relevant for flavour physics. Most of these results have been confirmed recently by numerical lattice methods. This gave the motivation to improve the accuracy of the 1986 calculations [9] and to investigate in [10] whether with improved accuracy new physics could also contribute to this issue. New heavy gauge bosons, still in the reach of the LHC, could indeed help, and it is exciting to see whether such gauge bosons, responsible for new forces, will be found when the LHC energy will be increased in 2015.

Selected Publications

[1] C. Bobeth, M. Gorbahn, and E. Stamou, "Electroweak corrections to $B_{s,d} \to l^+l^-$," *Phys. Rev. D*, vol. 89, no. 3, p. 34023, Feb. 2014.

[2] C. Bobeth, M. Gorbahn, T. Hermann, M. Misiak, E. Stamou, and M. Steinhauser, "$B_{s,d} \to l^+l^-$ in the standard model with reduced theoretical uncertainty," *Phys. Rev. Lett.*, vol. 112, no. 10, p. 101801, Mar. 2014.

[3] A. J. Buras, F. De Fazio, and J. Girrbach, "331 models facing new $b \to s\mu^+\mu^-$ data," *J. High Energy Phys.*, vol. 2014, no. 2, p. 112, Feb. 2014.

[4] A. J. Buras, F. De Fazio, and J. Girrbach-Noe, "Z-Z' mixing and Z-mediated FCNCs in $SU(3)_C \times SU(3)_L \times U(1)_X$ models," *J. High Energy Phys.*, vol. 2014, no. 8, p. 39, Aug. 2014.

[5] F. Beaujean, C. Bobeth, and D. van Dyk, "Comprehensive Bayesian analysis of rare (semi)leptonic and radiative B decays," *Eur. Phys. J. C*, vol. 74, no. 6, p. 2897, Jun. 2014.

[6] R. Barbieri, D. Buttazzo, F. Sala, and D. M. Straub, "Flavour physics and flavour symmetries after the first LHC phase," *J. High Energy Phys.*, vol. 2014, no. 05, p. 105, May 2014.

[7] A. J. Buras, D. Buttazzo, J. Girrbach-Noe, and R. Knegjens, "Can we reach the Zeptouniverse with rare K and $B_{s,d}$ decays?," *J. High Energy Phys.*, vol. 2014, no. 11, p. 121, Nov. 2014.

[8] A. J. Buras and J. Girrbach, "Towards the identification of new physics through quark flavour violating processes," *Reports Prog. Phys.*, vol. 77, no. 8, p. 86201, Aug. 2014.

[9] A. J. Buras, J.-M. Gérard, and W. A. Bardeen, "Large N approach to Kaon decays and mixing 28 years later: $\Delta I = 1/2$ rule, $\hat{B}_K$ and ΔM_K," *Eur. Phys. J. C*, vol. 74, no. 5, p. 2871, May 2014.

[10] A. J. Buras, F. De Fazio, and J. Girrbach, "ΔI=1/2 Rule, ε'/ε and $K \to \pi\nu\bar{\nu}$ in Z'(Z) and G' Models with FCNC Quark Couplings," *Eur. Phys. J. C.*, vol. 74, no. 7, p. 63, Apr. 2014.

Publications by this Focus Group can also be found on page 160.


500

Surface, Interface, Nano- and Quantum Science

New in this Research Area

Focus Group **Electrochemical Interfaces in Batteries**

Dr. Peter Lamp (BMW Group) | Rudolf Diesel Industry Fellow
Roland Jung | Doctoral Candidate
Prof. Hubert A. Gasteiger, Technical Electrochemistry, TUM

Peter Lamp

Participants of the Munich Battery Discussions 2014: “Reliable High Energy Materials - Perspectives for Future Energy Storage”

The large-scale commercialization of electric and hybrid vehicles will depend on the ability to improve battery characteristics such as energy and power density, safety, lifetime, and cost. The loss of capacity and the increase of internal resistance over battery life are the main phenomena that reduce the lifetime of battery cells. Both phenomena originate from a large number of simultaneous physico-chemical processes that occur under both battery storage and working conditions. The majority of these degradation processes involve chemical interactions taking place at the interface between the solid electrodes and the liquid electrolyte.
The research activity of this Focus Group is dedicated to the investigation of one of the most critical degradation mechanisms: the dissolution of transition metals from the cathode (typically a transition metal oxide or transition metal phosphate) into the electrolyte (typically a solution of a lithium-containing salt, such as $LiPF_6$, in an organic solvent). The transition metal dissolution is an intricate process that depends on several causes, including phase transitions in the cathode material and corrosion from electrolyte contaminants, hydrofluoric acid (HF) in particular. Transition metal dissolution not only causes loss of active material at the cathode side but also contributes to the increase of cell resistance via formation of insulating layers on the cathode particles. Moreover, the subsequent deposition of the transition metal at the anode will impair the anode stability through the disruption of the anodic surface protective layer.

The research activity started at the beginning of December 2014 after Roland Jung joined as a doctoral candidate. In 2015 we will start to investigate transition metal dissolution for those cathode materials that are considered the most serious candidates for the future generation of lithium batteries for automotive applications. These include high-voltage cathodes, for instance cobalt olivine $LiCoPO_4$, as well as high-capacity ones, including nickel-rich layered oxides $Li(Ni_{1-X-Y}Co_XMn_Y)O_2)$. The effect of water contamination, additive concentration, positive potential, and temperature will be considered using a combined electrochemical, chemical, and spectroscopic approach taking advantage of both *ex-situ* and *in-situ* techniques.

Munich Battery Discussions

Peter Lamp co-organized, together with his group at BMW and the TUM-IAS, the 2nd annual Munich Battery Discussions, March 17–18, 2014. This is an international conference dedicated to the hottest topics in the field of research and development of future battery materials and systems. After a 2013 conference dedicated to “Lifetime and Ageing of Battery Materials and Systems,” this year the topic of the conference was “Reliable High Energy Materials – Perspectives for Future Energy Storage.” Sixteen speakers from European, North American, and Asian universities and research centers presented their latest results on materials and design development toward high-energy and high-power battery propulsion systems for a viable large-scale automotive market. A selected audience of around 140 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.

This year, we also started a 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 2014 we had three presentations dedicated respectively to solid-state electrolytes, high-energy conversion cathodes, and novel approaches to safely exploit high-capacity metal lithium anodes.

Peter Lamp received his MSc in physics from TUM in 1989. In 1993, he obtained his PhD in general physics. His PhD thesis “Investigation of photoelectric injection of electrons in liquid argon” was prepared at the Max Planck Institute for Physics, Munich. Between 1994 and 2000 he was group leader at the Department of Energy Conversion and Storage of the Bayerischen Zentrum für angewandte Energieforschung (ZAE) in Garching. After a short period as project leader for fuel cell systems at Webasto Thermo Systems International GmbH, he joined BMW AG in 2001 as a development engineer for fuel cell systems. Since 2004 he has been leader of the “Technology and Concepts Electric Energy Storage” group and, since 2012, of the “Battery Technology” department at BMW.

Focus Group **Functional Interfaces**

Prof. Matthias Batzill (University of South Florida) | Hans Fischer Fellow
Yuanqin He | Doctoral Candidate
Prof. Johannes Barth, Molecular Nanoscience and Chemical Physics of Interfaces, TUM

Matthias Batzill

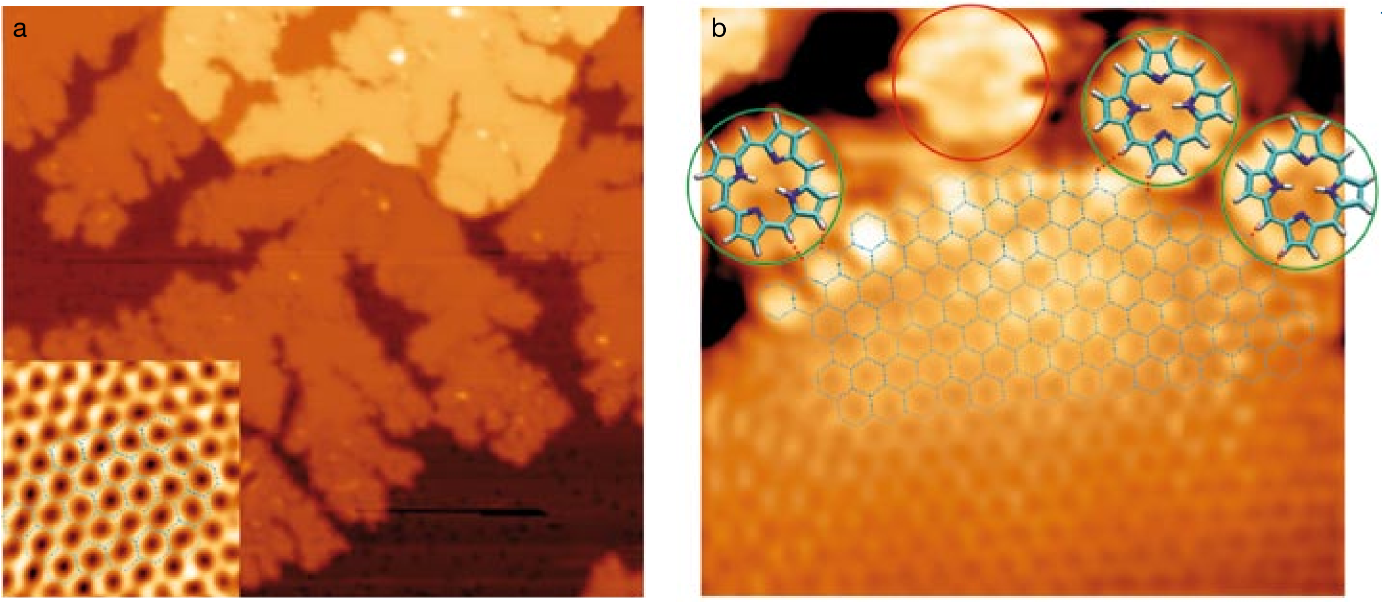
Symposium: Interfaces of two-dimensional materials – graphene and beyond

In May 2014 the Focus Group held the kick-off symposium for Hans Fischer Fellow Matthias Batzill. The topic of this stimulating event was "Interfaces of Two-Dimensional Materials: Graphene and Beyond." The audience comprised TUM researchers from the Physics and Chemistry Departments, including members of the Catalysis Research Center and the Walter Schottky Institute. As a guest, Thomas Michely (University of Cologne) gave an impressive presentation on fundamental studies of new graphene-based compound materials.

Graphene-porphyrin heterostructures:

A main goal for the project is to functionalize graphene with molecular modules and to atomistically investigate the properties of the resulting materials. Graphene/organic heterostructures have a wide spectrum of potential applications ranging from drug delivery vehicles to nanoelectronic or catalytically active hybrids and energy harvesting. In the latter, we envision charge separation of photoexcited chromophores attached to graphene, which exhibits a high electron affinity. In addition, the high electron mobility of graphene may enable electron conduction to chemically active sites. This scheme would effectively spatially separate photooxidation and reduction reactions and thus to some extent mimic photosynthesis in plants. The main challenge we are currently addressing is to understand how to combine different components providing specific functions into a complex molecular architecture. Our approach notably employs surfaces and sheet materials as platforms on which molecules self-assemble. This method also enables us to monitor these processes and to directly study functional properties using advanced scanning probe microscopy techniques.

2014 was the first year of this project and thus we are in the initial stages of optimizing new instrumentation and growth conditions for graphene. Important work done by Yuanqin He, the main doctoral candidate on this project, was setting up the qPlus-sensor atomic force microscope and exploring the preparation of graphene model systems to study attachment of porphyrins to graphene edges. Graphene is directly grown on a metal support in vacuum. The substrate of choice is Ag(111) because recent studies confirmed the extremely weak interaction between the close-packed silver surface and graphene. An important factor is that the graphene edges remain free; i.e., they do not laterally attach to Ag atomic steps, and this enables us to anchor porphyrin or other molecules at the carbon edge atoms. First results, shown in figure 1 (a), illustrate our successful growth of graphene islands by direct evaporation of C atoms. Subsequent deposition of porphines under the right conditions showed that these molecules indeed decorate the free graphene edges, thus forming a lateral heterostructure between graphene and the tetrapyrrole units; cf. data shown in figure 1(b). These results are a first demonstration of the proof of concept of surface-assisted assembly of such large covalently bonded structures to graphene edges. For applications, control over the size of the graphene "islands" or the embedding of porphine units in the graphene layer would be desirable, and this will be one direction for future experiments.



1 | Scanning tunneling microscopy characterization of porphyrin-functionalized graphene edges. (a) Graphene grown on a silver substrate by carbon-vapor deposition (the inset shows an atomic-resolution image of the graphene honeycomb structure). (b) Single porphyrin molecules attached to the graphene edge. The porphyrin molecular structure and the graphene honeycomb lattice are superimposed on the experimental data. While three of the porphyrin molecules (green circles) are stable, indicating their covalent linking to the graphene edge, one porphyrin molecule (red circle) is mobile and appears "fuzzy," suggesting surface mobility and weak non-covalent lateral interactions.

◯ stable, covalently bonded

◯ movable, not covalently bonded

It will be important, especially for energy harvesting, to understand the interface electronic structure between organic macromolecules and graphene. This can be probed by scanning tunneling spectroscopy in our experimental set-up and will be supported by computational modeling using density functional theory.

Selected Publications

[1] J. Li, S. Wieghold, M. A. Öner, P. Simon, M. V. Hauf, E. Margapoti, J. A. Garrido, F. Esch, C.-A. Palma, J. V. Barth, "Three-dimensional bicomponent supramolecular nanoporous self-assembly on a hybrid all-carbon atomically flat and transparent platform," *Nano Lett.*, vol. 14, no. 8, pp. 4486–4492, Aug. 2014.

[2] H. Coy Diaz, J. Avila, C. Chen, R. Addou, M. C. Asensio, and M. Batzill, "Direct observation of interlayer hybridization and dirac relativistic carriers in graphene/MoS_2 van der Waals heterostructures," *Nano Lett.*, vol. 15, no. 2, pp. 1135–1140, Jan. 2015.

[3] A. Dahal and M. Batzill, "Graphene-nickel interfaces: a review," *Nanoscale*, vol. 6, no. 5, pp. 2548–62, Mar. 2014.

Matthias Batzill is currently a tenured associate professor of Physics at the University of South Florida (USF) in Tampa, USA. He received his Diploma degree in physics from the University of Göttingen in 1996 and his PhD from the University of Newcastle, UK, in 2000. After two postdocs at the University of Southern California in Los Angeles and Tulane University in New Orleans, he joined the faculty of USF in 2006. His current research interests are mainly in oxide surfaces, photocatalysis, and materials science of graphene and other 2D materials. His research has been supported by the National Science Foundation, Department of Energy, and the Office of Naval Research in the USA. His over 80 peer-reviewed articles received 680 citations in 2013 alone.

Publications by this Focus Group can also be found on page 161.

Focus Group **Metal-Organic Superlattices of Quantum Magnets**

Prof. Harald Brune (EPFL) | Hans Fischer Senior Fellow
Raphael Hellwig, Georg Michelitsch | Doctoral Candidates

Harald Brune

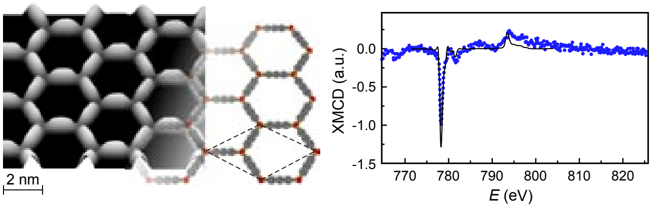
Metal-Organic Superlattices of Quantum Magnets

Low-dimensional magnets are of interest for ultrahigh-density data storage and as bits in quantum computers. In order to be useful, these magnets have to be adsorbed at surfaces. These surfaces can for instance be the electrodes, accessing and influencing their magnetic state. Significant progress has been made in the understanding and control of the magnetic properties of single-ion magnetic molecules and of individual magnetic atoms adsorbed onto surfaces [1]. The present project aims at the equidistant creation of such magnets. The approach is the self-assembly of well-ordered metal-organic networks at surfaces [2]. One doctoral candidate (Raphael Hellwig) explores the assembly with scanning tunneling microscopy (STM) and will investigate the magnetic properties with X-ray magnetic absorption spectroscopy. The second doctoral candidate (Georg Michelitsch) works on density functional theory methods describing the X-ray absorption and the magnetic properties of the metal atoms and clusters linked to organic molecules. The project started with a kick-off meeting held at the TUM-IAS on November 7, 2013, notably featuring several recognized external speakers (J. R. Galan-Mascaros, ICIQ, Taragona, Spain; W. Kuch, Freie Universität Berlin; and N. Atodiresei, Forschungszentrum Jülich) and a series of internal oral and poster contributions.

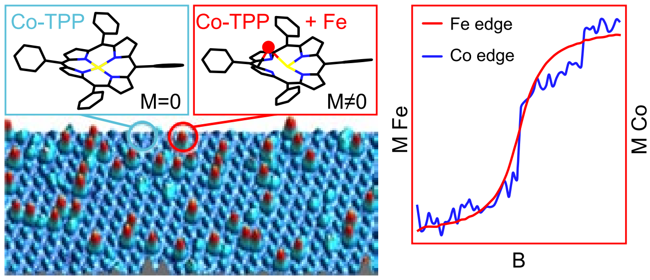
Figure 1 shows a well-ordered superlattice formed by the co-adsorption of dicarbonitrilepolyphenyl molecules and Co atoms on an Ag(111) surface. One sees that the Co atoms form the coordination nodes with three molecules producing a honeycomb open network structure. The magnetic properties are accessed by synchrotron measurements, where Co core electrons are excited into the conduction band formed by the hybridization between Co atom and surface. If the synchrotron radiation is polarized, only transitions between certain spin orientations can take place, thus giving magnetic sensitivity. The difference between the absorption for left and right circularly polarized X-rays is called X-ray magnetic circular dichroism (XMCD); it is shown as blue dots together with a theoretical calculation of the signal expected for the magnetic ground state and crystal field environment of the Co atom [1]. The spectra are very narrow, showing that only a single Co species is present and thus confirming the excellent order in the superlattice. In addition, this proves that there is little hybridization of the Co and substrate electronic states. The atoms have their magnetization oriented out-of-plane and possess appreciable magnetic moments. However, they are paramagnetic and thus have only short spin-relaxation times.

Figure 2 shows one example where a network of metal-organic species has been achieved by adsorbing entire metal-organic molecules. Co-porphyrin (Co-TPP) forms a well-ordered square lattice on Ag(111). It was quite surprising when we found that the Co magnetic moment is entirely quenched by the interaction with the surface. However, deposition of Fe, which decorates specific sites close to the Co atoms in an unusual coordination geometry elucidated by computational modeling, restores the magnetic moments of the Co atoms. In addition, the Fe atoms themselves carry a moment that is ferromagnetically aligned with the one of Co [3].

Prof. Johannes Barth, Molecular Nanoscience and Chemical Physics on Interfaces, TUM
Prof. Karsten Reuter, Theoretical Chemistry, TUM



1 | STM image and structure model of metal-organic network on an Ag(111) surface. The organic species are dicarbonitrile-polyphenyl molecules, and the metal coordination nodes are Co atoms. The magnetic properties are studied with X-ray magnetic absorption spectroscopy at low temperature and high magnetic fields. The out-of-plane XMCD spectrum shows sharp features of the atoms, indicating little substrate hybridization (T = 6 K, B = 6 T).



2 | STM image of self-assembled Co-TPP superlattice on a Ag(111) surface. The red protrusions are Fe atoms that site-selectively adsorb close to the Co sites of the complexes. The element-specific magnetization curves have been recorded with XMCD and show that Fe and Co have their magnetization ferromagnetically aligned. Both atoms are paramagnetic and exhibit out-of-plane easy magnetization direction (T = 8 K) [3].

Again, the spin-relaxation times are short, and the magnetization changes fully reversibly as seen in the out-of-plane magnetization curves of both elements shown on the right side. The next steps will be to find systems that are equally well ordered but exhibit long spin relaxation and/or spin coherence times.

Selected Publications

[1] I. G. Rau, S. Baumann, S. Rusponi, F. Donati, S. Stepanow, L. Gragnaniello, J. Dreiser, C. Piamonteze, F. Nolting, S. Gangopadhyay, O. R. Albertini, R. M. Macfarlane, C. P. Lutz, B. A. Jones, P. Gambardella, A. J. Heinrich, and H. Brune, "Reaching the magnetic anisotropy limit of a 3d metal atom," *Science*, vol. 344, no. 6187, pp. 988–92, May 2014.

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[2] W. Auwärter, D. Ecija, F. Klappenberger, and J. V. Barth, "Porphyrins at interfaces,“ *Nat. Chem.*, vol. 7, no. 2, pp. 105–120, Jan. 2015.

[3] S. Vijayaraghavan, W. Auwärter, D. Écija, K. Seufert, S. Rusponi, T. Houwaart, P. Sautet, M. L. Bocquet, P. Thakur, S. Stepanow, et al., "Restoring the Co Magnetic Moments at Interfacial Co-Porphyrin Arrays by Site-Selective Uptake of Iron," *ACS Nano*, accepted for publication (2015).

Publications by this Focus Group can also be found on page 161.

Harald Brune is a full professor at the Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland. In 1989, he obtained his Diploma in Physics from the Ludwig-Maximilians Universität München and in 1992 his PhD in Physical Chemistry under the guidance of Gerhard Ertl (2007 Nobel Laureate in Chemistry) and Jürgen Behm at the Fritz Haber Institute of the Max Planck Society in Berlin. He joined the group of Klaus Kern as postdoctoral fellow at EPFL, where he earned the Latsis Award 1996 for his studies on the self-assembly of metal nanostructures at metal surfaces. In 1998, Harald Brune was nominated Reader (MER) in Nanophysics at EPFL, received an offer for a Chair (C4) at Philipps-Universität Marburg, and accepted the counteroffer of EPFL. He is a fellow of the American Physical Society and member of the research council of the Swiss National Science Foundation (SNSF). In 2014, he was elected president of the Mathematics, Natural and Engineering Sciences division of the Research Council of SNSF.

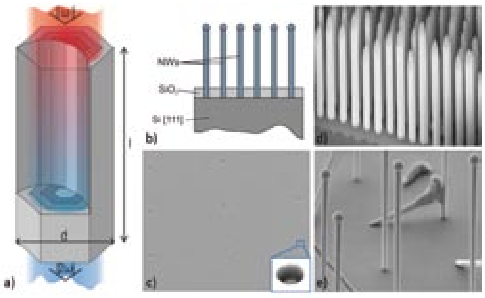
Focus Group **Nanophotonics and Quantum Optics**

Prof. Jelena Vuckovic (Stanford University) | Hans Fischer Senior Fellow
Armin Regler | Doctoral Candidate
Prof. Jonathan Finley, Semiconductor Quantum Nanosystems, TUM

Jelena Vuckovic

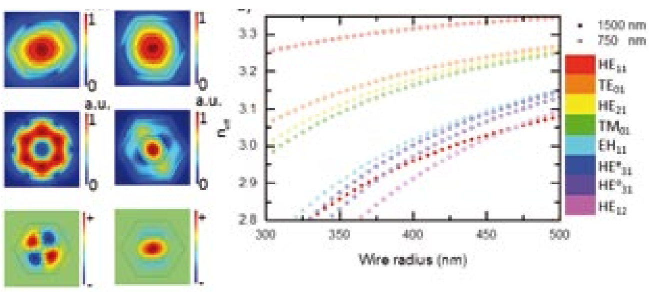
Splicing, splitting, and detecting quantum light using nanowires

For many applications ranging from medicine and environmental sensing to imaging and emerging quantum technologies, it is necessary to develop novel optical sources at well-defined frequencies. This is particularly true in the green and mid-infrared regions of the electromagnetic (EM) spectrum where efficient light-emitting materials simply do not exist. An attractive alternative involves using *nonlinear* optical phenomena, whereby an efficient optical source is built at a practically accessible frequency but then the output is frequency-converted. Here, green laser pointers are the most commonly encountered devices in which pairs of infrared photons are *spliced together* to form green light. Three-five (III-V) semiconductors are highly nonlinear optical materials; they can be used, e.g., for sum-frequency generation where two input fields, with frequencies ω_1 and ω_2, are mixed to produce a third output wave at a frequency $\omega_{SFG} = \omega_1 + \omega_2$, or difference frequency generation where infrared photons are combined to produce an output wave at $\omega_{DFG} = \omega_1 - \omega_2$. Unfortunately, in a macroscopic optical medium the three EM waves having different frequencies (ω_1, ω_2 and $\omega_{D/SFG}$) continually run into and out of phase with each other, limiting the overall efficiency of the nonlinear conversion process. As a result, several tricks have to be applied, including the use of wavelength scale nano-resonators to recirculate light many times through the medium and precisely match the phase of the input and output fields.



1 | (a) Core-shell-NW geometry used for 2nd harmonic generation consisting of four $Al_xGa_{1-x}As$ shells with dissimilar Al-content and a well defined thickness. (b) Schematic of the NW growth mode on silicon, (c) SEM image of the nano-apertures in the SiO_2 layer acting as nucleation sites for NWs. (d) InAs and (e) GaAs NWs grown site-selectively on such a Si/SiO_2 substrate.

This Focus Group is exploring the use of III-V semiconductor nanowires (NWs) grown directly on silicon substrates to generate quantum light produced by nonlinear optical processes (see figure 1a). The semiconductor NWs are grown by molecular beam epitaxy at predefined positions on the silicon substrate, defined by <100nm diameter holes using electron beam lithography in the few nm thick SiO_2 (oxide/layer) (figures 1b and 1c). After growth of an AlGaAs NW-core, having a typical diameter of ~100nm and length >10µm, a series of AlGaAs shells are formed around the core to carefully tailor the refractive index of modes at ω_1, ω_2 and $\omega_{D/SFG}$ and, thereby, enhance the efficiency of the nonlinear optical process. Figure 1 depicts schematically the growth of such nanowires (figure 1b) and shows scanning electron microscopy images of the pre-patterned substrate before the growth of the NWs (figure 1c) and post-growth images of InAs (figure 1d) and GaAs (figure 1e) NWs. The thickness of the NWs can be precisely controlled to facilitate guiding of an optical beam in a manner similar to the way light is guided along an optical fiber. Figure 1a shows a typical nanowire structure design for a waveguide supporting second harmonic generation at 750nm, i.e., $2 \times \omega$ photons → $1 \times 2\omega$ photon. In this case, the diameter of the NW should be large enough to facilitate refractive index matching of the participating modes. Figure 2a shows finite element simulations of the fundamental waveguide mode (HE_{11}) at 1.5 µm and the desired 2nd harmonic mode (HE_{12}) at 750 nm. A sufficiently small refractive index difference can be achieved by using a layered radial NW profile as shown in figure 1a, where a four-layer core-shell NW was modeled with varying layer thickness and Al-content.



2 | a) - mode profiles of the fundamental HE11 mode at a wavelength of 1.5 µm, two modes at 750 nm. The overlap for 2nd harmonic generation of the modes on top to the modes in the middle is shown in the lower panels. By integrating over the entire NW profile, the nonlinear signal vanishes for the leftmost mode at 750 nm, whereas in the right case a nonlinear signal is obtained. b) Calculated effective refractive indices for the lowest order modes at pump and 2nd harmonic frequencies for different NW diameters at a uniform NW aluminum content of 15%. For diameters > 800 nm they effectively reproduce a non-linear output.

Figure 2a shows the mode profile of the fundamental mode (HE_{11}) at 1500 nm (leftmost panel), two typical 2nd harmonic modes at 750 nm (HE^{o}_{31} left and HE_{12} right-middle panel) and the calculated mode overlap of the HE_{11} mode 2nd order polarization with the 2nd harmonic mode (bottom-most panel). The integral of this overlap over the whole waveguide region vanishes in the case of the HE^{o}_{31} mode, whereas the case of the HE_{12} mode yields a finite value indicating that 2nd harmonic conversion will occur. Nanowire structures geometrically optimized according to the simulated values for the effective refractive indices have been designed and are currently being fabricated and tested.

In related work, the Focus Group is exploring the use of superconducting NWs to detect photons propagating in silicon waveguides. Here, absorption of a single photon in the NW locally destroys the superconductivity and leads to a measurable signal in the attached readout circuit. Such superconducting NW-detectors promise near-unity detection quantum efficiencies, low dark count rates (<10 Hz), and ultrafast (<80ps) timing resolution. By integrating *superconducting* NW single-photon detectors and *semiconductor* nonlinear frequency conversion elements onto a single silicon ridge waveguide, the Focus Group aims to frequency-convert, distribute, and detect single photons on a silicon chip.

Selected Publications

[1] G. Reithmaier, F. Flassig, P. Hasch, S. Lichtmannecker, K. Müller, J. Vučković, R. Gross, M. Kaniber, and J. Finley, "A carrier relaxation bottleneck probed in single InGaAs quantum dots using integrated superconducting single photon detectors," *Appl. Phys. Lett.*, vol. 105, no. 8, p. 081107, Aug. 2014.

[2] G. Reithmaier, M. Kaniber, F. Flassig, S. Lichtmannecker, K. Müller, A. Andrejew, J. Vučković, R. Gross, and J. Finley, "On-chip generation, routing and detection of quantum light," Aug. 2014.

Publications by this Focus Group can also be found on page 161.

Jelena Vuckovic is a professor of Electrical Engineering and, by courtesy, of Applied Physics at Stanford, where she leads the Nanoscale and Quantum Photonics Lab. She is also a faculty member of the Ginzton Lab, Bio-X, and the Pulse Institute at Stanford. Upon receiving her PhD degree in Electrical Engineering from the California Institute of Technology (Caltech) in 2002, she worked as a postdoctoral scholar at Stanford. In 2003, she joined the Stanford Electrical Engineering Faculty, first as an assistant professor (until 2008), then an associate professor with tenure (2008–2013), and finally as a professor of electrical engineering (since 2013). As a Humboldt Prize recipient, she has also held a visiting position at the Institute for Physics of the Humboldt University in Berlin, Germany (since 2011). In addition to the Humboldt Prize (2010) and the Hans Fischer Senior Fellowship (2013), Vuckovic has received many awards including the Marko V. Jaric award for outstanding achievements in physics (2012), the DARPA Young Faculty Award (2008), the Chambers Faculty Scholarship at Stanford (2008), the Presidential Early Career Award for Scientists and Engineers (PECASE in 2007), the Office of Naval Research Young Investigator Award (2006), the Okawa Foundation Research Grant (2006), and the Frederic E. Terman Fellowship at Stanford (2003). She is on the editorial advisory board of Nature Quantum Information and ACS Photonics, and was on the editorial board of the New Journal of Physics.

Focus Group **Nanoscience for Renewable Energy Sources**

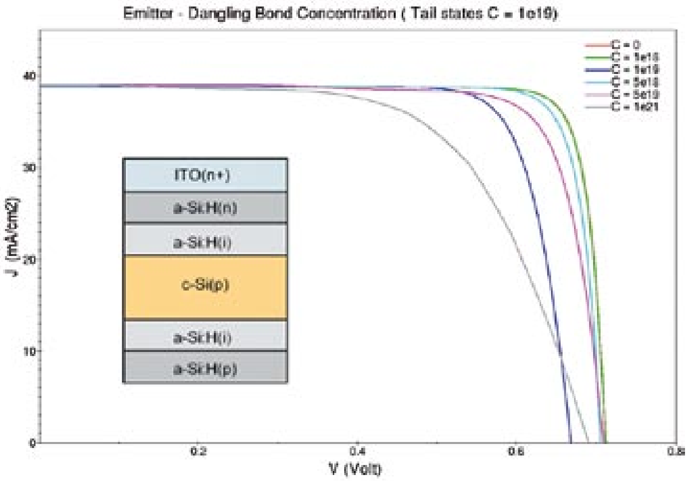
Prof. Stephen Goodnick (Arizona State University) | Hans Fischer Senior Fellow
Pietro Luppina | Doctoral Candidate
Prof. Paolo Lugli, Nanoelectronics, TUM

Stephen Goodnick

This Focus Group is concerned with the modeling and simulation of advanced-concept photovoltaic devices that utilize nanostructure materials for their realization. The development of sustainable and efficient energy conversion processes and systems is one of the grand challenges globally. The limited availability of fossil fuels as primary energy sources and the concomitant emission of pollutants are leading to negative local and global effects on the environment and pose an enormous challenge for our future. Solar energy is by far the most abundant clean energy source available today. However, the efficiency of present-day solar cells is well below the maximum conversion efficiency dictated by thermodynamics.

The motivation for our project comes from the necessity to develop tools that can help to improve the efficiency of existing solar energy conversion systems or to design novel advanced-concept devices. Current commercial modeling tools lack the sophistication and necessary physics to accurately model novel new energy conversion concepts that may significantly improve photovoltaic efficiencies. The project aims at setting up a simulation framework based on a series of physical models and Monte Carlo tools able to describe the fundamental processes determining the operation of PV devices, and ultimately to provide accurate design tools for their optimization. While the use of such tools is widely established for the design of electronic devices, this is not the case for solar cells and other energy conversion devices. The theoretical effort is supporting experimental efforts at both TUM and Arizona State University in realizing high-efficiency solar cells.

Stephen Goodnick and Paolo Lugli participated in a special symposium at the annual meeting of the American Association for the Advancement of Science (AAAS) in Chicago on February 16, 2014, organized by Patrick Regan of the TUM Corporate Communications Center. The title of the symposium was “Nanoelectronics for Renewable Energy: How Nanoscale Innovations Address Global Needs.” Stephen Goodnick presented a talk entitled “Pathways to Next-Generation Photovoltaics” while Prof. Lugli presented a talk entitled “Large-Area Nanoimprinting for Energy Harvesting Applications.” Wolfgang Porod (University of Notre Dame, USA), Alumnus Hans Fischer Senior Fellow, presented a talk as well on “Nanoantenna Thermocouples for Energy Harvesting.” Other speakers included Stephen Chou from Princeton University and Anna Fontcuberta I Morral from EPFL. Overall the symposium was well attended and very well received.



1 | Effect of the amorphous Si defect tail density of states on the device performance of an amorphous Si/crystalline Si heterojunction solar cell. The inset shows the illuminated IV curve. Inset: Schematic of a Si heterojunction solar cell (HIT cell).

From July to December of 2014, Stephen Goodnick was on sabbatical leave at the TUM. The research during this period focused on two main areas: on modeling and simulation of high-efficiency Si photovoltaics based on crystalline Si/amorphous Si heterojunctions, and on utilization of III–V compound nanowires for photovoltaic applications.

Stephen Goodnick was co-organizer of the 2014 Workshop on Integrated Nanoscale Devices and Systems (WINDS) held Nov. 30–Dec. 5 on Kohala Coast, Hawaii, USA, where he presented a paper entitled “Ultrafast Carrier Relaxation in Nanowire Structures for Photovoltaic Applications,” related to his work on nanowire photovoltaics as part of the Focus Group.

Selected Publication

[1] R. Hathwar, Y. Zou, C. Honsberg, P. Lugli, M. Saraniti, and S. Goodnick, “Ultrafast Carrier Relaxation in Nanowire Structures for Photovoltaic Applications,” in Workshop on Innovative Nanoscale Devices and Systems, p. 58, 2014.

Publications by this Focus Group can also be found on page 162.

Publications

Angewandte Reviews
P. L. Arnold et al.
DOI: 10.1002/anie.201404613

C–H Activation

C–H Bond Activation by f-Block Complexes

Polly L. Arnold, Max W. McMullon, Julia Rieb, and Fritz E. Kühn*

Keywords:
actinides · asymmetric catalysis · polarity reversal catalysis · radical addition · rare earths

NANO LETTERS
Letter
pubs.acs.org/NanoLett

Controlled Manipulation of Gadolinium-Coordinated Supramolecules by Low-Temperature Scanning Tunneling Microscopy

José I. Urgel, David Ecija,* Willi Auwärter,* and Johannes V. Barth
Physik Department E20, Technische Universität München 85748 Garching, Germany

Supporting Information

ABSTRACT: Coordination bonding between para-quaterphenyl-dicarbonitrile linkers and gadolinium on ... to construct pentam... exploited ... isting of a ... employing ... tocol was ... dition, the ... tetrameric, ... arrange- ... brication ... lity of metal–ligand interactions and atomistic manipulation
...olecules, coordination chemistry, lanthanides

Global Change Biology
Global Change Biology (2014) 20, 3767–3779, doi: 10.1111/gcb.12637

Patterns of drought tolerance in major European temperate forest trees: climatic drivers and levels of variability

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Abstract

The future performance of native tree species under climate change conditions is frequently discussed, since increasingly severe and more frequent drought events are expected to become a major risk for forest ecosystems. To improve our understanding of the drought tolerance of the three common European temperate forest tree species Norway spruce, silver fir and common beech, we tested the influence of climate and tree-specific traits on the inter and intra-site variability in drought responses of these species. Basal area increment data from a large tree-ring network in Southern Germany and Alpine Austria along a climatic cline from warm-dry to cool-wet conditions were used to calculate indices of tolerance to drought events and their variability at the level of individual trees and populations. General patterns of tolerance indicated a high vulnerability of Norway spruce in comparison to fir and beech and a strong influence of bioclimatic conditions on drought response for all species. On the level of individual trees, low growth rates prior to drought events, high competitive status and low age favored resilience in growth response to drought. Consequently, drought events led to heterogeneous and variable response patterns in forests stands. These findings may support the idea of deliberately using spontaneous selection and adaption effects as a passive strategy of forest management under climate change conditions, especially a strong directional selection for more tolerant individuals when frequency and intensity of summer droughts will increase in the course of global climate change.


RESEARCH

RESEARCH ARTICLES

MOLECULAR MAGNETISM

Reaching the magnetic anisotropy limit of a 3d metal atom

Ileana G. Rau, Susanne Baumann, Stefano Rusponi, Fabio Donati, Sebastian Stepanow, Luca Gragnaniello, Jan Dreiser, Cinthia Piamonteze, Frithjof Nolting, Shruba Gangopadhyay, Oliver R. Albertini, Roger M. Macfarlane, Christopher P. Lutz, Barbara A. Jones, Pietro Gambardella, Andreas J. Heinrich, Harald Brune

Designing systems with large magnetic anisotropy is critical to realize nanoscopic magnets. Thus far, the magnetic anisotropy energy per atom in single-molecule magnets and ferromagnetic films remains typically one to two orders of magnitude below the theoretical limit imposed by the atomic spin-orbit interaction. We realized the maximum magnetic anisotropy for a 3d transition metal atom by coordinating a single Co atom to the O site of an MgO(100) surface. Scanning tunneling spectroscopy reveals a record-high zero-field splitting of 58 millielectron volts as well as slow relaxation of the Co atom's magnetization. This striking behavior originates from the dominating axial ligand field at the O adsorption site, which leads to out-of-plane uniaxial anisotropy while preserving the gas-phase orbital moment of Co, as observed with x-ray magnetic circular dichroism.

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PLOS ONE

Enhancing Genome-Enabled Prediction by Bagging Genomic BLUP

Daniel Gianola, Kent A. Weigel, Nicole Krämer, Alessandra Stella, Chris-Carolin Schön

OPEN ACCESS Freely available online

PLOS ONE

Imaging Liver Lesions Using Grating-Based Phase-Contrast Computed Tomography with Bi-Lateral Filter Post-Processing

Julia Herzen, Marian S. Willner, Alexander A. Fingerle, Peter B. Noël, Thomas Köhler, Enken Drecoll, Ernst J. Rummeny, Franz Pfeiffer

nature COMMUNICATIONS

ARTICLE

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DOI: 10.1038/ncomms3947 OPEN

Submicron structures provide preferential spots for carbon and nitrogen sequestration in soils

Cordula Vogel, Carsten W. Mueller, Carmen Höschen, Franz Buegger, Katja Heister, Stefanie Schulz, Michael Schloter & Ingrid Kögel-Knabner

The sequestration of carbon and nitrogen by clay-sized particles in soils is well established, and clay content or mineral surface area has been used to estimate the sequestration potential of soils. Here, via incubation of a sieved (<2 mm) topsoil with labelled litter, we find that only some of the clay-sized surfaces bind organic matter (OM). Surprisingly, <19% of the visible mineral areas show an OM attachment. OM is preferentially associated with organo-mineral clusters with rough surfaces. By combining nano-scale secondary ion mass spectrometry and isotopic tracing, we distinguish between new labelled and pre-existing OM and show that new OM is preferentially attached to already present organo-mineral clusters. These results, which provide evidence that only a limited proportion of the clay-sized surfaces contribute to OM sequestration, revolutionize our view of carbon sequestration in soils and the widely used carbon saturation estimates.

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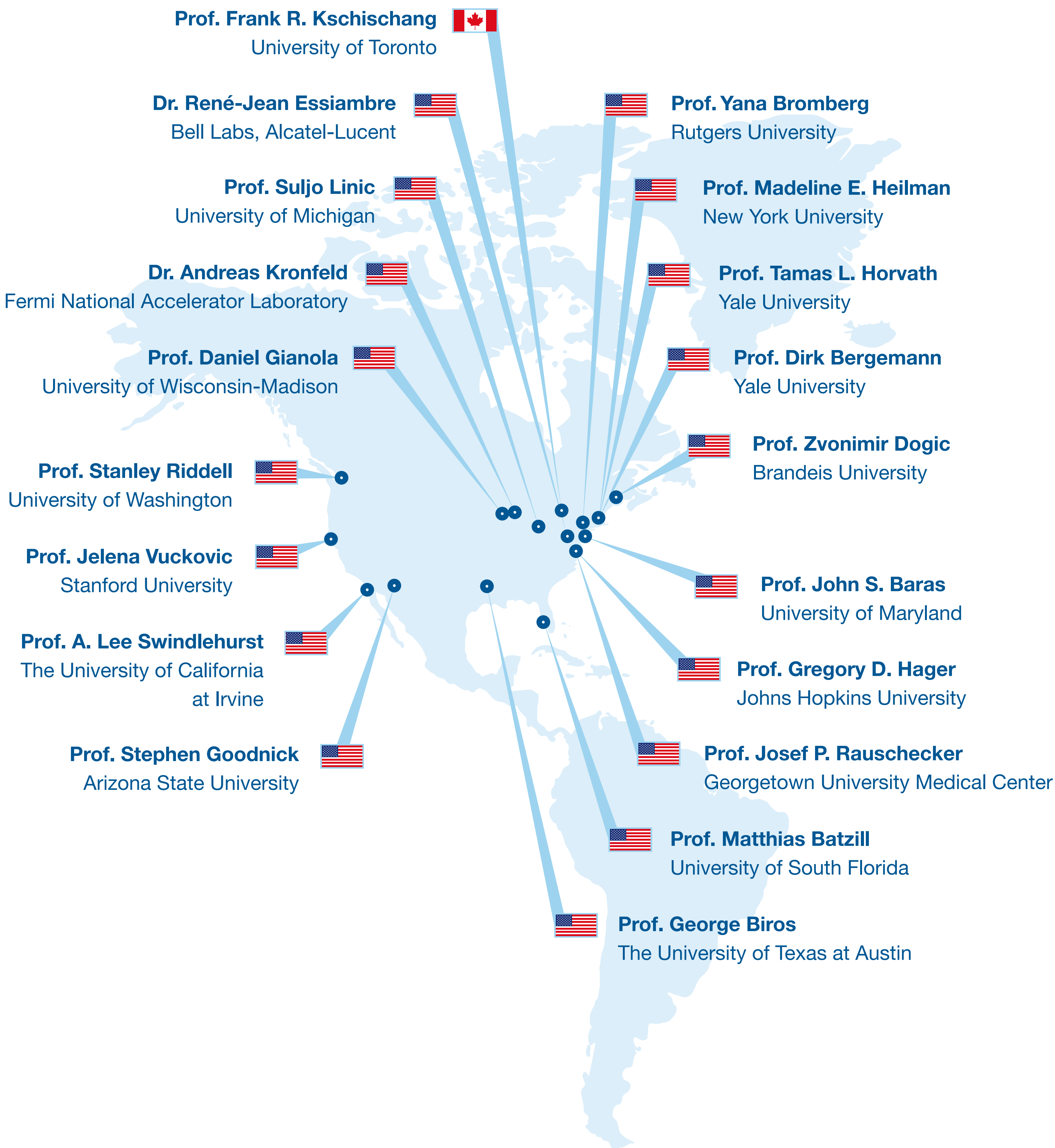
Facts and Figures

Where do the TUM-IAS Fellows come from?

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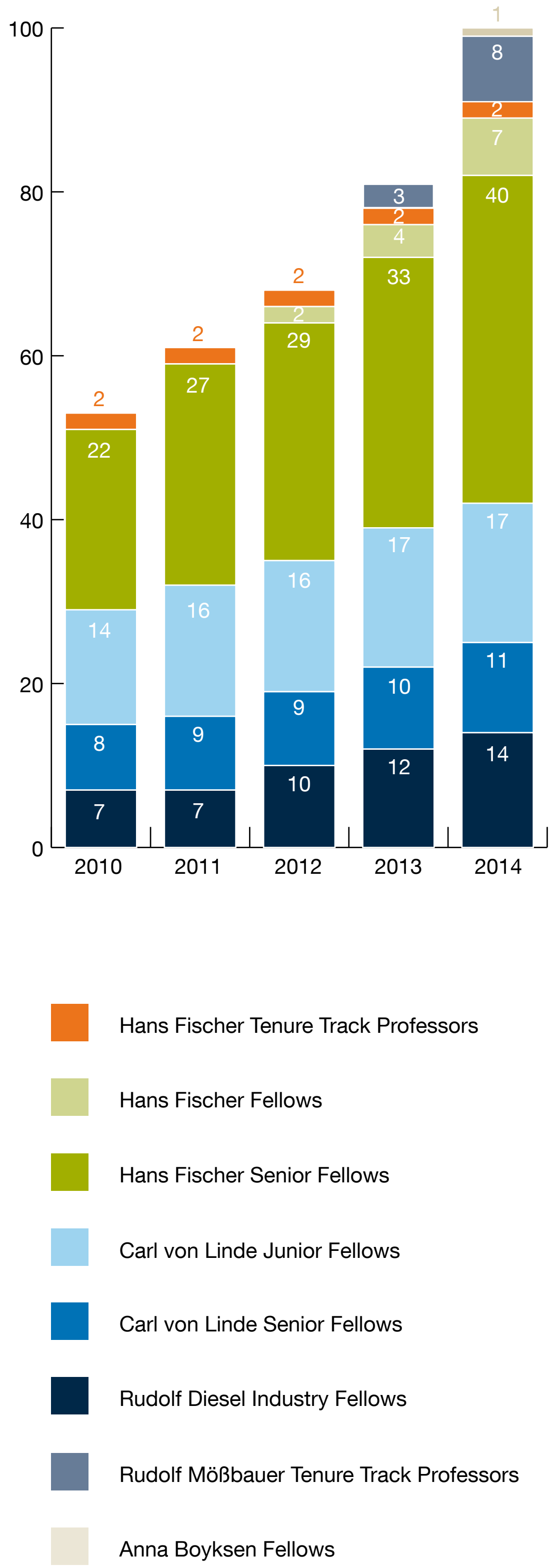
Prof. Kathrin Lang
Prof. Dongheui Lee
Prof. Bjoern Menze
Prof. Annette Menzel
Prof. Alessio Zaccone

Fellow Distribution

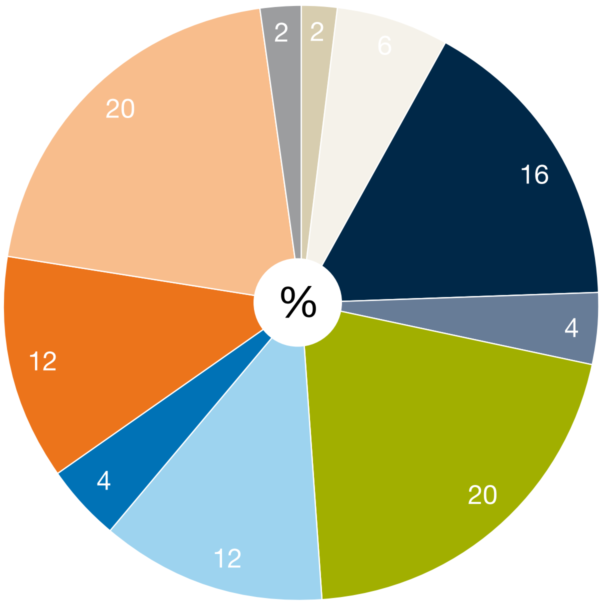
In 2014, TUM-IAS appointed 20 new Fellows, which means that for the first time since the Fellowship program's first days in 2007, the total number of active and alumni Fellows has risen to more than 100. The Hans Fischer program for international scientists experienced a visible growth with seven new Hans Fischer Senior and four Hans Fischer Fellows, strengthening TUM's connection to prestigious research institutions abroad. Two newly appointed Rudolf Diesel Industry Fellows and one Carl von Linde Senior Fellow show the well established nature of these two programs. TUM-IAS is especially proud of the success of its Rudolf Mößbauer Tenure Track Professorship program, which attracted five high-potential early-career scientists to TUM in 2014 (one of them a former Hans Fischer Fellow), bringing the total number of Mößbauer Professors at the university up to eight. The Anna Boyksen Fellowship brought a new dimension – aimed at gender- and diversity-related issues in natural sciences and technology; it is the first Fellowship with a topical focus.

Regrettably, the Carl von Linde Junior Fellowship program had to be brought to an end. However, the high numbers of new Hans Fischer Fellows and Rudolf Mößbauer Tenure Track Professors show that TUM-IAS has not relinquished its strategic aim to offer attractive career and research opportunities for early-career scientists. TUM-IAS continues to attach great importance to its interdisciplinary nature: With the TUM School of Management being involved for the first time, 11 of the 13 TUM faculties now host Fellows.

Total Number of Fellows and Alumni Fellows

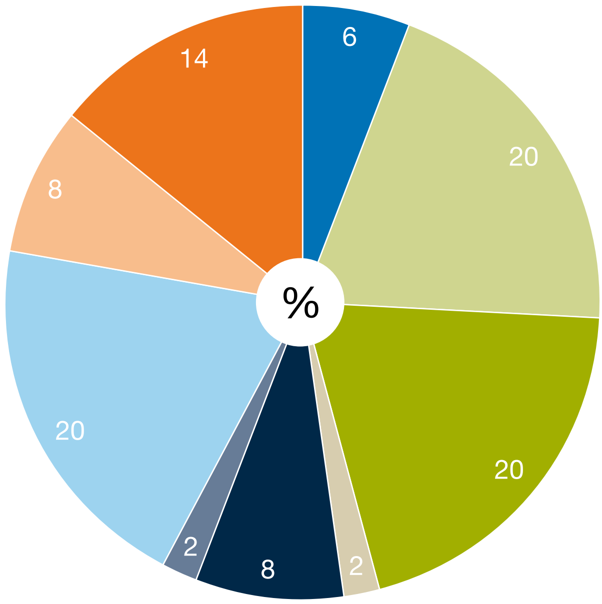


Distribution of Active Fellows According to Faculties



- Architecture
- Center of Life and Food Sciences Weihenstephan
- Chemistry
- Civil, Geo and Environmental Engineering
- Electrical Engineering and Information Technology
- Informatics
- Mechanical Engineering
- Medicine
- Physics
- TUM School of Management

Distribution According to Research Areas

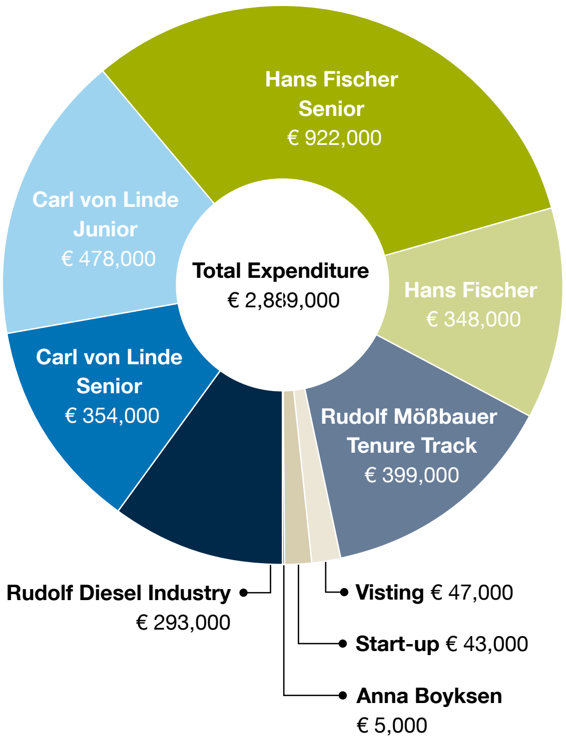


- Advanced Computation and Modeling
- Biomedical Engineering, Bio-Imaging, Neuroscience
- Bio-related Natural Sciences
- Gender and Diversity in Science and Engineering
- Communication and Information
- Fundamental Physics
- Surface, Interface, Nano- and Quantum Science
- Control Theory, Systems Engineering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

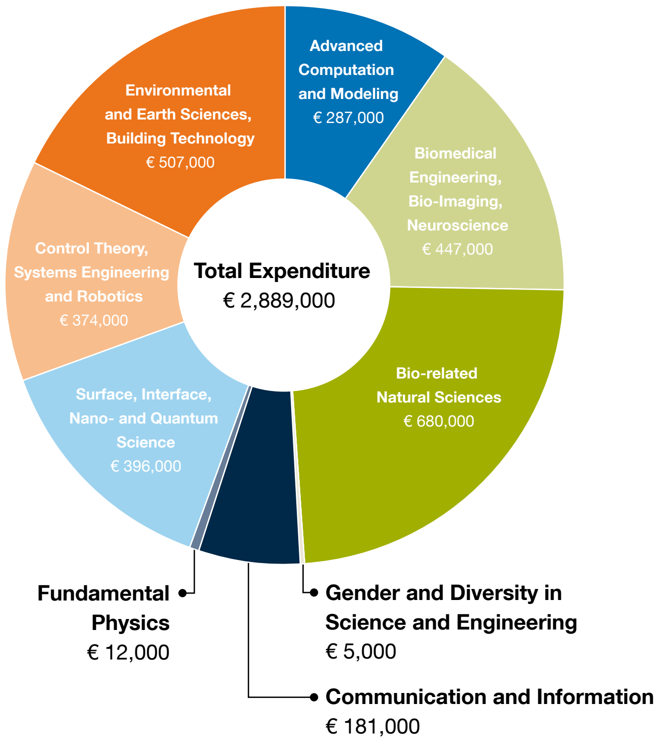
Finances

In this section we present a brief survey of the financial data of the TUM-IAS. The expenditure are covered by the “third funding line” of the German Excellence Initiative as well as by the European Union Seventh Framework Program (Marie Curie COFUND).

Expenditure per Fellowship Category in 2014



Expenditure per Research Area in 2014

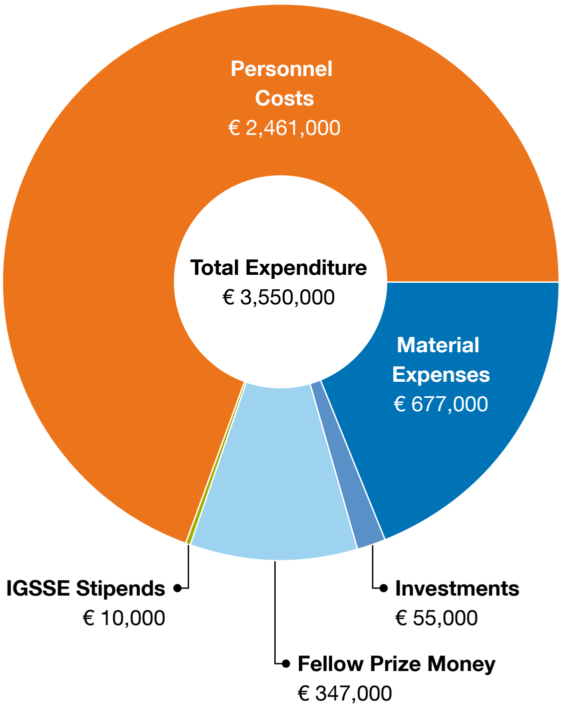


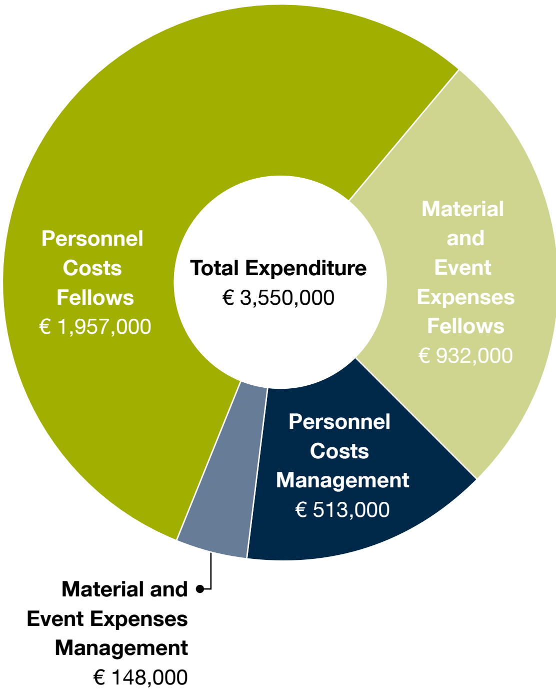
This chart illustrates the expenditure in 2014 for each Fellowship category, along with expenditure from the Start-up and Visiting Fellowship programs. Most dominant in terms of costs – with 32% of the total expenditure – is the Hans Fischer Senior Fellowship; these Fellowships are an integral part of the TUM internationalization strategy and are immensely valuable in terms of the exchange of complementary expertise and the grooming of emerging fields. Expenditure for the Carl von Linde Senior Fellowship category underwent no significant change in 2014. In contrast, the Rudolf Diesel Industry Fellows received less than before, the primary reason being that doctoral candidates are no longer financed in this category.
Expenditure for the Hans Fischer Fellowship category and the new Rudolf Mößbauer Tenure Track Professorships increased – with more than a quarter spent for the funding of outstanding, high-potential early-career scientists who have the ambition of developing a new field of endeavor upon joining the TUM-IAS. The Anna Boyksen Fellowship category was newly established in 2014, and as one might expect, this led to very low costs for the year.

In 2014, TUM-IAS has established eight Research Areas with Focus Groups, running Start-up projects and Visiting Fellows fitting in one of these broad topical areas. In addition, TUM-IAS has created the Research Area Gender and Diversity in Science and Engineering for the Anna Boyksen Fellowship program. Nevertheless, TUM-IAS continues to be a Fellow-driven Institute with a bottom-up approach.

This chart shows the TUM-IAS Fellowship expenditure grouped into the TUM-IAS Research Areas, including the expenditure from the Start-up and Visiting Fellowship programs, also according to the TUM-IAS Research Areas.

This financial chart as well as the illustration of the distribution of Fellows demonstrate very nicely the diverse and interdisciplinary nature of the Institute (see pages 168–169 “Fellow Distribution”).





On this chart, total TUM-IAS expenditure is displayed, including Fellowships, Start-up funding, Visiting Fellowships, events, and management. The total expenditure reached approximately the same level as in 2013, due to full-capacity operation of the Institute. It has become a policy of the Institute to offer working contracts to doctoral candidates (instead of stipends), and this is reflected in an increase in personnel costs and a decrease in IGSSE stipends.

This chart devides the total TUM-IAS expenditure into expenses related to the TUM-IAS management and related to expenses of the Fellows. The chart displays personnel costs, and material, travel, and event costs for the TUM-IAS management and for the Fellows respectively.

Cover and inside cover: Julian Treu, Walter Schottky Institute.

4, 10, 15 (Schmid, Sturm), 21 (Hagn), 23, 27, 43, 68, 76 (Menze), 86 (Koehler), 94 (Dogic), 96, 98, 100, 104, 110, 112 (Buss) 115, 134 (Lamp), 136, 163: Andreas Heddergott.

5, 6, 11 (Herrmann), 15 (Abstreiter, Merz, Steinberger, Fischer, Höchtl, Jelinek, Schwarzer), 29, 46, 48, 49, 51, 52, 53, 54, 56, 57, 58, 59, 60, 61, 64, 74 (Riddell), 78, 80, 120, 122, 124, 131: Astrid Eckert.

11 (Aufderheide), 12 (Rüland): Eric Lichtenscheidt.

13 (Rummel; Sakman), 112 (Lee): Astrid Eckert/Andreas Heddergott.

30, 33 (bottom rows), 39 (photograph), 40 (photographs), 42, 129, 134 (group picture): TUM-IAS.

33, 35 (poster): Brigitte Steinbüchler.

38, 39, 40, 41 (banner „Nachbarn“): Julie Rousset.

11 (Aebischer): Alain Herzog; (Bjarklev): Sten Brogaard.

12 (Carrier): Vincent Leifer; (Engel): Evonik; (Gallini): Martin Dee, UBC; (Hofmeister): Jon Reis; (Kronthaler): Oliver Jung; (Lang): Christian Kruppa; (Neugebauer): Axel Griesch.

13 (Sakaki): Masayuki Shioda; (Schwaiger): Matthias Meyer; (Tye): HKUST.

21 (Lang): Neil Grant.

33: J. Leo van Hemmen (top row).

34, 35: Chair for Strategy and Organization (photographs).

38 (top row, left to right): V. Tritschler, S. Hickel, X. Hu and N. A. Adams, Physics of Fluids 25: 071701, 2013 (artwork: Li Su); G. De Nayer and Michael Breuer (Fluid Mechanics, Helmut-Schmidt University, Hamburg), realized at Leibniz-Rechenzentrum; L. Han, X. Hu and N. A. Adams ,Journal of Computational Physics 262, 131–152, 2014 (artwork: Li Su); (bottom row, left to right): A. Garon, R. Zeier and S. J. Glaser,“Visualization of Multi-spin operators”, in preparation; N. Thuerey, C. Wojtan, M. Gross and G. Turk,

ACM Transactions on Graphics (SIGGRAPH), ACM Press, 2010; E.R. McNellis, Ch. Bronner, J. Meyer, M. Weinelt, P. Tegeder and K. Reuter, *Phys. Chem. Chem. Phys. 12*, 6404 (2010).

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72: Focus Group High-Performance Computing.

74: Luca Gattinoni, “Memory T Cells Officially Join the Stem Cell Club,” *Immunity*, vol. 41, pp. 7–9, Jul. 2014 (illustration).

76 (illustration): Bjoern Menze.

79: Michael Friebe.

81: Giaime Rancan.

82: Georgetown University.

83, 85: Focus Group Neuroimaging.

86 (illustration), 87: Focus Group Phase Contrast Computed Tomography.

89 Focus Group Regenerative Medicine.

92 (Kessler): facesbyfrank; (illustration): D. Pallarola, A. Bochen, H. Boehm, F. Rechenmacher, T. R. Sobahi, J. P. Spatz, and H. Kessler, “Interface immobilization chemistry of *c*RGD-based peptides regulates integrin mediated cell adhesion,” *Adv. Funct. Mater*, vol. 24, no. 7, pp. 943–956, Feb. 2014 (illustration).

93: F. Rechenmacher, K. Steigerwald, B. Laufer, S. Neubauer, T. G. Kapp, L. Li, C. Mas-Moruno, M. Joner, and H. Kessler, “The integrin ligand *c*(RGDf(*N*Me)Nal) reduces neointimal hyperplasia in a polymer-free drug-eluting stent system,” *ChemMedChem*, vol. 9, no. 7, pp. 1413–8, Jul. 2014.

94, 95: Focus Group Biologically Inspired Material Science (illustrations).

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99: Focus Group Statistical and Quantitative Genomics.

101: Focus Group Structural Membrane Biochemistry.

102 (Lang): Neil Grant.

102 (illustration), 103: Focus Group Synthetical Biochemistry.

105: Focus Group Theory of Soft Matter.

111: Alkurdi et al., 2015, in preparation.

113: Focus Group Control and Robotics.

114 (top row and bottom left): TUM-FSD; (bottom center): ERC Advanced Grant; (bottom right): TUM-IAS/FSD.

115 (illustration): Focus Group SADAS.

118: Edith Stenhuys.

119: Stefano Boeri Architteti.

121: Robert Vanis.

122 (illustration), 123: Christian Hirt.

125: Ingrid Kögel-Knabner.

137: Focus Group Functional Interfaces.

138: Photo Tornow.

139: Focus Group Metal-Organic Superlattices of Quantum Magnets.

140 (Vuckovic): Craig Lee, Stanford University; (figure 1 a, b): Focus Group Nanophotonics and Quantum Optics; (figure 1 c, d, e): Daniel Rudolph, "Growth of GaAs-based nanowires on silicon for optical applications", doctoral thesis, Walter Schottky Institute, Technische Universität München.

141: Focus Group Nanophotonics and Quantum Optics.

143: Focus Group Nanoscience for Renewable Energy Sources.

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147 (top to bottom): I. G. Rau, S. Baumann, S. Rusponi, F. Donati, S. Stepanow, L. Gragnaniello, J. Dreiser, C. Piamonteze, F. Nolting, S. Gangopadhyay, O. R. Albertini, R. M. Macfarlane, C. P. Lutz, B. A. Jones, P. Gambardella, A. J. Heinrich, and H. Brune, "Reaching the magnetic anisotropy limit of a 3d metal atom," *Science*, vol. 344, no. 6187, pp. 988–92, May 2014; D. Gianola, K. A. Weigel, N. Krämer, A. Stella, and C.-C. Schön, "Enhancing genome-enabled prediction by bagging genomic BLUP," *PLoS One*, vol. 9, no. 4, p. e91693, Jan. 2014; J. Herzen, M. S. Willner, A. A. Fingerle, P. B. Noel, T. Koehler, E. Drecoll, E. J. Rummeny, and F. Pfeiffer, "Imaging liver lesions using grating-based phase-contrast computed tomography with bi-lateral filter post-processing," *PLoS One*, vol. 9, no. 1, p. e83369, Jan. 2014; C. Vogel, C. W. Mueller, C. Höschen, F. Buegger, K. Heister, S. Schulz, M. Schloter, and I. Kögel-Knabner, "Submicron structures provide preferential spots for carbon and nitrogen sequestration in soils," *Nat. Commun.*, vol. 5, p. 2947, Jan. 2014.

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Semiconductor Nanowires, seen with an electron microscope. Julian Treu, Walter Schottky Institut, TUM

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