MAX-PLANCK-INSTITUT
FÜR KOLLOID- UND
GRENZFLÄCHENFORSCHUNG

Jahresbericht
Annual Report

2019 | 2020 | 2021

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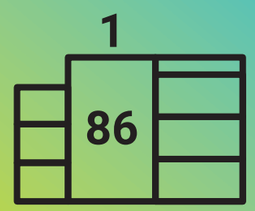

1 von 86 Max-Planck-Instituten
1 of 86 Max Planck Institutes

Labore
Laboratories

Gesamtfläche in m²
Total area in m²

↘ Max-Planck-Institut
für Kolloid- und Grenzflächenforschung
Am Mühlenberg, D–14476 Potsdam

www.mpikg.mpg.de/en

1 Vorwort
Preface

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von links nach rechts,
from left to right:
Prof. Dr. Dr.h.c. Peter Fratzl
Prof. Dr. Peter H. Seeberger
Prof. Dr. Dr. h.c. Markus Antonietti
Prof. Dr. Reinhard Lipowsky

Mit diesem Jahresbericht gibt das Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG) einen kurzen Einblick in seine Tätigkeit während der Jahre 2019 bis 2021. Für zusätzliche Informationen verweisen QR-Codes auf webbasierte Inhalte.

Die Forschungstätigkeit des MPIKG konzentriert sich auf sehr kleine Strukturen im Nano- und Mikrometerbereich, auf deren Synthese, Analyse und modellhafter Beschreibung, was für neue nachhaltige Materialien, für Impf- und Wirkstoffe und auch für regenerative Therapien von größter Bedeutung ist. Das MPIKG wird kollegial geleitet und gliedert sich in vier Abteilungen: Biomolekulare Systeme (Peter H. Seeberger), Kolloidchemie (Markus Antonietti), Biomaterialien (Peter Fratzl) und Theorie & Bio-Systeme (Reinhard Lipowsky) sowie die Max-Planck-Forschungsgruppe Mechano(bio)chemie (Kerstin Blank). Gegen Ende des Jahres 2021 wechselte Kerstin Blank auf eine Professur an der Johannes Kepler Universität Linz und die Abteilung Theorie & Bio-Systeme wurde mit der Emeritierung von Reinhard Lipowsky geschlossen. In Übereinstimmung mit unserem Fachbeirat sowie mit der Chemisch-Physikalisch-Technischen Sektion der Max-Planck-Gesellschaft wird die Strategie des Instituts zukünftig stärker in Richtung nachhaltige Chemie und Materialwissenschaft ausgerichtet. Die frei gewordene Abteilung wird sich in Einklang mit dieser Thematik experimenteller Forschung widmen.

Zum Zeitpunkt der Drucklegung dieser Broschüre wird mit einer höchstqualifizierten Physikerin über die Besetzung der offenen Direktorenstelle verhandelt.

Wir wünschen viel Vergnügen beim Durchblättern und Lesen dieses Berichts.

Peter Fratzl
Geschäftsführender Direktor 2021–2022

With this report, the Max Planck Institute of Colloids and Interfaces (MPICI) intends to give a short overview of its activities in the years 2019 to 2021. QR codes provide links to additional web-based content.

Research at MPICI concentrates on materials and structures at a nano- and micrometer scale. Their synthesis, analysis, and modeling is of utmost importance for many fields, such as new sustainable materials, vaccines and therapeutics, or regenerative therapies. The MPICI consists of four departments: Biomolecular Systems (Peter H. Seeberger), Colloid Chemistry (Markus Antonietti), Biomaterials (Peter Fratzl), and Theory & Bio-Systems (Reinhard Lipowsky), as well as the Max Planck Research Group Mechano(bio)chemistry (Kerstin Blank). Towards the end of 2021, Kerstin Blank accepted a professor position at Johannes Kepler University Linz, and the Department of Theory & Bio-Systems was closed with the retirement of Reinhard Lipowsky. In agreement with our scientific advisory board and the Chemistry, Physics, and Technology Section of the Max Planck Society, the future strategy of the MPICI will be directed more strongly towards sustainable chemistry and materials.

At the moment where this report is printed, negotiations are ongoing to fill the open position with an outstanding experimental physicist in this area.

We hope you enjoy reading through this report.

Peter Fratzl
Managing Director 2021–2022

↘ Weitere Informationen finden Sie unter
www.mpikg.mpg.de/jahresbericht

↘ Further information can be found at
www.mpikg.mpg.de/annual-report

Von der Natur lernen – für eine nachhaltige Zukunft

Learning from nature—for a sustainable future

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Seit seiner Gründung im Jahr 1992 ist das Max-Planck-Institut für Kolloid- und Grenzflächenforschung eines der ersten, das die Max-Planck-Gesellschaft in den neuen Bundesländern unterhält. Knapp 30 Jahre später hat sich das Potsdamer Institut zu einer weltweit führenden Forschungseinrichtung mit etwa 300 internationalen Mitarbeitenden entwickelt.

Als Institut, an dem Grundlagenforschung auf Spitzenniveau betrieben wird, stellen wir uns den großen gesellschaftlichen Herausforderungen dieses Jahrhunderts. Für einen nachhaltigeren Einsatz unserer materiellen Ressourcen braucht es neue chemische und materialwissenschaftliche Lösungsansätze, die wir als innovative Forschungseinrichtung schaffen wollen. Wir forschen an Ideen für eine Kreislaufwirtschaft nach dem Vorbild der Natur, in der Materialien wiederverwendet und recycelt werden, selbstheilend sind oder sich an Umweltbedingungen anpassen. Dafür haben wir innerhalb unserer Forschungseinheiten am Institut die idealen Bedingungen, mit den richtigen Köpfen, der nötigen Expertise und den modernsten Geräten:

– Die Pionierleistung der Abteilung **Biomaterialien** von Peter Fratzl besteht in der systematischen Erforschung des Zusammenhangs von Strukturen und Eigenschaften biologischer Materialien wie z. B. Knochen, Holz oder Muschelschalen. Ziel ist es, von der Natur zu lernen, um Materialien und deren Einsatz besser und nachhaltiger zu machen. Materialwissenschaftliches Wissen am Knochen wird auch in der Medizin benötigt, um die Frakturheilung zu verbessern oder Osteoporose zu behandeln.

Founded in 1992, the Max Planck Institute of Colloids and Interfaces was one of the first Max Planck Society Institutes in the new, formerly East German, federal states. Almost 30 years later, the Potsdam institute has developed into a world-leading research institution with nearly 300 international employees.

As an institute where basic research is conducted at the highest level, we are addressing the major societal challenges of this century. If we are to use our material resources in a more sustainable manner, new chemical and material science solutions are needed, which we aim to develop through innovative research approaches. We are studying ideas for a circular economy modeled on nature, in which materials are reused and recycled, are self-healing, or adapt to environmental conditions. We have ideal conditions for this within the institute's research units with the right minds, the necessary expertise, and state-of-the-art equipment:

– The pioneering work of Peter Fratzl's Department of **Biomaterials** consists of systematic research into the interrelationship of the structures and properties of biological materials such as bones, wood, or mussel shells. The aim is to learn from nature how to make materials and the way we use them better and more sustainable. Materials science knowledge regarding bone is also needed in medicine to improve fracture healing and treat osteoporosis.

– Die Kernkompetenz von Peter H. Seebergers Abteilung **Biomolekulare Systeme** liegt in der Herstellung komplexer Zuckermoleküle mittels Syntheseautomat. Über dieses Verfahren werden Impfstoffkandidaten gegen multiresistente (Krankenhaus-)Keime sowie Wirkstoffe gegen andere Bedrohungen für die menschliche Gesundheit erforscht.

– Markus Antoniettis Abteilung **Kolloidchemie** konstruiert aus grüner Chemie einfach zugängliche und nachhaltige molekulare Bausteine für größere Einheiten und Materialien. Auf diese Weise entstehen hochmoderne Energiespeicher sowie preiswerte und nachhaltige Katalysatoren, die unter anderem eine „künstliche Photosynthese" möglich machen und dank grüner Chemie sollen „künstliche Huminstoffe" zukünftig unsere Böden verbessern.

– Ende 2021 emeritierte Reinhard Lipowsky. Bis dahin befasste sich die Abteilung **Theorie & Bio-Systeme** mit der Selbstorganisation von künstlichen Biosystemen, die unter anderem modular aus Biomembranen, molekularen Motoren, Filamenten sowie Nanotröpfchen aufgebaut sind. Durch die einzigartige Kombination aus Theorie, Experiment und Simulation sowie durch Bottom-Up und Top-Down Methoden konnten diesbezüglich tiefgreifende Erkenntnisse gewonnen werden.

Bis Oktober 2021 unterhielt die Biophysikerin Kerstin Blank eine unabhängige Max-Planck-Forschungsgruppe zum Thema **Mechano(bio)chemie**. Sie erforschte den Einfluss von mechanischen Kräften auf die Struktur und die Funktion von Molekülen und Materialien. Nun ist sie als Professorin für Experimentalphysik an die Johannes Kepler Universität in Linz gewechselt.

multi-resistant (hospital) germs and active agents against other threats to human health are being researched.

– Markus Antonietti's Department of **Colloid Chemistry** uses green chemistry to construct easily accessible and sustainable molecular building blocks for larger entities and materials. In this way, state-of-the-art energy storage devices are created, as well as inexpensive and sustainable catalysts that make "artificial photosynthesis" possible, among other things. And thanks to green chemistry, "artificial humic substances" should improve our soils in the future.

– Until Reinhard Lipowsky retired at the end of 2021, his Department of **Theory & Bio-Systems** was concerned with the self-organization of artificial biosystems, which are, among other things, modularly constructed from biomembranes, molecular motors, filaments, and nanodroplets. Through the unique combination of theory, experiment, and simulation, as well as bottom-up and top-down methods, profound insights could be gained in this respect.

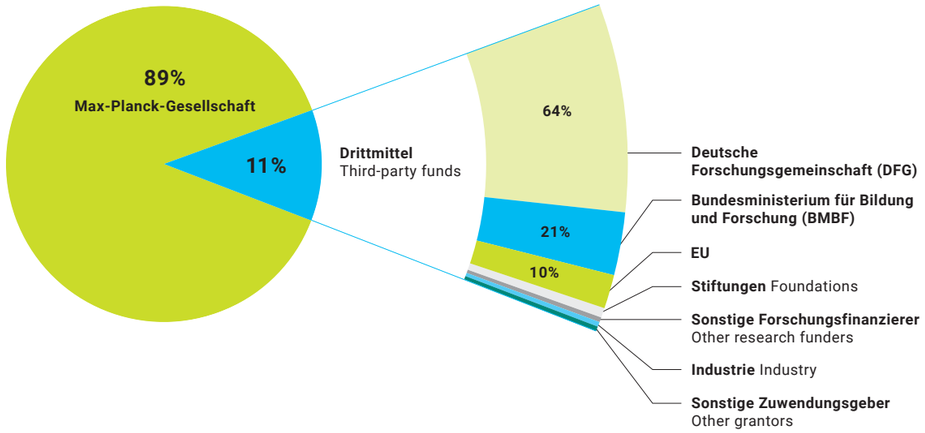
Until October 2021, biophysicist Kerstin Blank maintained an independent Max Planck research group on **Mechano(bio)chemistry**. She researched the influence of mechanical forces on the structure and function of molecules and materials. She has now moved to Johannes Kepler University Linz as a professor of experimental physics.

Zahlen & Fakten 1
Facts & Figures 1

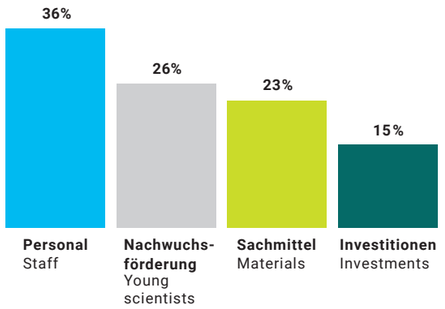
Unser Forschungsinstitut erhält jährlich ein Gesamtbudget von der Max-Planck-Gesellschaft. Diese bekommt die Fördergelder von Bund und Ländern und gibt sie an die 86 Max-Planck-Institute weiter. In den Diagrammen ist dargestellt, wofür diese Förderung verwendet wurde:

Our institute receives its annual budget from the Max Planck Society, which gets the funding from the federal and state governments and passes it on to the 86 Max Planck Institutes. The diagrams show what this funding has been used for.

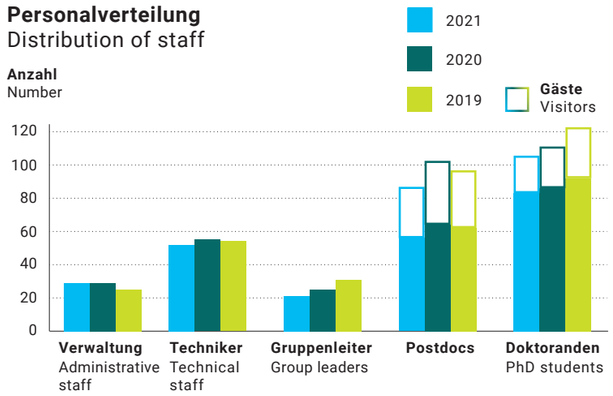
Gesamtbudget 2020
Total funding in 2020



Ausgaben 2020
Expenditure in 2020



Personalverteilung
Distribution of staff



Im Jahr 2020 belief sich die Drittmittelförderung auf rund 11,4 Prozent des Gesamtbudgets. Der höchste Anteil der Drittmittel entfällt mit 64 Prozent auf die Deutsche Forschungsgemeinschaft (DFG). Die Förderung des Bundesministeriums für Bildung und Forschung (BMBF) beläuft sich auf 21 Prozent der Gesamtsumme. Mit knapp 380 Mitarbeitenden entfielen im Jahr 2020 36 Prozent des Gesamtbudgets auf Personalkosten. 27 Prozent wurden zusätzlich für institutsfinanzierte Stellen der Nachwuchswissenschaftler/innen verwendet. Diese Gruppe und auch die Postdocs machen mehr als die Hälfte aller Mitarbeitenden aus. Zudem verzeichnet das Institut jedes Jahr eine hohe Zahl von Gastforschenden.

In 2020, third-party funding amounted to around 11.4 percent of the total budget. The highest share of third-party funding, 64 percent, was provided by the German Research Foundation (DFG). Funding from the German Federal Ministry of Education and Research (BMBF) amounted to 21 percent of the total. With a total of 380 employees, personnel costs accounted for 36 percent of the total budget in 2020. 27 percent was additionally used for institute-funded positions for young scientists. This group, including postdocs, also accounts for more than half of all employees. In addition, the institute has a high number of visiting researchers each year.

Zukunftsfragen
Questions for the Future

Wie werden Batterien preiswerter, nachhaltiger und gleichzeitig leistungsstärker?

Einfache Zink- oder Aluminium- und Natrium-Metallbatterien wären viel billiger, aus einfach verfügbaren Elementen aufgebaut, und damit auch auf der Skala des gesamten Energienetzes anwendbar.

How can we make batteries cheaper, more sustainable, and more powerful?

Simple zinc or aluminum and sodium metal batteries would be much cheaper, constructed of easily available elements, and thus employable on the scale of the entire energy grid.

Wie können wir Materialkreisläufe der Natur besser verstehen und als Vorbild für nachhaltigere technische Lösungen nutzen?

Die Struktur natürlicher Materialien passt sich auf vielen Größenskalen an die Bedingungen im Ökosystem an. Ein besseres Verständnis der Prozesse hilft uns, Konzepte für nachhaltige technische Kreisläufe zu entwickeln.

How can we better understand nature's material cycles and use them as a model for more sustainable technical solutions?

The structure of natural materials adapts to ecosystem conditions at many size scales. A better understanding of this helps us to develop concepts for sustainable technical cycles.

Wie können wir bezahlbare Medikamente für Entwicklungs- und Schwellenländer herstellen?

Kleine per Laptop gesteuerte Automaten mit eingebauter Qualitätskontrolle können aus einfachen Ausgangsstoffen überall auf der Welt Wirkstoffe in gleichbleibend hoher Qualität herstellen, indem Chemie im Rohr anstatt im Topf gemacht wird.

How can we produce affordable medicines for developing and emerging countries?

Small laptop-controlled synthesis machines with built-in quality control can produce active ingredients of consistently high quality from simple starting materials by taking chemistry out of the cooking pot and into the test tube. And they can do this anywhere in the world.

Wie können wir die Eigenschaften von molekularen Motoren durch künstliche Evolutionsprozesse verbessern und optimieren?

Eigenschaften von molekularen Motoren wie Geschwindigkeit und Lauflänge lassen sich systematisch durch die biotechnologische Methode des Phagen-Display optimieren.

How can we improve and optimize the properties of molecular motors through artificial evolution processes?

Properties of molecular motors such as velocity or run length can be optimized using the biotechnological method of phage display.

Vier Experten – ein Ziel

Four experts —one goal

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Prof. Dr. Dr.h.c. Peter Fratzl

2003 gründete Peter Fratzl die Abteilung **Biomaterialien** am Max-Planck-Institut für Kolloid- und Grenzflächenforschung, die er bis heute leitet und die aus sechs bis acht Forschungsgruppen besteht. Der an der École Polytechnique Paris und der Uni Wien ausgebildete Ingenieur und Physiker untersucht die Zusammenhänge zwischen der (hierarchischen) Struktur und den physikalischen Eigenschaften von biologischen und bioinspirierten Materialien. Diese Forschung an natürlichen Materialien wie Holz, Insektenpanzern, Muschelschalen, Proteinfasern und Knochen liefert Einblicke wie die Natur Materialien synthetisiert, wie diese heilen oder sich an geänderte Anforderungen anpassen. Das hat Auswirkungen auf die regenerative Medizin, es entstehen aber auch neue Konzepte für nachhaltige technische Materialien. Diese interdisziplinäre Forschung an der Schnittstelle von Physik, Chemie, Biologie, Ingenieurwissenschaften und Medizin ergänzt Fratzl durch enge Kooperationen mit Experten aus den Geisteswissenschaften und der Gestaltung im Rahmen eines Berliner Exzellenzclusters, den er auch als Co-Sprecher vertritt, um nachhaltige Materialkonzepte ganzheitlich zu erforschen.

Peter Fratzl ist Autor und Mitautor von mehr als 600 wissenschaftlichen Veröffentlichungen in Fachzeitschriften und Büchern. Er ist Träger des Max-Planck-Forschungspreises (2008), des Gottfried Wilhelm Leibniz-Forschungspreises (2010), sowie Ehrendoktor der Université Montpellier, Frankreich. Außerdem ist Fratzl Mitglied folgender Akademien: Österreichische Akademie der Wissenschaften, Berlin-Brandenburgische Akademie der Wissenschaften, Akademie der Wissenschaften und Literatur Mainz, Deutsche Akademie der Technikwissenschaften (acatech), sowie der United States National Academy of Engineering.

Since 2003, Peter Fratzl has headed the Department of **Biomaterials** at the Max Planck Institute of Colloids and Interfaces, which consists of six to eight research groups. Trained at the École Polytechnique Paris and the University of Vienna, Fratzl is an engineer and physicist who studies the relationships between the (hierarchical) structure and physical properties of biological and bioinspired materials. This research on natural materials such as wood, insect shells, mussel shells, protein fibers, and bones provides insights into how nature synthesizes materials and how they heal or adapt to changing requirements. This has implications for regenerative medicine, but new concepts for sustainable engineering materials are also emerging. Fratzl complements this interdisciplinary, research at the interface of physics, chemistry, biology, engineering, and medicine with close collaborations with experts from the humanities and design as part of a Berlin Cluster of Excellence, which he also co-chairs, in order to holistically explore sustainable material concepts.

Peter Fratzl is author and co-author of more than 600 scientific publications in journals and books. He is a recipient of the Max Planck Research Award (2008), the Gottfried Wilhelm Leibniz Research Award (2010), and an honorary doctorate from the University of Montpellier, France. Fratzl is also a member of the following academies: the Austrian Academy of Sciences, the Berlin-Brandenburg Academy of Sciences, the Mainz Academy of Sciences and Literature, the German Academy of Science and Engineering (acatech), and the United States National Academy of Engineering.

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Prof. Dr. Peter H. Seeberger

Der Chemiker und Biochemiker Peter H. Seeberger ist seit 2009 Direktor der Abteilung **Biomolekulare Systeme**. Mit seinen acht Arbeitsgruppen forscht er im Grenzgebiet von Chemie und Biologie. Die Wissenschaftler/innen nutzen synthetische Chemie als Basistechnologie zur Erforschung komplexer biologischer Systeme mit einem besonderen Schwerpunkt auf der Glykobiologie. Kohlenhydrate spielen eine entscheidende Rolle für Struktur, Energiespeicherung und molekulare Erkennungsvorgänge, die für lebende Organismen essentiell sind, aber auch bei Infektionen, der Immunantwort und der Krebsentwicklung. Komplexe Zucker, die die meisten Zellen umhüllen, bilden die Grundlage für Impfstoffe gegen Bakterien, Parasiten und Viren. Neben bahnbrechenden Erfindungen im Bereich der Synthese komplexer Zucker entwickelt seine Abteilung kontinuierlich neue automatisierte Synthesemethoden für die Totalsynthese von Wirkstoffen. Neben biologischen Arbeiten zur Aufschlüsselung von Signalübertragung steht die Erforschung der Materialeigenschaften komplexer Zucker im Vordergrund. Die Grundlagenforschung im Bereich der Immunologie hat zur Entwicklung von Impfstoffen beigetragen. Impfstoffe gegen Krankenhauskeime stehen nun kurz vor der klinischen Entwicklung.

Seebergers Forschung wurde in über 630 Artikeln, fünf Büchern und mehr als 50 Patentfamilien publiziert und in über 900 Vorträgen präsentiert. Unter den mehr als 40 Preisen sind besonders die Emil-Fischer-Medaille (2020), der Wissenschaftspreis des Stifterverbandes (2017), der Körber Preis für die Europäische Wissenschaft (2007) sowie der Claude S. Huson Award der American Chemical Society (2009) zu nennen. Seit 2013 ist er gewähltes Mitglied der Berlin-Brandenburgischen Akademie der Wissenschaften und seit 2021 Vize-Präsident der DFG. Zudem lehrt er als Professor an der Freien Universität Berlin und seit 2011 als Honorarprofessor an der Universität Potsdam.

Chemist and biochemist Peter H. Seeberger has been director of the Department of **Biomolecular Systems** since 2009. With his eight research groups, he conducts research at the interface of chemistry and biology. The scientists use synthetic chemistry as an enabling technology to study complex biological systems, with a particular focus on glycobiology. Carbohydrates play a critical role in structure, energy storage, and the molecular recognition processes essential to living organisms, as well as in infections, the immune response, and cancer development. Complex sugars that coat most cells form the basis for vaccines against bacteria, parasites, and viruses. In addition to breakthrough inventions in the field of automated synthesis of complex sugars, the department is developing new continuous synthetic methods for total drug synthesis. Alongside biological work on the breakdown of signal transduction, the focus is on research into the material properties of complex sugars. Basic research in immunology has contributed to the development of vaccines. Vaccines against hospital germs are now nearing clinical development..

Seeberger's research has been published in more than 630 articles, five books, and more than 50 patent families, and presented in more than 900 lectures. Among the more than 40 awards, special mention should be made of the Emil Fischer Medal (2020), the Stifterverband Science Prize (2017), the Körber Prize for European Science (2007), and the Claude S. Huson Award of the American Chemical Society (2009). He has been an elected member of the Berlin-Brandenburg Academy of Sciences and Humanities since 2013 and vice president of the DFG since 2021. He also teaches as a professor at Freie Universität Berlin and, since 2011, as an honorary professor at the University of Potsdam.

Prof. Dr. Dr. h.c. Markus Antonietti

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Mit nur 33 Jahren übernimmt Markus Antonietti als einer von drei Gründungsdirektoren im Jahr 1993 die Leitung der Abteilung **Kolloidchemie** am Institut. Sein Forschungsfeld ist die Kolloid- und Grenzflächenforschung, die sich mit kleinsten Teilchen im Größenbereich von Mikro- und Nanometern beschäftigt. In seinen derzeit acht Arbeitsgruppen liegt der Fokus im Bereich der nachhaltigen Chemie. Ihn beschäftigen von der Natur inspirierte Verfahren, wie die „künstliche Photosynthese", welche Sonnenenergie direkt in chemische Speicher- und Wertmoleküle umwandelt sowie „künstliche Huminstoffe" zur Verbesserung der Bodenqualität. Ziel ist es auch, hochwertige Materialien aus Bioabfällen herzustellen, die zur Energiespeicherung in Akkus oder Superkondensatoren dienen könnten. Als erster deutscher Chemiker hat Markus Antonietti von den weltweit ausgeschriebenen „Grants" des Europäischen Forschungsrats (European Research Council, ERC) bisher drei Auszeichnungen erhalten: 2020 bekam er den „Synergy Grant" für die Entwicklung einer nachhaltigen Batterie, einen der höchsten Forschungspreise in Europa. Energiespeichersysteme für eine zukünftig nachhaltige Stromversorgung der Haushalte und der Gesellschaft möchte er bezahlbar machen. In letzter Zeit gelangen ihm Durchbrüche in der Synthese funktionaler kohlenstoffbasierter Materialien auf Basis von erneuerbaren Ressourcen.

Mit seinen weit über 900 wissenschaftlichen Publikationen in Büchern und Fachzeitschriften zählt Markus Antonietti zu den meistzitierten deutschen Chemikern. Zudem hält er über 90 Patente und ist mit zahlreichen Auszeichnungen bedacht, darunter dem Hermann-Staudinger-Preis der Gesellschaft Deutscher Chemiker (2020), dem Bundesverdienstkreuz 1. Klasse (2018) und der Liebig-Denkmünze (2016), und er ist Mitglied der Berlin-Brandenburgischen Akademie der Wissenschaften.

In 1993, at the age of only 33, Markus Antonietti became one of the three founding directors of the Department of **Colloid Chemistry** at the institute. His research field is colloid and interface research, which deals with the smallest particles in the micro- and nanometer size range. In his current eight research groups, the focus is on sustainable chemistry. He is concerned with processes inspired by nature, such as "artificial photosynthesis," which converts solar energy directly into chemical storage and value molecules, and "artificial humic matter" to improve soil quality. The goal is also to produce high-value materials from biowaste that could be used to store energy in rechargeable batteries or supercapacitors. Markus Antonietti is the first German chemist to have received three awards from the European Research Council's (ERC) global grants: In 2020, he received the Synergy Grant for the development of a sustainable battery, one of the highest research prizes in Europe. He wants to make energy storage systems affordable for the future sustainable power supply of households and society. Recently, he has achieved breakthroughs in the synthesis of functional carbon-based materials based on renewable resources.

With well over 900 scientific publications in books and journals, Markus Antonietti is one of the most-cited German chemists. He also holds over 90 patents and is the recipient of numerous awards, including the Hermann-Staudinger Prize of the German Chemical Society (2020), the Federal Cross of Merit 1st Class (2018), and the Liebig Medal (2016). He is a member of the Berlin-Brandenburg Academy of Sciences and Humanities.

Prof. Dr. Reinhard Lipowsky

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Der Physiker Reinhard Lipowsky ist einer von drei Gründungsdirektoren, die im Jahr 1993 ihre Arbeit am Institut aufgenommen haben. Fortan leitet er die Abteilung **Theorie & Bio-Systeme**, in der analytische Theorie, Computer-Simulationen und experimentelle Methoden zum Einsatz kommen, um die grundlegenden Mechanismen und allgemeinen Prinzipien aufzuklären, die der Selbstorganisation von Biosystemen im Nanobereich zu Grunde liegen. Diese Biosysteme bestehen aus molekularen Bausteinen im Nanometerbereich, die sich von alleine zu Molekülverbänden zusammenfügen. Bis zu seiner Emeritierung Ende 2021 konzentrierte sich die Forschung seiner Abteilung auf die Fragen, was uns im Innersten zusammenhält und was uns im Innersten bewegt.

Reinhard Lipowsky ist Mitglied der Berlin-Brandenburgischen Akademie der Wissenschaften und Honorarprofessor an der Universität Potsdam und an der Humboldt-Universität zu Berlin. Seit Bestehen der Internationalen Max Planck Research School (IMPRS) über „Multiscale Bio-Systems" war er ihr Sprecher. Im Jahr 2017 wurde ihm der Wolfgang-Ostwald-Preis für hervorragende wissenschaftliche Lebensleistungen auf dem Gebiet der Kolloidwissenschaft verliehen. Nun führt Reinhard Lipowsky für weitere zwei Jahre eine Emeritus-Gruppe.

Diese wird die Aufklärung des supramolekularen Verhaltens synthetischer Biosysteme weiter erforschen, wobei der Schwerpunkt auf dem Umbau von Biomembranen liegt. Besonders faszinierende Themen bietet die rätselhafte Morphologie des endoplasmatischen Retikulums, einer faszinierenden Organelle, die in jeder menschlichen Zelle vorkommt und ein kontinuierliches Netzwerk von Membran-Nanoröhren bildet.

Physicist Reinhard Lipowsky was one of three founding directors who started working at the institute in 1993. From then on, he headed the Department of **Theory & Bio-Systems**, which uses analytical theory, computer simulations, and experimental methods to elucidate the fundamental mechanisms and general principles underlying the self-organization of nanoscale biosystems. These systems consist of molecular building blocks at a nanometer scale that self-assemble into molecular assemblies. Until his retirement at the end of 2021, his department's research focused on the questions of what holds us together and what moves us at our very core.

Reinhard Lipowsky is a member of the Berlin-Brandenburg Academy of Sciences and Humanities and an honorary professor at the University of Potsdam and the Humboldt University of Berlin. He has been the spokesperson of the International Max Planck Research School (IMPRS) on "Multiscale Bio-Systems" since its inception. In 2017, he was awarded the Wolfgang Ostwald Prize for outstanding lifetime scientific achievements in the field of colloid science.

For the next two years, Reinhard Lipowsky will be leading an emeritus group. This group will further elucidate the supramolecular behavior of synthetic biosystems, with a focus on the remodeling of biomembranes. Some particularly intriguing topics are provided by the puzzling morphology of the endoplasmic reticulum, a fascinating organelle that forms a continuous network of membrane nanotubes in each cell of the human body.

Aktive Nachwuchsförderung
Promotion of Young Scientists

Unsere Arbeit am Max-Planck-Institut fußt auf zwei großen Säulen: Zum einen ist das eine intensive Forschungstätigkeit mit dem Anspruch höchster wissenschaftlicher Exzellenz. Zum anderen die erstklassige Ausbildung des wissenschaftlichen Nachwuchses, wobei hervorragende junge Wissenschaftler/innen unter besten Bedingungen lernen und sich weiterentwickeln. Bei uns bekommen Gruppenleiter/innen Führungsverantwortung für ihr Team und arbeiten über mehrere Jahre an einem eigenen Forschungsthema mit all den hervorragenden Möglichkeiten, die das Max-Planck-Institut bietet. Postdoktorand/innen aus aller Welt forschen selbständig oder im Team und erwerben die Qualifikation für eine wissenschaftliche Karriere. Doktorand/innen arbeiten unter besten Bedingungen und intensiver Betreuung und bereiten sich auf ihre Laufbahn in Industrie, Akademie oder anderen Positionen vor.

Viele unserer Gruppenleiter/innen habilitieren sich an der Universität Potsdam oder an einer der Berliner Universitäten und lehren in großem Umfang an diesen Institutionen. Darüber hinaus arbeiten die Direktoren und Gruppenleiter/innen in DFG-geförderten Konsortien mit verschiedenen Universitäten zusammen, etwa in Sonderforschungsbereichen (SFB), Graduiertenschulen, Forschergruppen und Exzellenzclustern. Erworbenes Wissen aus unserem Institut wird in die Welt getragen und trägt zur Entwicklung unserer Forschungsgebiete bei. Unser Max-Planck-Institut bemüht sich in höchstem Maße um die Betreuung junger Forscher/innen. Im Schnitt promovieren jedes Jahr 25 Doktorand/innen.

Erstklassige Doktorandenausbildung

Das Institut verfügt über eine „International Max Planck Research School on Multiscale Bio-Systems“, an der begabte Studierende die Chance erhalten, unter exzellenten Bedingungen zu promovieren. Seit über 20 Jahren gehören diese englischsprachigen Graduiertenschulen, kurz IMPRS, zum festen Bestandteil in der Doktorandenförderung der Max-Planck-Gesellschaft. Gemeinsames Kennzeichen der Doktorandenprogramme an den Max-Planck-Instituten sind die Lehrpläne mit Forschungsseminaren und Workshops sowie die enge Kooperation mit Universitäten. Aufgrund der interdisziplinären Ausrichtung arbeitet unser Institut bei der Doktorandenausbildung mit den folgenden Universitäten eng zusammen: Universität Potsdam, Freie Universität Berlin und Humboldt-Universität zu Berlin. Für interdisziplinäre Forschung bieten wir unseren Doktorand/innen erstklassige Rahmenbedingungen und eine hervorragende Ausstattung.

Exzellente Netzwerke

Innerhalb der Exzellenzstrategie von Bund und Ländern zur Stärkung universitärer Spitzenforschung haben sich von der Deutschen Forschungsgemeinschaft (DFG) geförderte Exzellenzcluster gegründet. Wissenschaftler/innen verschiedener Disziplinen und Institutionen arbeiten gemeinsam an einem Forschungsvorhaben. Direktoren, Gruppenleiter/innen und Doktorand/innen unseres Instituts beteiligen sich im Raum Berlin/Potsdam an zwei interdisziplinären Clustern:

Matters of Activity. Image Space Material erforscht in mehr als 40 Disziplinen und sechs Projekten systematisch die Neuerfindung des Analogen im digitalen Zeitalter. Im Kern steht eine neue aktive Materialität, die die Forschung und den Alltag zu verändern beginnt.

Das Netzwerk **UniSysCat – Unifying Systems in Catalysis** besteht aus mehr als 260 interdisziplinären Forschenden, die in fünf Projekten Reaktionen in der Katalyse nutzen, um mit grüner Chemie energiesparende Geräte oder effiziente Möglichkeiten der Energiespeicherung zu entwickeln.

Max Planck Queensland Center (MPQC) Ende des Jahres 2021 wurde auf dem australischen Kontinent das erste Max Planck Center gegründet. Dies ist eine Kooperation zwischen unserem Max-Planck-Institut, dem MPI für Intelligente Systeme in Stuttgart und der Queensland University of Technology. Die Projektteams erforschen biologische Materialien, sogenannte extrazelluläre Matrizen.

Our work at the Max Planck Institute is based on two major pillars: The first is intensive research activity with a claim to the highest scientific excellence, and the second is the first-class training of young scientists, with outstanding young scientists learning and developing under the best conditions. With us, group leaders are given leadership responsibility for their team and work for several years on their own research area, with all the excellent opportunities that the Max Planck Institute offers. Postdocs from all over the world conduct research independently or in a team and acquire the qualifications for an independent scientific career. PhD students work under the best conditions and intensive supervision while preparing for their careers in industry, academia, or other positions.

Many of our group leaders habilitate at the University of Potsdam or at one of the Berlin universities, and they teach extensively at these institutions. In addition, the directors and group leaders collaborate in DFG-funded consortia with various universities, for example in Collaborative Research Centers (SFB), graduate schools, research groups, and clusters of excellence. Knowledge acquired at our institute is disseminated to the world and contributes to the development of our research areas. Our Max Planck Institute is highly committed to mentoring young researchers. On average, 25 of our PhD students complete their doctorates each year.

Excellent doctoral training

The institute includes an “International Max Planck Research School on Multiscale Bio-Systems”, where talented students are given the chance to do their PhD under excellent conditions. For more than 20 years, these English-language graduate schools, IMPRS for short, have been an integral part of the Max Planck Society’s doctoral funding. Common features of the doctoral programs at the Max Planck Institutes are the curricula, which include research seminars and workshops, as well as the close cooperation with universities. Due to its interdisciplinary orientation, the institute works closely with the following universities on doctoral training: the University of Potsdam, Freie Universität Berlin, and the Humboldt University of Berlin. For interdisciplinary research, we offer our doctoral students first-class conditions and excellent equipment.

Outstanding networks

Clusters of Excellence funded by the German Research Foundation (DFG) have been established as part of the Excellence Strategy of the German federal and state governments to strengthen top-level university research. They involve scientists from different disciplines and institutions working together on a research project. Directors, group leaders, and PhD students from our institute participate in two interdisciplinary clusters in the Berlin/Potsdam area:

Matters of Activity. Image Space Material systematically explores the reinvention of the analog in the age of the digital in more than 40 disciplines and six projects. At its core is a new active materiality that is central to sustainable development and requires a holistic approach between the humanities, natural sciences, engineering, and design disciplines.

The **UniSysCat—Unifying Systems in Catalysis** network consists of more than 260 interdisciplinary researchers working on five projects that use reactions in catalysis to develop energy-saving devices or efficient ways to store energy with green chemistry.

Max Planck Queensland Center (MPQC) At the end of 2021, the first Max Planck Center was founded on the Australian continent. This is a collaboration between our Max Planck Institute, the MPI for Intelligent Systems in Stuttgart, and the Queensland University of Technology in Brisbane. The project teams are researching the biological materials known as extracellular matrices.

Max-Planck-Forschungsgruppe
Max Planck Research Group

Prof. Dr.
Kerstin Blank

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Im Jahr 2014 kam nach einem strengen, zentral gesteuerten Auswahlverfahren Kerstin Blank als Leiterin einer Max-Planck-Forschungsgruppe auf eine W2-Stelle an unser Institut. Die Experimentalphysikerin verfolgt einen interdisziplinären Ansatz und kombiniert Methoden, um biophysikalische Fragen zu beantworten. Sie untersucht in biologischen Systemen vorkommende mechanische Prozesse. Proteine reagieren auf einen mechanischen Einfluss mit einer Konformationsänderung, der oft ein biochemisches Signal folgt. Ziel ihrer Forschung ist es, diese Mechanismen zu verstehen und auszunutzen, um künstliche Kraftsensoren mit neuen Eigenschaften zu entwickeln. Mechanische Prozesse spielen bei vielen Krankheiten eine Rolle. Mechanische Gewebeeigenschaften verändern sich beispielsweise bei Krebs oder Erkrankungen des Herz-Kreislauf-Systems. Genau an dieser Stelle möchte Kerstin Blank die molekularen Mechanismen noch besser erforschen, um gezielt eingreifen zu können.

Inzwischen lehrt sie als Professorin für Experimentalphysik an der Johannes Kepler Universität in Linz. Nach einer seit 1970 geführten internen Statistik der Max-Planck-Gesellschaft konnten 61 Prozent aller ehemaligen Forschungsgruppenleiter/innen ihre Karriere auf einer W2/W3-Stelle im In- oder Ausland fortsetzen. Elf Prozent wurden als Max-Planck-Direktorin oder Direktor berufen, elf Prozent blieben in wissenschaftlicher Funktion an einem MPI, 17 Prozent gingen an andere Forschungseinrichtungen oder in die Wirtschaft.

In 2014, after a rigorous, centrally managed selection process, Kerstin Blank joined our institute as head of a Max Planck research group in a W2 position. As an experimental physicist, she follows an interdisciplinary approach and combines methods to investigate mechanical processes in biological systems. Proteins respond to mechanical stimuli with a conformational change, which in turn causes a biochemical signal. The goal of her research is to understand and exploit these mechanisms to develop artificial molecular force sensors with novel properties. Mechanical processes play a role in many diseases. Mechanical tissue properties change, for example, in cancer or cardiovascular diseases. It is precisely at this point where Kerstin Blank wants to understand the molecular mechanisms and to intervene in a targeted manner.

She is now a professor of experimental physics at the Johannes Kepler University in Linz. According to internal statistics collected by the Max Planck Society since 1970, 61 percent of all former research group leaders continue their career as a W2/W3 professor in Germany or abroad. Eleven percent were appointed as Max Planck directors, eleven percent remained in a scientific position at an MPI, and 17 percent moved to other research institutions or to industry.

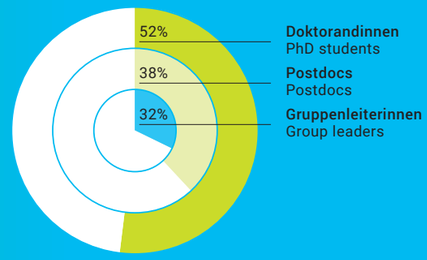
↘ Weitere Informationen finden Sie unter
www.mpikg.mpg.de/jahresbericht

↘ Further information can be found at
www.mpikg.mpg.de/annual-report

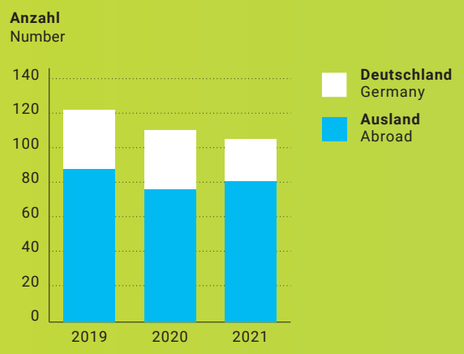
Zahlen & Fakten 2
Facts & Figures 2

Exzellente Forschungsergebnisse entstehen mit den besten Köpfen weltweit – der Frauenanteil in den Naturwissenschaften wächst
Excellent research results with the best minds worldwide—the proportion of women in the natural sciences is growing

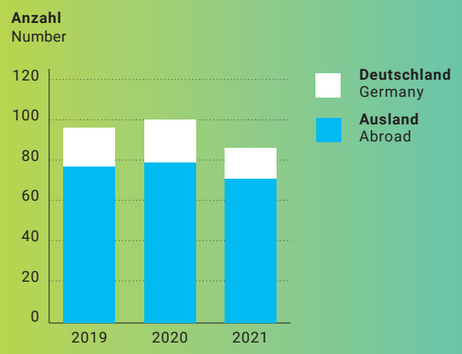
Anteil der Wissenschaftlerinnen am Institut 2019
Proportion of female scientists at the institute in 2019



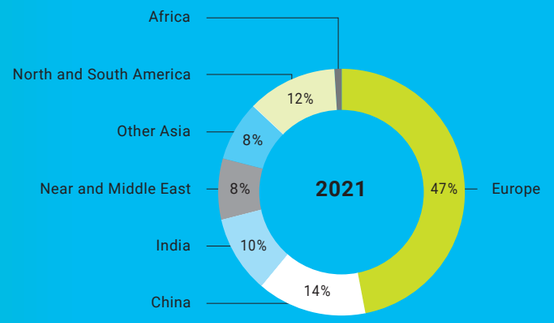
Entwicklung unserer Doktorandenzahlen
Development of PhD students



Entwicklung unserer Postdoc-Zahlen
Development of Postdocs



Nationalitäten
Nationalities



31
Promotionen 2020
Doctorates conferred in 2020

300
Publikationen im Durchschnitt pro Jahr
Average yearly publications

34 000
Zitierungen pro Jahr
Citations per year

Jedes Jahr betreuen wir an unserem Institut im Schnitt 110 Doktorand/innen, davon sind etwa 20 als Gäste bei uns. Der Großteil unserer Promovierenden sowie der Postdoktorand/innen kommt aus dem Ausland. Dieser internationale Austausch stellt eine Bereicherung für die wissenschaftliche Arbeit am Institut dar. Gleichzeitig werden auf diese Weise internationale Netzwerke auf- und ausgebaut. Für unsere internationalen Mitarbeitenden ist der Aufenthalt an unserem Institut in der Regel ein weiterer Schritt für die individuelle Qualifizierung und Karriereentwicklung. Die Zahl der Doktorand/innen ist in den Jahren 2020 und 2021 leicht gesunken, was auf die Emeritierung von Prof. Lipowsky und die damit einhergehende Schließung seiner Abteilung Ende 2021 zurückzuführen ist. Gleiches gilt für die Zahl der Postdoktorand/innen. Mit der für 2022 geplanten Neuberufung wird sich das wieder ausgleichen.

Bislang gelten Frauen in den Naturwissenschaften als unterrepräsentiert. An unserem Max-Planck-Institut stellten Frauen im Jahr 2019 mit 52 Prozent mehr als die Hälfte der Doktorand/innen. Das liegt zwei Prozentpunkte über dem Bundesschnitt. Bei den Postdoktorand/innen und Gruppenleiter/innen sind es hingegen nur halb so viele Frauen wie Männer. Diese Zahlen dürften sich in den kommenden Jahren erhöhen.

Wie in den vergangenen Jahren kommen knapp 50 Prozent unserer Mitarbeitenden aus Europa, wobei der Anteil der Westeuropäer überwiegt. Gleichbleibend ist mit 40 Prozent auch der Anteil unserer Nachwuchsforschenden und der Forschenden aus Asien. Mit zwölf Prozent unterscheidet sich auch die Zahl der nord- und südamerikanischen Mitarbeitenden nicht von den Zahlen der Vorjahre. Erstmals verzeichnen wir in den letzten drei Jahren Forschende aus Afrika.

Every year, we supervise an average of 110 PhD students at our institute, of which about 20 are with us as guests. The majority of our PhD students and postdocs come from abroad. This international exchange enriches the scientific work at the institute. At the same time, international networks are established and expanded in this way. For our international employees, the stay at our institute is usually a further step for their individual qualification and career development. The number of PhD students has slightly decreased in 2020 and 2021, which is due to the retirement of Prof. Lipowsky and the associated closure of his department at the end of 2021. The same applies to the number of postdocs. This will be balanced out again with the new appointment planned for 2022.

Women are still considered to be underrepresented in the natural sciences. At our Max Planck Institute, women made up more than half of the PhD students in 2019, at 52 percent. This is two percentage points above the national average. In contrast, among postdocs and group leaders, there are only half as many women as men. These numbers are likely to increase in the coming years.

As in previous years, 50 percent of our employees come from Europe, with a predominance of Western Europeans. The proportion of our junior researchers and researchers from Asia has also remained the same, at 40 percent. At twelve percent, the number of North and South American employees is also no different from the figures for previous years. For the first time in the last three years, we now have researchers from Africa.

Unsere Vision
Our Vision

In Anbetracht der Klima- und Ressourcenkrise mit all ihren Auswirkungen sehen wir es als unsere Aufgabe, unsere wissenschaftliche Expertise zunehmend in nachhaltige Materialforschung zu investieren.

Wir streben einen Dreiklang aus Chemie, Materialien und Nachhaltigkeit an. Unsere Forschungseinheiten arbeiten in den Bereichen Molekül- und Materialsynthese, physikalische Charakterisierung, theoretische Beschreibung und Werkstoffforschung.

Unsere Forschungsschwerpunkte sind dynamisch, weil jeder neue Gruppenleiter und jede neue Gruppenleiterin neue Schwerpunkte setzt und eine gewisse Neuausrichtung für die Abteilung bedeutet.

In view of the climate and resource crisis, with all its implications, we see it as our task to increasingly invest our scientific expertise in sustainable materials research.

We strive for a triad of chemistry, materials, and sustainability. Our research units work in the areas of molecular and materials synthesis, physical characterization, theoretical description, and materials engineering.

Our research's main areas of focus are dynamic because each new group leader sets new priorities, which therefore means some realignment for the department.

Department of Biomaterials

Department of Biomaterials

Natural material systems and their interaction with the environment are studied in order to develop new concepts for more sustainable engineering materials.

In the nearly 20 years since the creation of the Department of Biomaterials, it has been pursuing research in biological materials science. This relatively new scientific area (see Fig. 1) covers research on natural materials, such as wood or silk, and improves potential uses of bio-based materials. It also addresses healthcare materials, such as scaffolds for tissue engineering, in order to contribute towards better medical treatments. The Department of Biomaterials is active in both areas, but above all it has been pushing forward a most promising direction represented by the double arrow in Fig. 1. The concept of bioinspired materials research goes far beyond the mimicry of biological strutures for engineering purposes, which is sometimes described as biomimetic or bionic research. The idea is that biological materials interact with their spatial and temporal environment and also adapt to it, meaning that entire systems need to be considered in bioinspired materials research. Translating the results of this type of research will lead to materials innovations that may not only integrate into engineering cycles but also with the natural environment.

The innovation potential of this approach was analyzed under the leadership of the department's director in a publication by the German Academy of Science and Engineering (acatech), supported by the German Ministry of Science and Education. Based on this analysis, bioinspired materials research is likely to become an important pillar of development towards a more sustainable materials economy.

↘ https://www.acatech.de/publikation/materialforschung-impulsgeber-natur/)

Research in the Department of Biomaterials is carried out by a number of scientifically independent research groups, with diverse backgrounds including mathematics, physics, chemistry, materials science, physical chemistry, biochemistry, wood science, botany, and zoology. The group leaders were assembled based on their scientific excellence and their ability to collaborate—where needed—with the other groups in the department. This report features contributions from group leaders who spent at least part of the three-year period 2019—2021 in the Department of Biomaterials. They cover a broad range of biological materials, including those based on cellulose such as wood (see report by Michaela Eder), on chitin such as the spider cuticle (see report by Yael Politi), on protein such as tendon and bone collagen (see reports by Wolfgang Wagermaier and Richard Weinkamer), or on combinations of those such as in bacterial biofilms (see report by Cécile Bidan) or in cartilaginous fishes (see report by Mason Dean). Mineral-based materials such as seashells are studied by Shahrouz Amini's group, Angelo Valleriani's group focuses on population dynamics, Emanuel Schneck has been studying the structure and properties of cell membranes, and Amaia Cipitria, extracellular matrices in the context of bone metastases (see their respective reports).

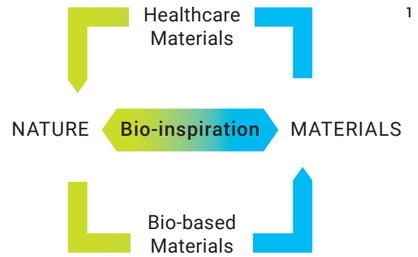


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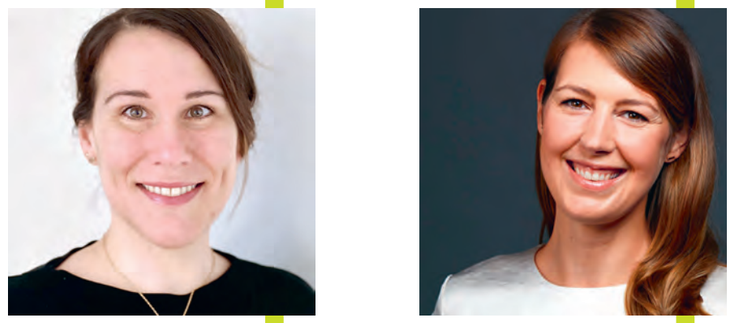
Fig. 1 The science of biological materials encompasses several research directions. Nature provides a wide range of bio-based materials for human use—wood, leather, or cotton would be prototypic examples. Healthcare materials correspond to engineered materials for use in biology or medicine, with implants being prototypic examples. The double arrow in the center represents bio-inspired science and engineering where technical materials are inspired by and collaborate with natural systems.



2

Fig. 2 Two new group leaders who start their groups in the Department of Biomaterials beginning in 2022: Emeline Raguin (left, joining from a postdoc at the Weizmann Institute, Israel) and Franziska Jehle (right, joining from a postdoc at McGill University, Montreal, Canada).

High-end materials characterization is key to the better understanding of structure-function relations. This includes micromechanical and microstructural characterization, based on electron and light microscopy, spectroscopy, as well as in-operando material studies with synchrotron radiation. The most recent addition is focused ion beam scanning electron microscopy (see report by Luca Bertinetti).

By studying these material classes, which all typically occur in most ecosystems, we try to improve our general understanding of how natural building blocks are used and combined in different ways to achieve a broad range of properties. For example, chitin in the spider cuticle is used to generate a variety of tools for grinding, piercing, cutting, adhering, for light manipulation, and much more [1]. Extracellular proteins are constituents of materials as different as wool, collagen, bone, skin, or silk [2], with properties determined by their hierarchical structure from supramolecular to macroscopic dimensions. Of particular interest are active materials that change shape or generate force due to a stimulus from the environment. Examples are plant-grown materials changing shape or acquiring motility due to water absorption from the ambient air [3] or collagen fibers that contract during mineralization [4]. Interdisciplinary studies of active materials [5] are carried out within a Cluster of Excellence that includes the collaboration of more than 40 disciplines.

↘ www.matters-of-activity.de

References: [1] Politi, Y.; Bertinetti, L.; Fratzl P. and Barth, F. G.: The spider cuticle: a remarkable material toolbox for functional diversity. Philosophical Transactions of the Royal Society A 379, 20200332 (2021). Harrington, M. J.; Fratzl, P.: Natural load-bearing protein materials. Progress in Materials Science 120, 100767/1—44 (2021).

[2] Harrington, M. J.; Fratzl, P.: Natural load-bearing protein materials. Progress in Materials Science 120, 100767/1—44 (2021).

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[4] Ping, H.; Wagermaier, W.; Horbelt, N.; Scoppola, E.; Li, C.; Werner, P.; Fu, Z.; Fratzl, P.: Mineralization generates megapascal contractile stresses in collagen fibrils. Science 376, 188—192 (2022).

[5] Fratzl, P.; Friedman, M.; Krauthausen, K.; Schäffner, W.: Active Materials. 387 pages. De Gruyter, Berlin (2022).

The goal is to develop a holistic view on materials and their functions based on natural sciences, humanities, engineering, and design. In early 2022, we also started the Max Planck Queensland Center, co-directed by Dietmar Hutmacher (Queensland University of Technology) and Peter Fratzl, to study the materials science of extracellular matrices in a collaborative effort between Australia and Germany.

The department's environment is highly dynamic and five group leaders left to tenured and/or professor positions in the three-year period of this report: Yael Politi and Luca Bertinetti to Technische Universität Dresden, Emanuel Schneck to Technische Universität Darmstadt, Mason Dean to City University of Hong Kong, and Amaia Cipitria to the Biodonostia Health Research Institute in San Sebastian, Spain. Moreover, Angelo Valleriani joined the Department of Biomaterials from the closing Department of Theory & Bio-Systems in 2021. Finally, two group leaders (Fig. 2) are joining the Department of Biomaterials in early 2022 and are, therefore, not yet represented in this report. Emeline Raguin will study bone development and its early mineralization patterns. For this, she is developing a highly promising experimental approach based on cryo-FIB/SEM. In this technique, shock-frozen (and, therefore, nearly unmodified) specimens are imaged in 3D by using scanning electron microscopy (SEM) and serial thinning of the specimen using a focused ion beam (FIB). Franziska Jehle will work on slime-based materials secreted by snails, for example. These have a multitude of functions from gilding to adhesion and protection. Her approach is primarily biochemical, but will also use high-end imaging methods such as cryo-FIB/SEM.

Our experimental approach is generally based on multi-method correlative imaging, where different probes are used to image the same specimen. This provides information on different features of the materials such as micro-structure, chemical composition, or mechanical properties in a position-resolved manner with micron-range resolution. We are currently combining X-ray tomography, (focused ion beam) scanning electron microscopy, scanning X-ray diffraction and tomography, as well as spectroscopic imaging to characterize micro- and nanostructures and many levels of structural hierarchy. We use nano-indentation as well as acoustic microscopy to estimate local mechanical properties. In addition to our dedicated beamline end station for scanning small- and wide-angle scattering and fluorescence spectroscopy, which is operated at the synchrotron BESSY at the Helmholtz Zentrum Berlin, we have now started a new emphasis on electron microscopy. In addition to transmission electron microscopy, where the institute (specifically the Department of Colloid Chemistry) is running a new facility, the Department of Biomaterials has started an operation for (cryo)-focused ion beam 3D electron imaging. This is an extremely promising technique that has the potential to revolutionize our understanding of cell and tissue structure, in particular mineralized tissues. These characterization approaches are accompanied by a significant effort in mathematical modeling, which is always closely tied to the experimental work in the department. Typically, modeling and experimentation go hand in hand with the research projects. The majority of the research in the Department of Biomaterials involves collaborations—within the department, with other departments in the institute, and with many outside partners around the world to whom we all extend our sincere gratitude for cultivating and fostering such wonderful partnerships.

Prof. Dr. Dr.h.c. Peter Fratzl

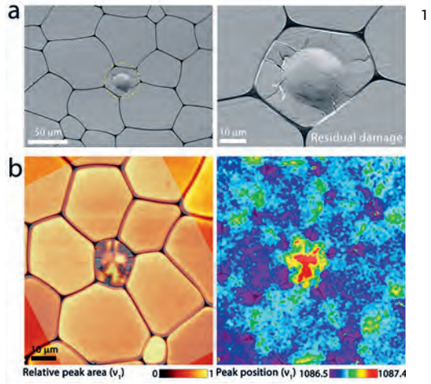
Ingénieur Diplômé de l'École Polytechnique Paris;
Dr. rer. nat. Universität Wien;
Dr. honoris causa Université de Montpellier.

2012 Leibniz Award
Member of several Academies of Science in Berlin, Mainz, and in Austria, as well as of the German National Academy of Science and Engineering (acatech) and the US National Academy of Engineering (NAE)

Since 2003 Director at MPICI and **Honorary Professor** at the University of Potsdam and the Humboldt University of Berlin; **Co-director** of the Excellence Center "Matters of Activity" (EXC 2025), HU Berlin

Selected Board Memberships:
Ludwig Boltzmann Institute of Osteology Vienna; Institute of Science and Technology Austria; Wyss Institute @Harvard; MIT Department of Civil and Environmental Engineering; Materials Science Institute of Sorbonne University Paris; Leibniz Institute for Polymer Research Dresden; Rostock Centre for Interdisciplinary Implant Research; Center for Molecular Bioengineering Dresden; Reviewing Editors @Science Magazine.

↘ Further information can be found at https://www.mpikg.mpg.de/bm



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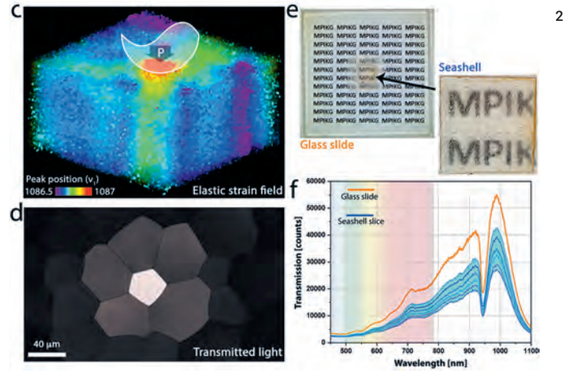


2

Fig. 1 Localization of the induced damage in a prismatic seashell, revealed by post-indentation a) electron micrographs and b) confocal Raman maps. **Fig. 2** Interaction of a prismatic seashell with mechanical load and light. c) Development of the elastic field and d) distribution of the transmitted light are modulated by the prismatic microarchitecture. e, f) Light transmission through the prismatic shell compared to a glass slide.

In the course of evolution, nature is honed to solve the maze puzzle of "try, match, and combine" by means of the adaptation and integration of unlike characteristics to offer complex biological functions. For instance, an eggshell should protect the embryo from physical damage and bacterial penetration, control the inner shell humidity, and act as a mineral reservoir required for the development of the embryo, all in one. Remarkably, such multi-functionalities are often crafted through innovations in structural and architectural arrangements and location-specific physical alterations (rather than chemical modifications). These strategies can result in material design frameworks that can push the boundaries of classical engineering materials and address long-standing challenges for the development of advanced engineering materials.

In our group, we investigate the physical principles deployed in biological composites and explore the ways the architecture arrangement, interfaces, and morphologies modulate the interaction of the materials with their environmental stimuli (force, hydration, light, and temperature). By combining and developing vibrational spectroscopy and tribological and optical characterization techniques, we investigate the elastic-inelastic responses and mechanical performance of the biological materials (Figs. a, b) and study the real-time evolution of stress/strain fields in biogenic ceramics (Fig. c). Moreover, we explore the optical performance of the translucent tissues and investigate the possibilities of their involvement in light-sensing or light-tracking functions (Figs. d—f). Understanding and translating these fascinating architecture-function correlations unveils the development of architecturally modulated (multi)functional materials and promotes sustainability by avoiding unnecessary chemical diversity.

References: [1] Amini, S.; Razi, H.; Seidel, R.; Werner, D.; White, W. T.; Weaver, J. C.; Dean, M. N.; Fratzl, P.: Shape-preserving erosion controlled by the graded microarchitecture of shark tooth enameloid. Nature Communications. (2020). 11, 5971.
[2] Eder, M.; Amini, S.; Fratzl, P.: Biological composites—complex structures for functional diversity. (2020) Science 362(6414) 543.

Dr. Shahrouz Amini

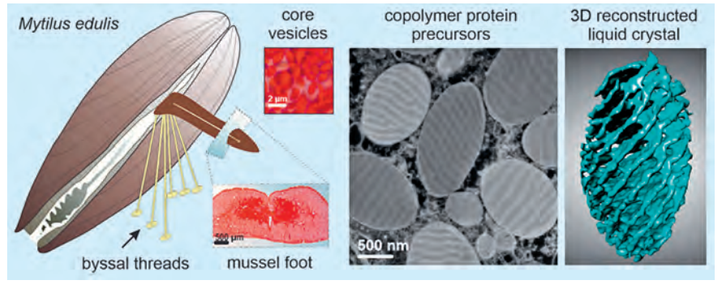
Group Leader since 2020

2017—2020 Max Planck Research Fellow
MPICI, Department of Biomaterials (Potsdam, Germany)

2016—2017 Postdoctoral Researcher
Energy Research Institute, Nanyang Technological University (NTU) (Singapore)

2015—2016 Postdoctoral Research Assistance
Materials Science and Engineering (MSE), Nanyang Technological University (NTU) (Singapore)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm



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Our research group focuses on the molecular and supramolecular principles and processes underlying the production of biological materials. In recent years, we have been developing theoretical approaches to describe water-mediated ionic, molecular, supramolecular, and macroscopic interactions, as well as multiscale analytical tools for in- and ex-situ characterization of the bonding state, structure, and mechanics of building blocks of biological materials. Using these tools, we formulated the fundamental hypothesis that specific aminoacidic sequences in the collagen molecule, when subjected to small osmotic pressure differences, can contribute to generate stresses in living tissues. Indeed, we could demonstrate that small collagen model peptides change their length as a response to an increase in water crowding and that the sign and the magnitude of this change depends on the aminoacidic sequence [1].

After having established a state-of-the art FIB/SEM-based volume imaging in cryogenic conditions, our group had access to the exciting world of the cellular and supramolecular processes underlying the production of biological materials and tissues. In collaboration with Matt Harrington (McGill University, Canada), we revealed insights into the self-organization and self-assembly of proteins smectic liquid crystals in the core fibers as well as the cuticle of the byssus of mussels [2]. Also, in collaboration with Yael Politi (MPIKG) we could investigate the fundamental mechanisms underlying the deposition and assembly of the (chitin-based) cuticular materials (in locusts) [3]. Furthermore, we reported for the first time the presence of an extended network of secondary channels in mineralizing tissues, like in the turkey leg tendon and in bone, which we hypothesize could act as passageways for the transport of ions, mineral precursors, and possibly mineralization inhibitors. In parallel, we have developed computational tools, also based on artificial intelligence techniques (within the BigMax network), for artifact removal, semi-automated 3D shape-based and texture-based segmentation, as well as for weekly-supervised label analysis of the acquired tomographic datasets.

References: [1] Ruiz-Rodriguez, L.; Loche, P.; Thornfeldt Hansen, L.; Netz, R. R.; Fratzl, P.; Schneck, E.; Blank, K.; Bertinetti, L.: Sequence-specific response of collagen-mimetic peptides to osmotic pressure. Mrs Bulletin 1—13 (2021) doi:10.1557/s43577-021-00138-9.
[2] Jehle, F.; Premiel, T.; Strauss, M.; Fratzl, P., Bertinetti, L.; Harrington, M.: Collagen Pentablock Copolymers Form Smectic Liquid Crystals as Precursors for Mussel Byssus Fabrication. Acs Nano (2021) doi:10.1021/acsnano.0c10457.
[3] Sviben, S.; Spaeker, O.; Bennet, M.; Albéric, M.; Dirks, J.-H.; Moussian, B.; Fratzl, P.; Bertinetti, L.; Politi, Y.: Epidermal Cell Surface Structure and Chitin-Protein Co-assembly Determine Fiber Architecture in the Locust Cuticle. ACS applied materials & interfaces (2020).

Fig. 1 Marine mussels fabricate hierarchically structured collagenous fibers with self-healing capacity known as byssal threads via supramolecular assembly of protein precursors.

Dr. Luca Bertinetti

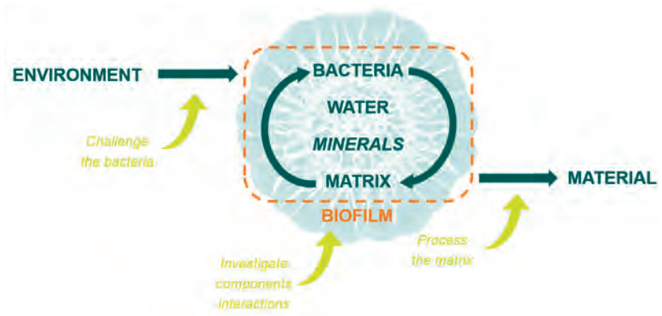
Group Leader 2017–2020

2010—2016 Independent Researcher
Water interactions in complex biological materials, MPICI (Potsdam, Germany)

2006 PhD in Chemical Sciences
Nanomaterials for biomedical applications: synthesis and surface characterization, University of Torino (Italy)

2001 Master of Science (110/110 cum laude)
Majoring in Materials Science, from solvated atoms to nanoparticles: a study on hydrogenation catalysts, University of Torino (Italy)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm



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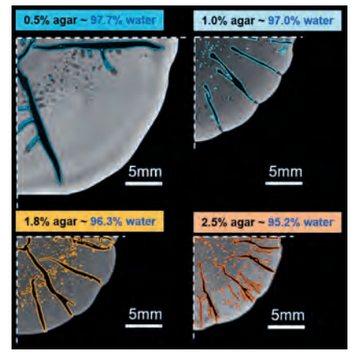

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Fig.1 Schematic representation of our approach to tuning and understanding biofilm-based materials properties.
Fig. 2 *E. coli* biofilm morphology on nutritive substrates with various agar concentrations after 90 h of growth. Colored contours outline delaminated buckles (adapted from [2] under Creative Commons BY license).

As bio-sourced materials are raising interest for their sustainability, using the ability of bacteria to produce biofilms made of a protein and polysaccharide matrix has become a new strategy to make "engineered living materials" with various functionalities. Our group aims to contribute to this emerging field of research by clarifying how bacteria adapt biofilms to their environment, and to use this knowledge to engineer the materials properties of these microbial tissues.

For this, we culture *E. coli* producing curli amyloid and phosphoethanolamine-cellulose fibers, plate them on nutritive agar substrates with varying physico-chemical properties, and study the growth, morphology, and mechanical properties of the resulting biofilms. For example, we demonstrated that changing the surface properties of the agar with cationic polyelectrolyte coatings limits biofilm spreading but increases their surface density via extended wrinkling in the third dimension [1]. Following similar strategies, we also showed that *E. coli* adapt their biofilm growth, morphology, and mechanical properties to the water content of their substrate [2]. Finally, we demonstrated that adding calcium and organic phosphate into the nutritive agar enables bacteria to mineralize the biofilm with hydroxyapatite crystals, thereby turning the soft tissue into a hybrid organic-inorganic material.

In collaboration with (bio)chemists, we also explore how post-processing biofilms can help further tune their properties (e.g. by treatment with ionic solutions) and investigate the interactions between matrix components (e. g. curli, cellulose, and water) at the molecular level to clarify their contribution to the ultimate materials properties [3].

References: [1] Ryzhkov, N. V.; Nikitina, A. A.; Fratzl P.; Bidan, C. M. *; Skorb E. V.*: Polyelectrolyte substrate coating for controlling biofilm growth at solid-air interface. Advanced Materials Interfaces (2021).
[2] Ziege, R.; Tsirigoni, A. M.; Large, B.; Serra, D. O.; Blank, K. G.; Hengge, R.; Fratzl, P.; Bidan, C. M.: Adaptation of E. coli biofilm growth, morphology, and mechanical properties to substrate water content. ACS Biomaterials Science & Engineering (2021).
[3] Siri, M.; Celej, M. S.; Fratzl, P.; Bidan, C. M.: Understanding biofilm physical and chemical properties at the molecular level. Biophysical Journal 66th Biophysical Society Annual Meeting, San Francisco, California, USA (2022).

Dr. Cécile Bidan

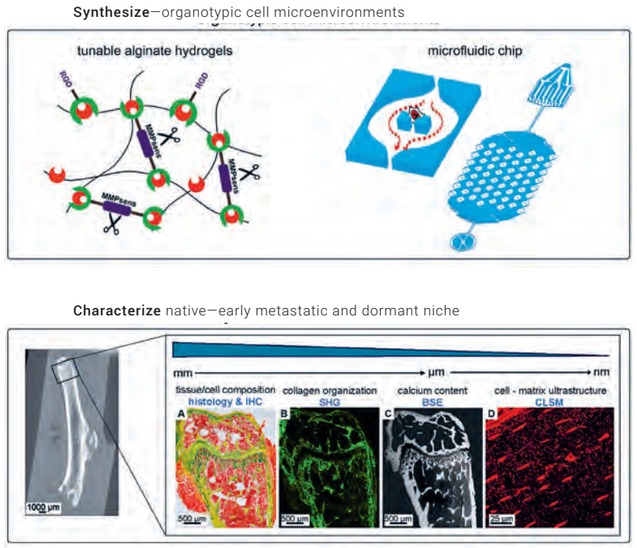
Group Leader since 2017

Since 2021 Principal Investigator in the Research Unit "InterDent" School of Dentistry, Charité Universitätsmedizin (Berlin, Germany)

2014—2017 Postdoctoral Researcher in Biophysics University Grenoble-Alpes, CNRS, Laboratory for Interdisciplinary Physics (LIPhy), Optics and mechanics instrumentation to decode mechanotransduction (France)

2013—2014 Postdoctoral Researcher in Biomechanics Groningen University, Department of Molecular Pharmacology (Netherlands), Medical Center BIDMC—Harvard Medical School (Boston, USA)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm



Our interdisciplinary group is interested in clinically-inspired basic and translational research at the intersection between bioengineering and biomedicine. We aim to understand how biophysical and biochemical properties of native extracellular matrix and synthetic biomaterials guide cell response in tissue regeneration, cancer dormancy, and bone metastasis. Our group activities are focused on two main research areas and the approach originates from a bioengineering, biotechnology, and/or biomaterials perspective:

1. Bioengineering and cancer research.
We investigate the effect of biophysical mechanisms in controlling cancer dormancy and bone metastasis [1—2], with special emphasis on breast cancer and multiple myeloma. Our experimental approach uses (i) engineering systems such as hydrogels [3] or microfluidic systems that obtain inspiration from (ii) in vivo models, investigated using in vivo imaging and ex vivo multiscale correlative characterization (Fig. 1). We are developing mathematical models based on evolutionary game theory to gain new insights about the interactions between disseminated cancer cells and their microenvironment, specifically in the organ bone. From a translational point of view, we have a strong collaboration with oncologists that allows us to extend our work to human bone biopsies of multiple myeloma patients at different stages of the disease, as well as human pancreatic tumor tissue.

2. Biomaterials and regenerative medicine.
We investigate the effect of biomaterial physical properties, such as stiffness, geometry, or degradation properties of 3D printed scaffolds or hydrogels [3], on cell response and in vivo tissue regeneration, using small and large animal models. We perform multiscale characterization of hierarchical biological tissues, with particular attention to the biomaterial-tissue interface. From a translational point of view, we participate in the European project HEALIKICK, where we will develop a modular strategy for the repair of critical-sized bone fractures.

This work is performed together with collaboration partners at the MPICI as well as national and international researchers.

References: **[1]** Bakhshandeh, S.; Werner, C.; Fratzl, P.; Cipitria, A.: Microenvironment-mediated cancer dormancy: Insights from metastability theory. Proceedings of the National Academy of Sciences (2022).
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[3] Lueckgen, A.; Garske, D.; Ellinghaus, A.; Mooney, D. J.; Duda, G. N.; Cipitria, A.: Dual alginate crosslinking for local patterning of biophysical and biochemical properties. Acta Biomaterialia 115, p. 185—196 (2020).

Dr. Amaia Cipitria

Group Leader 2017—2021

2021 Permanent position as Principal Investigator Biodonostia Health Research Institute, Ikerbasque Research Associate (Spain)

2020—2022 Graduation of three doctoral students Aline Lueckgen (2020), Sadra Bakhshandeh (2022), Hubert M. Taïeb (2022), TU Berlin (Germany)

2017 DFG (German Research Foundation) Emmy-Noether grant Principal investigator of project: "Extracellular matrix biophysical cues in dormancy and bone metastasis"

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm

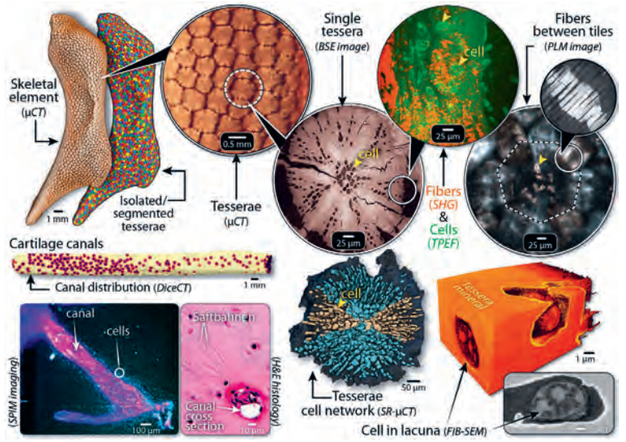

Fig. 1 Multimodal, correlative imaging approaches for characterizing shark/ray cartilage. The techniques used (listed with each image) allow tissue characterization from diverse perspectives and across a huge range of size scales.
© M. Dean, J. Chaumel, B. Wang, J. Ciecierska-Holmes

Skeletal tissue biology research is dominated by work on a few model mammal species, although mammals are < 10 % of living vertebrates. A wider view on natural tissue diversity is needed to understand how nature builds and regulates structure and the complex relationships between structural hierarchy and mechanical properties.

In our group, we focused particularly on fishes, which have hugely diverse ecologies and skeletal tissues, providing unique views into how anatomy and performance interrelate and evolve. Our recent work centers on shark/ray skeletons (Fig. 1), a platform for understanding cartilage biology and development, but also for probing general concepts in multi-scale structure-function. Shark/ray cartilage has a distinct outer crust of mineralized tiles (tesserae) linked by collagen fibers. The limited regeneration of human cartilage remains a major medical challenge; since shark/ray cartilage/cells have long lifespans and high performance, we are particularly interested in factors that distinguish shark/ray cartilage from ours.

We recently revealed an extensive vascular network in adult ray cartilage, with matrix passages (cartilage canals: Fig. 1; [1]) known only in young mammal cartilage. Our staining/imaging protocols allow 3D mapping of canals and nearby cells [2] to explore cell/ECM/canal interactions. Juxtaposed soft and hard tissues challenge imaging, but J. Chaumel's work—developing structure-sensitive fixation, clearing, and label-free imaging (e.g. using autofluorescence, non-linear microscopy [3])—allowed individual detection of cell/ECM components in bulk cartilage, even without staining (Fig. 1), a huge boon for 3D mapping tissue structure. Similarly, synchrotron µCT and FIB-SEM allow us to image tissue/cell interactions at cartilage mineralization fronts at high resolution. With B. Yang's ongoing work mapping 3D tesserae development and labeling growing tissues (w/ M. Debiais-Thibaud, Univ. of Montpellier), we can now explore finescale interplays of hard and soft tissues, even as they are assembled.

Our techniques allow in situ characterization and imaging of diverse (soft-hard) tissue components, key to the intriguing properties of many biological materials. In J. Ciecierska-Holmes' work, we now use these approaches to understand broader structure-mechanics links across varied natural tiled architectures in the "Tessellated Materials Systems" group of the Humboldt Excellence Cluster (w/ John Nyakatura, Humboldt Univ.).

References: [1] Dean M. N. et al. Cartilage canals in ray skeletons: Morphology, homology and putative role in mineralization. Integrative and Comparative Biology (2020).
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[3] Chaumel, J. et al. Autofluorescence of stingray skeletal cartilage: Hyperspectral imaging as a tool for histological characterization. Discover Materials (2021).

Dr. Mason Dean

Group Leader 2017—2021

Since 2021 Associate Professor
City University of Hong Kong (China)

2011—2017 Independent Researcher and HFSP Workgroup Leader (2011—2017), Group Leader (2017—2021)
MPICI, Department of Biomaterials (Potsdam, Germany)

2009—2011 Alexander von Humboldt Fellow
MPICI, Department of Biomaterials (Potsdam, Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm

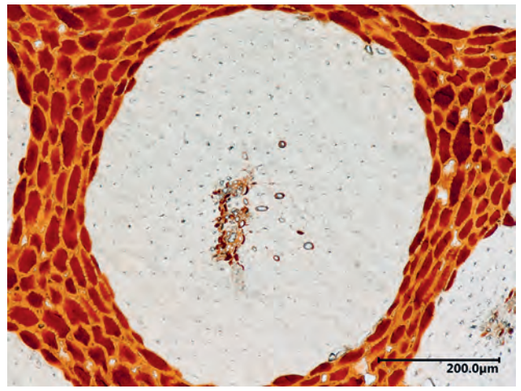

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Foto: Alexander Mageri

The MoA research group "Adaptive Fibrous Materials" investigates interactions between fibrous biological materials and their environments. Plants, sessile by nature, are particularly suited regarding their adaptability and optimization strategies since there is no way for them to escape the environment after germination. Remodeling processes, such as those found in the animal kingdom, are absent and adaptation occurs by growth. A large proportion of newly formed cells dies after a short period of time to take over water-transport, mechanical, or protective functions [1]. Over time the properties and functions of these dead cells can change; but at any time they are influenced by the temperature and humidity of the environment. This requires an intrinsic activity of the material [2]. Prominent examples are wood swelling and environmentally triggered seed capsule opening or seed dispersal.

We work towards a deep understanding of material activity and adaptation and optimization strategies, as well as exploring material properties under consideration of developmental stages and the environmental conditions in the field or in the lab. The results provide information about functions of the organism and hint how changing environmental conditions affect the organism. Furthermore, we create fundamental knowledge for the usage and applications of biogenic materials. The extracted material concepts can serve as inspiration for biomimetic applications. By combining materials science tools with design experiments, first steps towards applications are done, e.g. in the bark project, where bark, often seen as a large-scale waste material, is transformed into products, such as textiles or panels [3]. The creation of a woven bark sphere, a boundary object, should initiate discussions related to a more sustainable use of natural, renewable resources.

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[2] Eder, M.; Schäffner, W.; Burgert, I.; Fratzl, P.: (2021) Wood and the Activity of Dead Tissue, Advanced Materials, 33(28) 2001412.
[3] Wenig, C.; Dunlop, J. W. C.; Hehemeyer-Cürten, J., Reppe, F. J.; Horbelt, N.; Krauthausen, K.; Fratzl, P.; Eder, M.: (2021) Advanced materials design based on waste wood and bark. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 279 (2206) 20200345.

Fig. 1 Cross section of a mesocarp fiber bundle of a Banksia seed pod.
Fig. 2 Woven bark sphere.

Dr. Michaela Eder

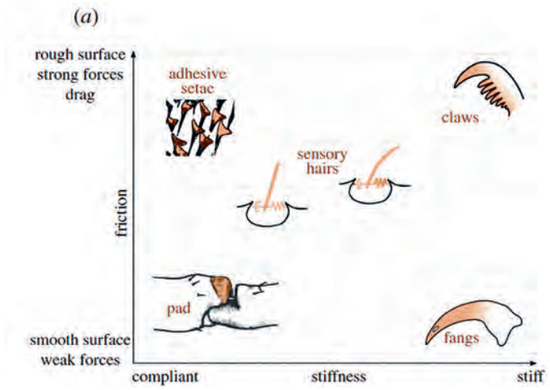
Group Leader since 2011

Since 2020 Principal Investigator in the Cluster of Excellence "Matters of Activity"
MPICI, Department of Biomaterials (Potsdam, Germany)

2007—2011 Postdoc
MPICI, Department of Biomaterials (Potsdam, Germany)

2003—2007 PhD Student
BOKU University of Natural Resources and Applied Life Sciences (Vienna, Austria) and MPICI (Potsdam, Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm



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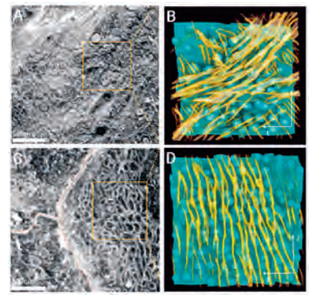

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The arthropod cuticle is a fascinating system with which to study how biological materials are formed and their properties determined. Multifunctionality emerged through evolution as a common solution to various, sometimes competing, requirements, leading to a material with remarkable versatility [1].

The cuticle supports locomotion and forms tools for piercing and cutting, sensors, structural colors lenses, and more. Unlike human technology, which led to a huge diversification of the material's composition, all this is achieved by local architectural variations of the basic building blocks. We believe that this research could inspire new ways of tuning materials properties without increasing the diversity of material compositions, leading to more sustainable materials and device production. To that end, we strive to understand how cuticle architecture is determined [2] and what the effect of minor compositional variations is [3]. In the cuticle, chitin is arranged in the form of nanofibrils wrapped by an organized protein coat. These fibers arrange into two-dimensional sheets of parallel fibers. The sheets are then stacked on top of each other, where the orientation of the fibers between sheets is either unchanged or slightly rotated. The result is a parallel stack arrangement or a helicoidal structure akin to an aligned nematic or cholesteric liquid crystal organization, respectively.

Studying the circadian-clock-regulated cuticle deposition in the locust, *Locusta migratoria*, which involves alternating deposition of helicoidal and plywood structured layers, we discovered that the epidermal cell surface determines an initial fiber orientation from which chitin-protein co-assembly leads to the final fiber architecture [2].

References: [1] Politi, Y.; Bertinetti, L.; Fratzl, P.; Barth. F. G.: The spider cuticle: a remarkable material toolbox for functional diversity. Philosophical Transactions of the Royal Society A. (2021).
[2] Sviben, S.; Spaeker, O.; Bennet, M.; Albéric, M.; Dirks, J.-H.; Moussian, B.; Fratzl, P.; Bertinetti, L.; and Politi, Y.: Epidermal cell surface structure and chitin-protein co-assembly determine fiber architecture in the Locust cuticle. ACS Applied Materials & Interfaces. (2021).
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Fig. 1 Cuticle versatility in C. salei. A mechanical design space contrasting friction vs. stiffness. Top left: adhesive setae. Top right: tarsal claws. Bottom right: fangs. Bottom left: the cuticular pad—a high pass filter for surface vibration. Center: sensory setae.
Fig. 2 FIB/SEM micrographs (left) and reconstructed volume (right) of the assembly zone and apical surface of epidermal cells in L. migratoria. Compare the apical microvilli and fiber orientation in the deposition of helicoidal (upper) and parallel arrangement (bottom panel). In the latter, microvilli arrange in ridges.

Prof. Dr. Yael Politi

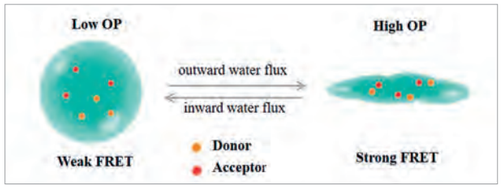
Group Leader 2012—2019

Since 2022 Director of the B CUBE-Center for Molecular Bioengineering
at TU Dresden (Germany)

Since 2019 Chair of Bioprospecting
at TU Dresden (Germany)

2009—2012 Postdoctoral Scientist
Alexander von Humboldt fellow, MPICI, Department of Biomaterials (Potsdam, Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm



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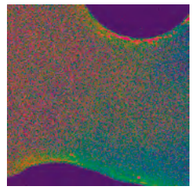

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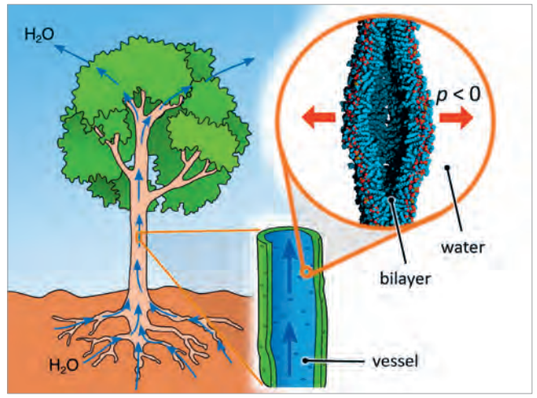

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Fig. 1 (a) Illustration of the measurement principle of OP sensors. (b) Imaging of OP in the coalescence region of two droplets with different initial OPs.
Fig. 2 Negative pressure ($p < 0$) induces cavities in lipid bilayers which destabilize the liquid in plant conduits.

Biological soft matter is composed of water and a great variety of biomolecules that are often organized in the form of supramolecular assemblies. We investigate soft matter of biological or biotechnological relevance, such as lipid membranes, biopolymers, or protein layers. While much of our work concerns the study of biomolecules at interfaces, we have recently extended our activities towards phenomena in the bulk phase, in particular towards special forms of what is commonly simply referred to as "pressure".

One of these forms, osmotic pressure (OP), is used by organisms to dehydrate certain molecular assemblies or tissue compartments. As previously demonstrated by MPICI researchers, OP can generate directed forces through its dehydrating action on fibrous biopolymers. The force-inducing contraction exhibits a strong dependence on the polymer chemistry [1]. With the mid-term goal of imaging the distribution of OP in vivo, we have recently developed micron-sized OP sensors based on liposomes loaded with fluorescent dyes exhibiting resonance energy transfer (FRET). Upon osmotic dehydration of the liposomes, the FRET efficiency increases (Fig. 1 top) and reports the local OP surrounding each sensor [2]. In this way, spatiotemporal OP imaging becomes feasible, see Fig. 1 (bottom).

Another form of pressure, namely negative pressure, occurs in the conduits of plants when water is pulled from the soil into the leaves (Fig. 2). The strongest negative pressures observed in plants have a magnitude of about 80 bars, although water can tolerate much more before becoming unstable due to the formation of rapidly growing cavities. We found that the presence of lipid bilayer aggregates in the plant liquid catalyzes cavity formation and may thus be what limits negative pressures in plants [3].

References: **[1]** Ruiz-Rodriguez, L.; Loche, P.; Thornfeldt Hansen, L.; Netz, R. R.; Fratzl, P.; Schneck, E.; Blank, K. G.; Bertinetti, L.: Sequence-specific response of collagen-mimetic peptides to osmotic pressure; MRS Bulletin, 46, 889–901 (2021).
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[3] Kanduc, M.; Schneck, E.; Loche, P.; Jansen, S.; Schenk, H. J.; Netz, R. R.: Cavitation in lipid bilayers poses strict negative pressure stability limit in biological liquids; Proc. Natl. Acad. Sci. USA, 117, 10733 (2020).

Prof. Dr. Emanuel Schneck

Group Leader 2014–2019

Since 2019 Professor
Physics Department, Technische Universität Darmstadt (Germany)

2014 Emmy-Noether Grant by the German Research Foundation (DFG)

2012–2014 Marie-Curie Fellow
Institut Laue-Langevin (Grenoble, France)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm

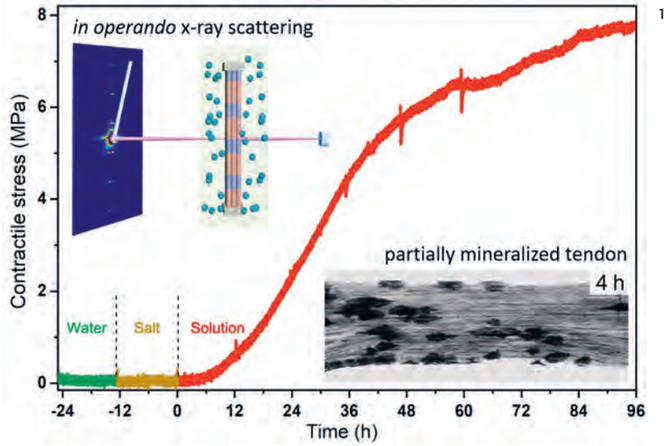

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Fig. 1 Contractile stress evolves during mineralization with $SrCO_3$ of a tendon (inset at lower right). Schematic of in operando synchrotron X-ray scattering measurements (inset on upper left).

References: [1] Schemenz, V.; Gjardy, A.; Chamasemani, F. F.; Roschger, A.; Roschger, P.; Zaslansky, P.; ... & Wagermaier, W. (2020). Heterogeneity of the osteocyte lacuno-canalicular network architecture and material characteristics across different tissue types in healing bone. Journal of Structural Biology, 212(2), 107616.
[2] Ping, H.; Wagermaier, W.; Horbelt, N.; Scoppola, E.; Li, C.; Werner, P.; Fu, Z.; Fratzl, P. (2022). Mineralization generates megapascal contractile stresses in collagen fibrils. Science, 376(6589): 188—192.
[3] Seidt, B.; Samsoninkova, V.; Hanßke, F.; Gjardy, A.; Fratzl, P.; Börner, H. G.; Wagermaier, W. (2020). Correlative analysis of specific compatibilization in composites by coupling in situ X-ray scattering and mechanical tensile testing. Frontiers in Materials, 348.

The research group addresses biological and bio-inspired materials from a materials science viewpoint and aims to devise material design concepts. In these materials, we characterize structure-function relations across several length scales by employing combinations of high resolution 2D and 3D imaging techniques, such as synchrotron X-ray scattering and microscopy techniques, and tailored mechanical testing equipment.

Numerous properties of bone are based on its character as a hybrid material, i.e. the structural interaction of soft, organic collagen fibers and the embedded hard, crystalline mineral particles. Bone also contains a lacuno-canalicular network (LCN) housing osteocytes. In healing bone, we visualized and correlated spatial variations in the LCN topology with mineral characteristics to detect interactions between cells and the surrounding material [1]. This approach revealed structural differences across several length scales during healing within calcified cartilage, bony callus, cortical bone, and the transition zones in between. The findings indicate that osteocytes contribute to (de)mineralization processes in bone.

Recently we discovered that the mineralization of tendons is accompanied by a shortening of collagen fibers, creating contractile stresses of up to several megapascals [2] (Fig. 1). By in operando X-ray scattering at the synchrotron BESSY in Berlin, we observed changes in the collagen structure during mineralization with six different minerals. The fiber contraction during mineralization puts the mineral under enormous pre-stress, which increases the overall strength of the composite material. This concept can potentially be transferred to technical hybrid materials to enhance their fracture resistance.

We also investigated synthetic hybrid materials based on magnesium fluoride nanoparticles coated with a glue-like conjugate phase, adhering the particles to a polymeric matrix [3]. In operando X-ray scattering revealed that the conjugation in these hybrid materials primarily generates non-agglomerated, nanometer-sized particles and that the mechanical performance improves with an increasing amount of conjugate.

Dr. Wolfgang Wagermaier

Group Leader since 2009

2015 Research stay
in the Department of Bioproducts and Biosystems, Aalto University (Finland)

Since 2013 Scientific and Administrative Leader
of the MPI synchrotron group at the µSpot beamline at BESSY II (Berlin) and MPICI, Department of Biomaterials (Potsdam, Germany)

2007–2009 Postdoc
Center for Biomaterial Development, GKSS Research Center Geesthacht GmbH, Teltow (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm

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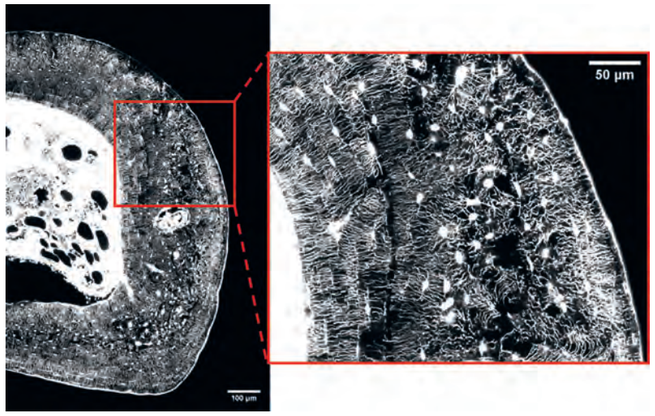


Fig. 1 Lacunocanalicular network (LCN) in mouse tibia with ellipsoidal lacunae accommodating the osteocyte cell bodies and canaliculi the cell processes.

Mechanobiology studies the structural response of biological systems to mechanical stimulation. In bone, structural adaptation occurs via a mechanically induced resorption of old and formation of new bone. This remodeling process has to be controlled by bone cells acting as mechanosensors. However, bone is very stiff, so mechanical strains are assumed to be too small to be directly sensed by cells. As a solution to this dilemma, the Fluid Flow Hypothesis was proposed, stating that a load-induced fluid flow through the lacunocanalicular network (LCN) acts as a mechanical stimulus. The LCN forms an intricate porosity (Fig. 1) permeating the bone and accommodates the cell network of osteocytes. The fluid flow through this network then creates shear and drag forces on the surface of the osteocytes.

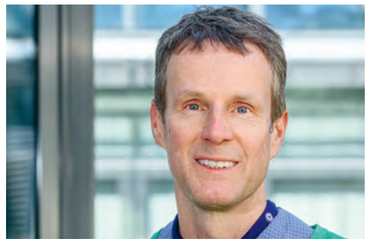
Recently, we performed a critical test of the Fluid Flow Hypothesis using a combination of three methods. First, the mechanoresponse to a controlled loading was measured in terms of newly formed and resorbed bone with time-lapsed in vivo µCT. Second, the 3D architecture of the LCN was obtained by confocal microscopy and image analysis. Third, circuit theory was used to calculate the fluid flow through the LCN. This new methodology was applied to the tibiae of three mice, and the measured mechanoresponse was compared to predictions based on fluid flow calculations. The consideration of the LCN architecture predicted correctly that (i) the mechanoresponse is similar on the outer periosteal and the inner endocortical surface of the tibia and (ii) individual differences in the mechanoresponse between mice [1].

Evidence is accumulating that the lacunocanalicular network also plays an important role in the mineralization process and in mineral homeostasis. We observed that bone mineralization starts first far away from canaliculi, leaving a zone around canaliculi free of mineral. We interpreted this as the LCN acting as the source of both mineral precursors and inhibitors [2]. In fully mineralized bone, we could show that regions with a denser network are more highly mineralized. This points to the LCN serving as an additional mineral reservoir [3].

References: [1] van Tol, A.F.; Schemenz, V.; Wagermaier, W.; Roschger, A.; Razi, H.; Vitienes, I.; Fratzl, P.; Willie, B.M.; Weinkamer, R.: The mechanoresponse of bone is closely related to the osteocyte lacunocanalicular network architecture. Proceedings of the National Academy of Sciences, 117, 32251 (2020).
[2] Ayoubi, M.; van Tol, A.F.; Weinkamer, R.; Roschger, P.; Brugger, P.C.; Berzlanovich, A.; Bertinetti, L.; Roschger, A.; Fratzl, P.: 3D interrelationship between osteocyte network and forming mineral during human bone remodeling. Advanced healthcare materials, 10, 2100113 (2021).
[3] Roschger, A.; Roschger, P.; Wagermaier, W.; Chen, J.; Van Tol, A.F.; Repp, F.; Blouin, S.; Berzlanovich, A.; Gruber, G.M.; Klaushofer, K.; Fratzl, P.; Weinkamer, R.: The contribution of the pericanalicular matrix to mineral content in human osteonal bone. Bone, 123, 76 (2019).

Dr. Richard Weinkamer

Group Leader since 2003



2012 Habilitation in Theoretical Physics
Humboldt University (Berlin, Germany)

2000—2003 Postdoctoral Scientist
Erich Schmid Institute of Materials Science (Leoben, Austria)

2000 PhD in Physics
University of Vienna (Austria)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bm

Department of Biomolecular Systems

Department of Biomolecular Systems

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Prof. Dr. Peter H. Seeberger

2021 Vice President
German Research Foundation, Bonn

2021 Fellow
Lincoln College, Oxford University

2021 ACS Award
for Affordable Green Chemistry

2020 Emil Fischer Medal
German Chemical Society

2021—2022 Newton-Abraham Visiting Professor
Oxford University (UK)

The Department of Biomolecular Systems uses synthetic chemistry as a tool to understand the role of biopolymers in biological systems by working at the interface of chemistry, engineering, biology, immunology, medicine, and materials science. The transdisciplinary approach often involves multiple groups in the department covering different areas of expertise. In addition to the core focus on the glycosciences, with efforts ranging from synthetic methods to vaccines, material science, antibody development, and X-ray crystallography, synthetic organic methods in the areas of catalysis and flow chemistry are being explored.

The department is operating in a steady state. In the past three years, four group leaders left the department to assume professorships at other institutions: Prof. Christoph Rademacher is now at the University of Vienna, Prof. Fabian Pfrengle moved to the University of Natural Resources and Life Sciences, Vienna, Prof. Kerry Gilmore is at the University of Connecticut, and Prof. Daniel Varón Silva at the University of Applied Sciences Basel. During the same period, two new group leaders joined the department, Dr. Dario Cambié is now in charge of the Continuous Flow Chemistry group, and Dr. John J. Molloy heads the Synthetic Methodology and Reaction Design group, having received a Liebig Fellowship to support his group. Dr. Thomas Weikl's group, Computational Biophysics, moved to our department from the Department of Theory & Bio-Systems after the retirement of Prof. Lipowsky. Together, we are actively pursuing different questions in the glycosciences, including the structure, function, and biological role of sugars found on the surface of mammalian and bacterial cells, particularly in the areas of immunology, biochemistry, and human disease.

Automated Glycan Assembly — AGA — our core technology developed in the department, has become a routine tool to prepare natural and unnatural oligosaccharides. A new generation of synthesizers is significantly faster and can access an unprecedented variety of ever-longer polysaccharides (current record: 151-mer). Synthetic glycans have been used to correlate glycan structure with glycan function, not only in biological systems but also for material science applications. Imaging techniques have allowed us to visualize single glycan molecules and study glycan folding and reaction mechanisms that had remained unexplained for over a century.

The medicinal chemistry approach to carbohydrate vaccine development has already yielded candidates entering clinical development. In the past three years, the focus has been on hospital-acquired bacterial infections such as *Klebsiella pneumoniae* as well as the zoonotic threat *Streptococcus suis*. Ready access to synthetic oligo- and polysaccharides has been the basis for the success of the Carbohydrate Materials group, which studies glycan structure and has made fundamental contributions to carbohydrate folding. The Synthetic Array Technologies group has developed methods for fully automated production of peptide microarrays and the synthesis of novel materials using combinatorial approaches. Anti- and nanobodies against glycans are powerful means to identify and eventually kill tumor cells, as studied in the Glycan Targeted Therapeutics group. The Carbohydrate Structure and Function group is using X-ray crystallography to study carbohydrate active enzymes.

The work on synthetic methodology and total synthesis is being pursued by three groups in the department. The most mature of these groups, Catalysis, has a heavy focus on photocatalysis, while the Synthetic Methodology and Reaction Design group is mainly concerned with organoboron chemistry. The Flow Chemistry group is working on new methods as well as the synthesis of important drug substances.

Publication selection

Le Mai Hoang, K.; Pardo-Vargas, A.; Zhu, Y.; Yu, Y.; Loria, M.; Delbianco, M.; Seeberger, P. H.: Traceless Photolabile Linker Expedites Chemical Synthesis of Complex Oligosaccharides by Automated Glycan Assembly. J. Am. Chem. Soc., 2019, 141, 9079—9086.

Chatterjee, S.; Guidi, M.; Seeberger, P. H.; Gilmore, K.: Automated Radial Synthesis of Complex Organic Molecules. Nature 2020, 579, 379—384.

Joseph, A.; Pardo-Vargas, A.; Seeberger, P. H.: Total Synthesis of Polysaccharides by Automated Glycan Assembly. J. Am. Chem. Soc., 2020, 142, 8561—8564.

Wu, X.; Delbianco, M.; Anggara, K.; Michnowicz, T.; Pardo-Vargas, A.; Bharate, P.; Sen, S.; Pristl, M.; Rauschenbach, S.; Schlickum, U.; Abb, S.; Seeberger, P. H.; Kern, K.: Imaging Single Glycans. Nature 2020, 582, 375—378.

Zhu, Y.; Delbianco, M.; Seeberger, P.H.: Automated Assembly of Starch and Glycogen Polysaccharides; J. Am. Chem. Soc., 2021, 143, 9758—9768.

↘ Further information can be found at https://www.mpikg.mpg.de/bs

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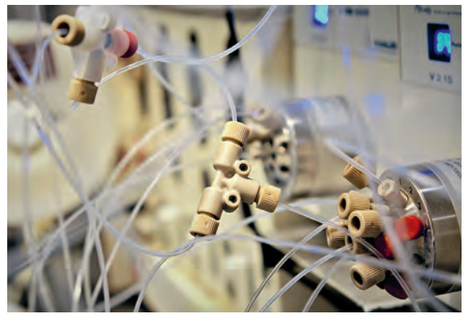

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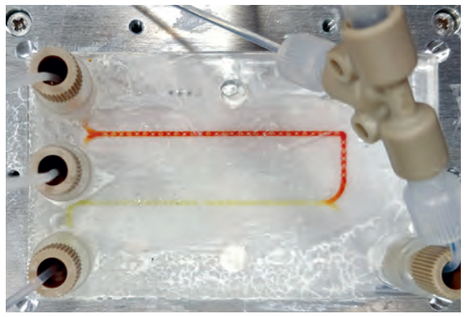

Often, in a research laboratory, the most valuable product of a reaction is not a pure chemical compound but rather information. In these cases, microreactor technology, where reactants are pumped in sub-millimeter-sized channels that replace conventional flasks, can reduce the amount of reactants needed to obtain such information. Key aspects of reactions performed in continuous flow are their reproducibility and scalability, ensured by the well-defined chemical engineering properties of the reactors. Moreover, microflow reactors can be easily automated, making them ideal to generate large datasets of reproducible and scalable reaction conditions to train statistical models on chemical reactivity.

In 2019 and 2020, the former Continuous Chemical Systems group trained a statistical model to predict the stereochemical outcome of glycosylations [1] based on results from an automated microreactor (an improved version of which is shown in Fig. 2).

Further research in 2021 focused on translating the reactivity trends observed in the microreactor to the parameters adopted in automated glycan assembly (AGA), such as the activation temperature.

Another significant result from the Continuous Chemical Systems group in 2020 was the introduction of an innovative automated flow reactor design, called the radial synthesizer [2] (shown in Fig. 1), where multi-step syntheses of targets are performed in a series of modules radially arranged around a central switching station.

In a continuation of that research, it was shown [3] that the reaction conditions optimized with the radial synthesizer can be easily translated to commercial flow reactors, obtaining similar results but with higher productivities and thus providing a solution for rapid process development, e.g. in case of sudden disruptions in the supply chain of fine chemicals.

References: [1] Moon, S.; Chatterjee, S.; Seeberger, P. H.; Gilmore, K.: Predicting glycosylation stereoselectivity using machine learning. Chemical Science (2021) 12, 2931—2939.
[2] Chatterjee, S.; Guidi, M.; Seeberger, P. H.; Gilmore, K.: Automated radial synthesis of organic molecules. Nature (2020) 579, 379—384.
[3] Guidi, M.; Moon, S.; Anghileri, L.; Cambié, D.; Seeberger, P. H.; Gilmore, K.: Combining radial and continuous flow synthesis to optimize and scale-up the production of medicines. Reaction Chemistry & Engineering (2021), 6, 220—224.

Fig. 1 Detail of the radial synthesizer. The valve on the right is part of the central switching station directing the reagents to the reaction modules (© 2020 Dario Cambié)
Fig. 2 The microreactor used for glycosylation mechanistic studies. The brownish color (iodine) generated upon activation is quenched in line. (© 2021 Dario Cambié)

Dr. Dario Cambié

Group Leader since 2020

2019—2020 Postdoc
University of Glasgow (Scotland)

2019 PhD cum laude (highest grade in NL)
Eindhoven University of Technology (Netherlands)

2018 SciFinder CAS Future Leader

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

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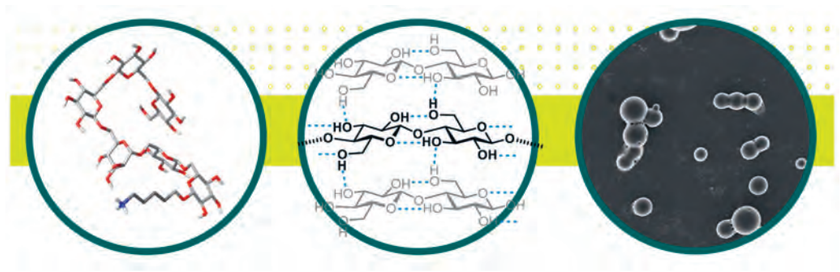

Polysaccharides can assemble into hierarchical architectures to generate materials, ranging from hard structural materials (e.g. cellulose) to dynamic hydrogels (e.g. glycosaminoglycans). Yet correlations between their chemical structure, conformation, and macroscopic properties have not been established. We prepared well-defined oligo- and polysaccharides resembling natural as well as unnatural structures using automated glycan assembly (AGA). With this approach, we generated polysaccharide probes, with full control over their length and modification, to study their fundamental properties. We employed computational methods, NMR spectroscopy, and single molecule imaging techniques to study polysaccharides' conformations [1]. We discovered that while some polymers form helices, others adopt rod-like structures; such three-dimensional structures are disrupted by single-site substitution [2].

Based on these insights, we designed synthetic oligosaccharides that self-assemble into supramolecular materials as models to understand the aggregation of natural polysaccharides. We combined several analytical techniques to reach a molecular level characterization of these carbohydrate materials. With microED analysis, we correlated the local crystal organization to the supramolecular architecture, allowing for the design of helical structures as well as flat lamellae [3]. These novel carbohydrate-based materials are crucial for a better understanding of biological process as well as for the creation of engineered platforms for biomedical applications.

References: [1] Wu, X.; Delbianco, M.; Anggara, K.; Michnowicz, T.; Pardo-Vargas, A.; Bharate, P.; Sen, S.; Pristl, M.; Rauschenbach, S.; Schlickum, U. et al.: Imaging single glycans. Nature 582 (7812), pp. 375—378 (2020).
[2] Yu, Y.; Tyrikos-Ergas, T.; Zhu, Y.; Fittolani, G.; Bordoni, V.; Singhal, A.; Fair, R. J.; Grafmüller, A.; Seeberger, P. H.; Delbianco, M.: Systematic hydrogen-bond manipulations to establish polysaccharide structure–property correlations. Angewandte Chemie International Edition 58 (37), pp. 13127—13132 (2019).
[3] Gim, S.; Fittolani, G.; Nishiyama, Y.; Seeberger, P. H.; Ogawa, Y.; Delbianco, M.: Supramolecular assembly and chirality of synthetic carbohydrate materials. Angewandte Chemie International Edition 59 (50), pp. 22577—22583 (2020).

Fig. 1 Three aspects of the research conducted in the Carbohydrate Materials group. Chemical synthesis, structural analysis, self-assembly.

Dr. Martina Delbianco

Group Leader since 2018

2017—2020 Minerva Fast Track Fellow
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

2015—2016 Postdoctoral Fellow
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

2012—2014 PhD in Chemistry
Durham University (UK)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

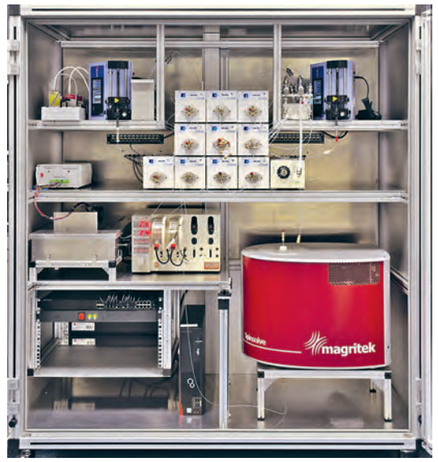

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Fig. 1 An automated platform for organic synthesis was developed that uses flow chemistry equipment arranged in a radial fashion.

The focus of the research group was the development of tools to better understand and perform organic chemistry. The foundation of these tools was a technique called flow chemistry, where chemistry is performed in thin tubing and reagents are passed through a set of environmental conditions, as opposed to a round-bottom flask to which conditions are applied. This subtle difference in approach has significant benefits to safety, reproducibility, and accessible reaction protocols. Over the years, we have developed a number of innovative approaches utilizing the intrinsic benefits of this technique to advance both single- and multi-step syntheses, as well as mechanistic understanding.

In the past two years, two major projects were realized that built on our foundational expertise. The first was the development of an automated platform for synthesis. This remotely-accessible instrument is capable of a wide variety of transformations and is designed in such a way that no manual reconfiguration is required between processes. Featuring in-line analytics, this instrument is fully capable of remote data generation, route exploration, and reaction/process optimization, see Fig. 1.

The second project saw the expansion of our work into data sciences. Using a previously gathered dataset of glycosylation selectivities, we trained a machine-learning algorithm to accurately predict the stereoselectivity of glycosylation reactions—transformations that are both mechanistically ambiguous and highly sensitive. Using this powerful approach, we were also able to gain valuable insights into the mechanistic variables influencing the selectivity.

During the 2019—2021 window, we published a number of additional studies not directly related to the two themes outlined above. The most notable of which was our discovery of and investigation into the activity of artemisinin, artemisinin-derivative, and even extract from the plant Artemisia annua (which produces artemisinin) against COVID-19.[3] This highly collaborative work showcased the potential of these compounds outside of their currently prescribed uses (malaria) and has spawned several new investigations currently ongoing into the broader activity of these compounds.

References: [1] Chatterjee, S.; Guidi, M.; Seeberger, P. H.; Gilmore, K.: Automated Radial Synthesis of Small Molecules. Nature 2020, 579, 379—384.
[2] Moon, S.; Chatterjee, S.; Seeberger, P. H.; Gilmore, K.: Predicting Glycosylation Stereoselectivity Using Machine Learning. Chemical Science 2020, 49, 8910—8932.
[3] Zhou, Y.; Gilmore, K.; Ramirez, S.; Settels, E.; Gammeltoft, K. A.; Pham, L. V.; Fahnoe, U.; Feng, S.; Offersgaard, A.; Trimpert, J.; Bukh, J.; Osterrieder, K.; Gottwein, J.; Seeberger, P. H.: In Vitro Efficacy of Artemisinin-Based Treatments Against SARS-CoV-2. Scientific Reports 2021, 11, 1—14.

Prof. Dr. Kerry Gilmore

Group Leader 2014—2020

Since 2020 Assistant Professor
University of Connecticut (USA)

2019—2020 W2 Research Group Leader
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

2014—2019 Group Leader
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

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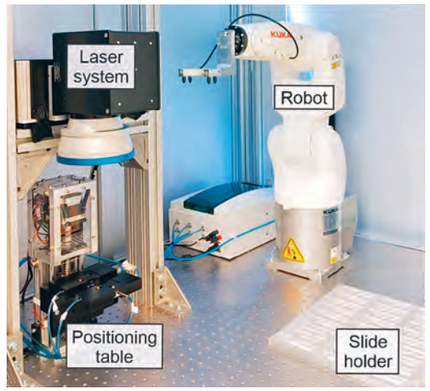

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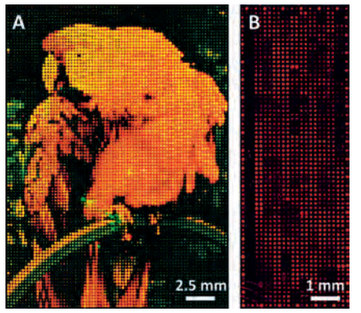

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Fig. 1 The laser-based synthesizer for automated synthesis of microarrays [1].
Fig. 2 Microarray generated by defined chemical mixing (A) and screening an Ebola virus peptide microarray (B) [1].

The Synthetic Array Technologies group pursues highly multi- and interdisciplinary research in chemistry, materials science, biology, engineering, physics, and computer science. The group develops novel microarray synthesis technologies for parallel and miniaturized chemical reactions by combining state-of-the-art laser processing with a polymer nanoreactor synthesis strategy. Instead of liquid solvents, solid polymers are used as a medium for the delivery of chemicals and reaction control. Similar to standard 3D printing, polymers, which can embed different chemicals, are printed in high resolution on surfaces by laser transfer. Heating the polymer above its glass transition temperature, the diffusion inside the polymer reactors can be "switched on" without losing its shape and position. Thus, many different reactions can be well controlled in small polymer nanoreactors in parallel, allowing the rapid synthesis of large libraries of different biomolecules or nanomaterials. The resulting libraries are used to discover novel diagnostic targets or catalysts in high-throughput.

As one core achievement, an automated laser-based synthesis machine was constructed, which offers fully automated production of diverse microarrays [1], now with a spot density of more than 100,000 spots per cm^2 [2]. Together with medical collaboration partners, the group has synthesized and applied peptide microarrays in high-throughput disease research and diagnostics, screening the proteomes of pathogens (e. g. Ebola) for vaccine research. Furthermore, they recently advanced their technology for printing while at the same time driving chemical reactions: They flash synthesized defined metal oxide nanoparticles [3] or performed photochemical reactions [2] within milliseconds.

References: [1] Paris, G.; Heidepriem, J.; Tsouka, A.; Liu, Y.; Mattes, D. S.; Dallabernardina, P.; Mende, M.; Lindner, C.; Wawrzinek, R.; Rademacher, C.; Seeberger, P. H.; Breitling, F.; Bischoff, F. R.; Wolf, T.; Loeffler, F. F.: Automated laser-transfer synthesis of high-density microarrays for infectious disease screening. Advanced Materials, 2200359 (2022).
[2] Zhang, J.; Liu, Y.; Ronneberger, S.; Tarakina, N. V.; Merbouh, N.; Löffler, F. F.: Nanolayer laser absorber for femtoliter chemistry in polymer reactors. Advanced Materials 34 (8), 2108493 (2022).
[3] Zhang, J.; Zou, Y.; Eickelmann, S.; Njel, C.; Heil, T.; Ronneberger, S.; Strauß, V.; Seeberger, P. H.; Savateev, A.; Löffler, F. F.: Laser-driven growth of structurally defined transition metal oxide nanocrystals on carbon nitride photoelectrodes in milliseconds. Nature Communications 12, 3224 (2021).

Dr. Felix Löffler

Group Leader since 2017

2020 Early Career Advisory Board
Chemistry—A European Journal

2019 ERC Starting Grant 2019
reserve list candidate (rated "A")
not funded due to budgetary cutoff

2017 NanoMatFutur
Research Group Award (€2.25 m)
German Federal Ministry of Education and Research (BMBF)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

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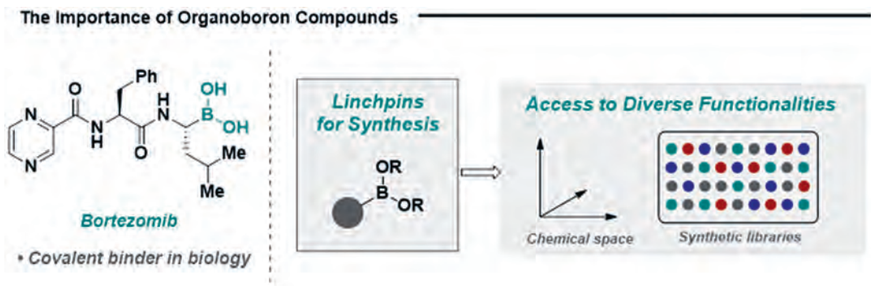

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Fig. 1 The importance of organoboron compounds in organic chemistry.
Fig. 2 Harnessing photocatalysis as an enabling technology for new reaction design.

New sustainable catalytic strategies which allow expedient access to structurally complex scaffolds from simple, easily accessible precursors is a highly desirable goal in modern synthetic chemistry. The group focuses on generating a firm understanding of reactivity at the molecular level through in-depth mechanistic analyses via various spectroscopic methods. These serve as a guiding principle for novel reaction design by translating the knowledge of reactivity to operationally simple synthetic methods in a laboratory paradigm. There are two key areas the group look to investigate:

Organoboron Chemistry
Organoboron motifs hold a privileged role in synthetic organic chemistry, particularly due to their versatility as a functional group, with many landmark transformations already well-established. The group is currently focused on synthetic strategies which transcend all reactivity aspects of organoboron chemistry, including methods which incorporate or retain the boron functionality. This enables access to small 3D fragments as well as structurally complex carbogenic frameworks bearing a boron linchpin for downstream synthetic manipulations.

Photocatalysis
The use of light as a cost-effective energy source to elicit chemical transformations has become an area of great interest. Compounds that absorb light and enable subsequent photochemical processes such as energy transfer or photo-induced electron transfer represent a sustainable strategy for future synthetic methods. The group looks to develop new transformative photocatalytic protocols that allow simple feedstock molecules to be readily converted into significantly more synthetically useful frameworks.

Dr. John J. Molloy

Group Leader since 2021

2022 Daimler and Benz Scholarship

2021 Liebig Fellowship
German Chemical Industry Funds (VCI)

2019 Alexander von Humboldt Postdoctoral Scholarship

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

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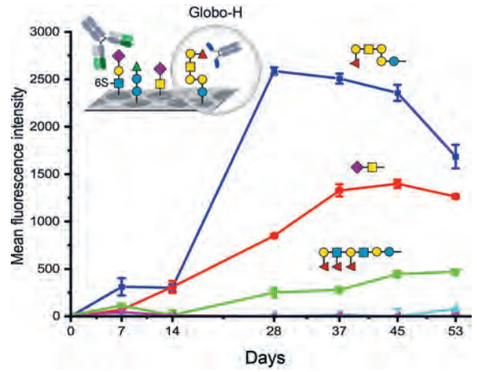

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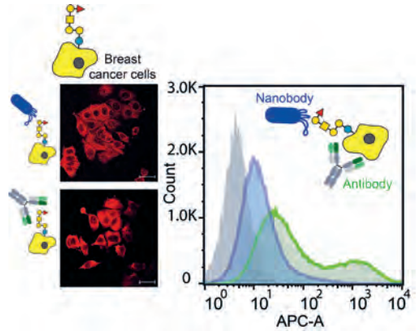

Glycans are the predominant molecules on our cell surface, and aberrant glycosylations or Tumor Associated Carbohydrates Antigens (TACAs) have served as a hallmark of cancer for more than 70 years, with TACAs expression being correlated with most aspects of cancer biology. Nevertheless, TACAs involvement in cancer or our immune response to TACAs expression on cancer cells is still far from fully understood. This is mainly due to insufficient molecular tools able to recognize specific glycan epitopes.

In my group, we utilize well-defined synthetic glycans to develop glycan-targeting compounds that are used for basic research, therapeutics, and diagnostics purposes. We have recently developed several antibodies and alpaca-derived single domain antibodies (or "nanobodies") against different TACA targets. Current work in my group focuses on two main topics: anti-Globo-H nanobody development (1) and novel TACA identification in blood sera of cancer patients (2).

(1) Previous work in my group produced nanobodies that target Globo-H [1]. Globo-H is an embryonic glycolipid that is uniquely over-expressed as TACA on roughly 80% of all human cancers. The nanobodies generated by immunizing alpaca with a synthetic Globo-H and additional TACAs (Fig. 1) are highly specific, also for the native Globo-H structures on cancer cells (Fig. 2). Our current work further exploits the versatility of nanobodies and the ease by which they can be engineered. We couple the nanobodies with fluorescent probes and anti-cancer drugs for further tests against breast cancer tumors in patient-derived xenograft (PDX) mouse models.

(2) In parallel, we collaborate closely with hospitals to screen sera and tissue samples from cancer patients. We first use synthetic glycan arrays to identify TACA-related antibody responses. Next, we stain the patient cancer tissues using antibodies and glycan-binding lectins. Finally, we measure the expression of the enzymes that assemble the TACAs in the cancer tissue. We combined the results to reveal glycan structures specific to tumors and different tumor stages. These novel insights then contribute to developing specific pharmaceuticals that broaden our limited anti-cancer toolbox.

References: [1] Khan Khilji, S.; Goerdeler, F.; Frensemeier, F.; Warschkau, D.; Lühle, J.; Zeinab Fandi, Z.; Schirmeister, F.; Angel Chen, Z.; Turak, O.; Mallagaray, A.; Boerno, S.; Timmermann, B.; Rappsilber, J.; Seeberger, P. H.; Moscovitz, O.: Generation of glycan-specific nanobodies. Cell Chemical Biology (2022).

Fig. 1 Synthetic glycan array analysis showing the generation of specific antibodies against tumor-associated carbohydrate antigens. We then use the alpaca serum to develop anti-TACA antibodies.
Fig. 2 Anti-Globo-H nanobodies bind native structures on breast cancer cells. Confocal microscopy (left) and flow cytometry (right) analysis prove specific binding of our nanobody and a control antibody to cancer cells.

Dr. Oren Moscovitz

Group Leader since 2018

2019 Co-founder of Tacalyx GmbH
Discovery and development of novel anti-TACA therapeutics

2014—2017 Research Fellow
Alexander von Humboldt Foundation

2013 Young Scientist Award
Israeli Society for Mass Spectrometry

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

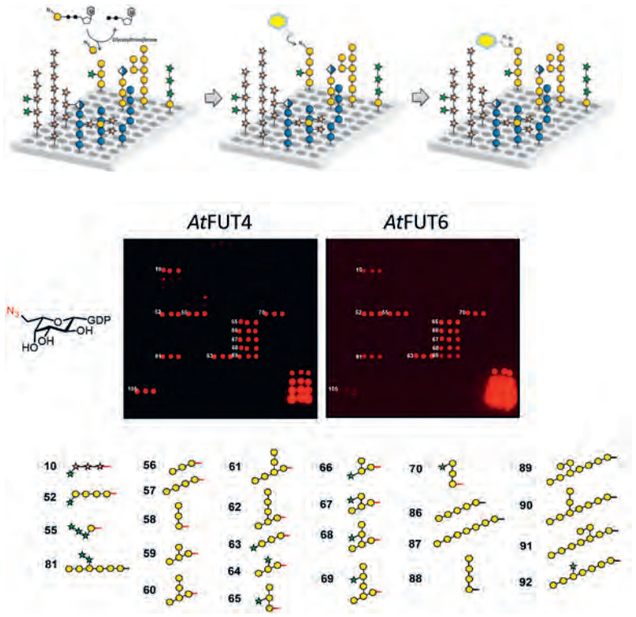

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Fig. 1 Glycan array-based assay for the identification and characterization of plant GTs. The array is incubated with a chemically modified nucleotide sugar donor and a putative GT, followed by visualization of any transferred monosaccharide by an "on chip" reaction with an alkynyl-functionalized-dye.

References: [1] Bartetzko, M. P.; Pfrengle, F.: Automated Glycan Assembly of Plant Oligosaccharides and Their Application in Cell Wall Biology. ChemBioChem 2019, 20, 877—885.
[2] Ruprecht, C.; Bartetzko, M. P.; Senf, D.; Lakhina, A.; Smith, P. J.; Soto, M. J.; Oh, H.; Yang, J.-Y.; Chapla, D.; Varon Silva, D.; Clausen, M. H.; Hahn, M. G.; Moremen, K.W.; Urbanowicz, B. R.; Pfrengle, F.: A Glycan Array-Based Assay for the Identification and Characterization of Plant Glycosyltransferases. Angew. Chem. Int. Ed. 2020, 59 (30), 12493—12498.
[3] Ruprecht, C.; Geissner, A.; Seeberger, P. H.; Pfrengle, F.: Practical considerations for printing high-density glycan microarrays to study weak carbohydrate-protein interactions. Carb. Res. 2019, 481, 31—35.

Plant biomass, which is comprised of carbohydrate-rich plant cell walls, represents the most abundant renewable resource on Earth. Plant cell walls represent a cellular exoskeleton that provides mechanical support for the growth and development of the plant. Oligosaccharide fragments of cell wall polysaccharides are valuable molecular tools for investigating the structure and function of this complex matrix of biopolymers. They can serve as acceptor molecules for glycosyltransferases, substrates for glycosyl hydrolases, epitopes for antibodies and glycan binding modules, and as ligands for plant immune receptors. Despite the importance of such molecules, the availability of well-defined and pure oligosaccharide samples is very limited. The major research scheme in the Synthetic Plant Carbohydrates group was the development of molecular tools for investigating the structure and biosynthesis of plant cell wall glycans. We have used automated glycan assembly to synthesize collections of oligosaccharides related to different classes of plant cell wall glycans. [1] These oligosaccharides were printed as glycan arrays to establish a high-throughput assay for the identification and characterization of plant cell wall biosynthetic glycosyltransferases. [2] Incubation of the array with putative glycosyltransferases and azido-functionalized nucleotide sugars followed by visualization of transferred monosaccharides by reaction with a fluorescent dye allowed the simultaneous screening of large numbers of individual combinations of enzyme, donor, and acceptor. En route to establishing this glycan array assay, we evaluated different printing buffers and compared slides from different manufacturers to provide practical advice for selecting the right printing conditions tailored to particular applications. [3] The long-term goal of our studies is to provide enabling knowledge for breeding plants with improved material properties and resistance to pathogens.

Prof. Dr. Fabian Pfrengle

Group Leader 2013—2020

2015—2020 DFG Emmy Noether Program

2010—2013 Research Associate
(Advisor: Prof. James Paulson)
Department of Chemical Physiology,
The Scripps Research Institute
(La Jolla, USA)

2010 PhD in Organic Chemistry
Graduated with Highest Honors,
Freie Universität Berlin (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

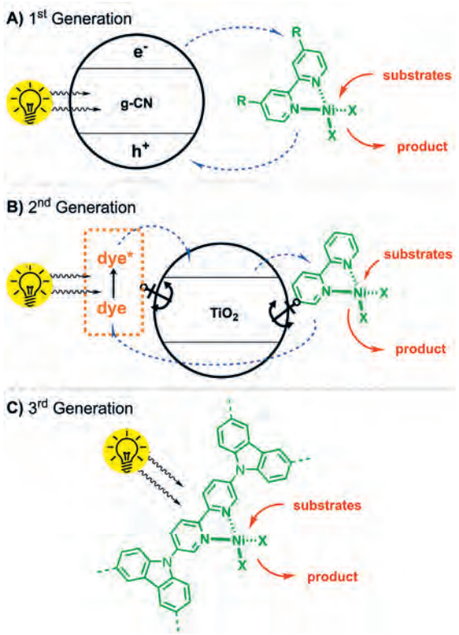

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Fig. 1 Our developments towards sustainable visible-light-mediated cross-couplings.

References: [1] Gisbertz, S.; Reischauer, S.; Pieber, B.: Nat. Catal. 2020, 3, 611.
[2] Reischauer, S.; Strauss, V.; Pieber, B.: ACS Catal. 2020, 10, 13269.
[3] Cavedon, C.; Gisbertz, S.; Vogl, S.; Richter, N.; Schrottke, S.; Teutloff, C.; Seeberger, P. H.; Thomas, A.; Pieber, B.: ChemRxiv 2021, DOI: 10.33774/chemrxiv-2021-kt2wr.

Our group develops sustainable catalytic transformations and new catalysts for organic synthesis with a strong focus on visible-light photocatalysis. We are particularly interested in carbon–heteroatom cross-coupling reactions using heterogeneous photocatalysts.

We showed that selective cross-couplings can be achieved using a combination of a homogeneous nickel catalyst and a heterogeneous carbon nitride photocatalyst (Fig. 1, A). During our studies on the scope and limitations of such transformations, we identified severe reproducibility issues and recycling problems that are caused by catalyst deactivation. [1] We found that over-reduction of the nickel catalyst produced inactive Ni nanoparticles that deposit on the photocatalyst. Studying the mechanism of catalyst deactivation allowed us to overcome this problem and expanded the scope of this transformation.

The main drawbacks of the carbon nitride approach are that the nickel co-catalyst could not be recycled and that the photocatalyst is limited to short wavelengths that can cause unwanted side-reactions. We therefore turned our attention to an alternative strategy. Inspired by dye-sensitized solar cells, we developed a modular, self-assembling catalyst system for cross-couplings (Fig. 1, B). [2] Key to success was the use of organic dyes and nickel complexes with functionalities that attach to the surface of a heterogeneous semiconductor. By studying different dyes and nickel complexes, we identified catalysts that harvest the entire visible light spectrum. This approach also enabled us to attach the nickel complex and the dye permanently on the semiconductor to create a recyclable, bifunctional catalyst for light-mediated cross-couplings.

The results of mechanistic investigations during these studies inspired a visible-light-mediated approach to nickel-catalyzed carbon-heteroatom cross-couplings that does not require an exogenous photocatalyst (Fig. 1, C). [3].

Dr. Bartholomäus Pieber

Group Leader since 2018

2016—2017 Postdoctoral Researcher
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

2015 Postdoctoral Researcher
Institute of Chemistry, University of Graz (Austria)

2015 PhD in Natural Science
(with distinction)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

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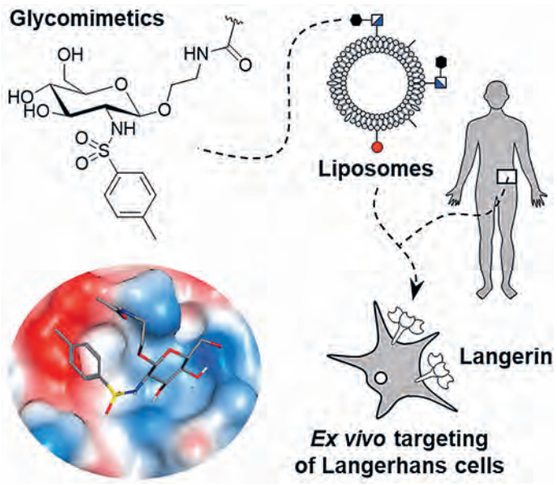

Fig. 1 A glycomimetic ligand is used for targeted delivery of lipid-based nanoparticles to Langerhans cells in the human skin [2].

References: **[1]** Wawrzinek, R.; Wamhoff, E. C.; Lefebre, J.; Rentzsch, M.; Bachem, G.; Domeniconi, G.; Schulze, J.; Fuchsberger, F. F.; Zhang, H.; Modenutti, C.; Schnirch, L.; Marti, M. A.; Schwardt, O.; Bräutigam, M.; Hauck, D.; Seeberger, P. H.; Seitz, O.; Titz, A.; Ernst, B.; Rademacher, C.: A Remote Secondary Binding Pocket Promotes Heteromultivalent Targeting of DC-SIGN. J Am Chem Soc, 2021, 143, 18977—18988.
[2] Wamhoff, E. C.; Schulze, J.; Bellmann, L.; Rentzsch, M.; Bachem, G.; Fuchsberger, F. F.; Rademacher, J.; Hermann, M.; Del Frari, B.; van Dalen, R.; Hartmann, D.; van Sorge, N. M.; Seitz, O.; Stoitzner, P.; and Rademacher, C.*: A Specific, Glycomimetic Langerin Ligand for Human Langerhans Cell Targeting. ACS Cent Sci 2019, 5, 808—820.

The Rademacher lab has a strong focus on members of the C-type lectin protein family, which are expressed on cells of the innate immune system. These cell surface receptors promote pathogen recognition and also, in some cases, endocytosis. This recognition process is based on the interaction of the lectins with glycans found on the invading pathogen, with sufficient avidity often being gained by homooligomerization of the receptor.

In our search for small molecule modulators of C-type lectin receptor function, we make use of the structural plasticity of these lectins. We found that, besides the shallow and featureless carbohydrate recognition site, several secondary sites exist that are partially druggable and offer possibilities for inhibitor design against C-type lectins. These insights are complemented by our studies into receptor flexibility using protein NMR in combination with molecular dynamics simulations, revealing an allosteric network of communicating amino acid sidechains. This network regulates the Ca^{2+} affinity and partially its pH sensitivity in human langerin. Based on these insights on the existence of druggable secondary sites and the presence of allostery, we were able to develop a series of allosteric inhibitors of langerin and other CLRs [1].

As an application of the specific CLR ligands, we have focused our efforts on the development of langerin ligands as warheads for skin-based targeted delivery purposes. The skin represents an attractive organ for the application of novel vaccines since it harbors a large reservoir of resident immune cells capable of eliciting a systemic response against antigens. In particular, Langerhans cells (LCs) are located in the epidermis, the upper layer of the skin. These responses were primarily investigated using antibody-based delivery of antigens to LCs and were especially effective when langerin was used as a targeted receptor. We have developed a small molecule ligand specific to langerin that we are exploring as the basis for antigen delivery via liposomal formulations [2]. Overall, these highly specific nanoparticles potentially build the basis for innovative delivery of vaccines via the skin.

Prof. Dr. Christoph Rademacher

Group Leader 2011—2020

Since 2020 Full Professor
University of Vienna, Department of Pharmaceutical Sciences (Austria)

Since 2017 ERC Starting Grant Holder

2012—2016 Emmy-Noether Young Research Group Leader

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

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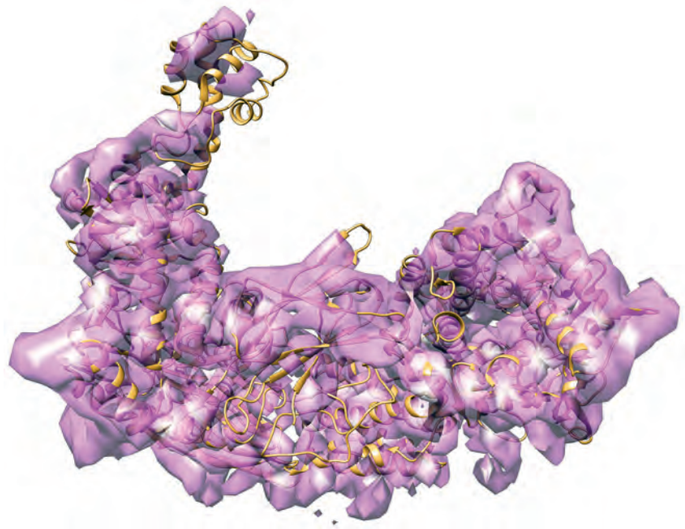


Fig. 1 Cryo-EM reconstruction of hGDE to 3.4 Å resolution. The structural model of Candida glabrata GDE (pdb-ID:5d06) was fitted into the EM-map.

Carbohydrates are involved in all processes of life, for example cell signaling, nutrition and as building blocks for cell walls and other biomaterials. Carbohydrate synthesis, turnover, and remodeling is a result of orchestrated actions of numerous enzymes. We want to shed light on how proteins and enzymes interact with carbohydrate. We seek to understand how the enzymes catalyze their reaction and achieve exquisite regio- and stereoselectivity. To reach these goals, we are using biophysical methods, mainly X-ray crystallography and cryo-EM. Two projects are highlighted to show our contribution to the field: glycosylated antimicrobial peptides and glycogen remodeling.

Multiresistant microorganisms are a threat to human health and require the development of novel antimicrobials. An interesting subclass are glycosylated antimicrobial peptides, glycocins. Glycocins harbor up to two glycosylations at a serine or cysteine, resulting in O- or unusual S-glycosylation, installed by a specific glycosyltransferase. We aim to understand the catalytic mechanism and the structural motifs responsible for the substrate specificity and selectivity in respect of their donor and acceptor. This may lead to a better understanding of S-glycosylation and may establish a new family of glycosyltransferases for the chemoenzymatic synthesis of glycocins.

Glycogen is the most important quickly accessible resource of carbon and energy in procaryotes and eucaryotes. In humans, complete degradation is achieved by two enzymes, the glycogen phosphorylase and the glycogen debranching enzyme (hGDE). Despite the critical role of hGDE, structural data are available for yeast homologs only. We have recently determined the structure of hGDE using cryo-EM (Fig. 1) and are now starting to determine the role of each domain in the catalytic cycle. This will help to understand how mutations in the enzyme are responsible for the onset of various diseases, for example glycogen storage disorders.

Dr. Christian Roth

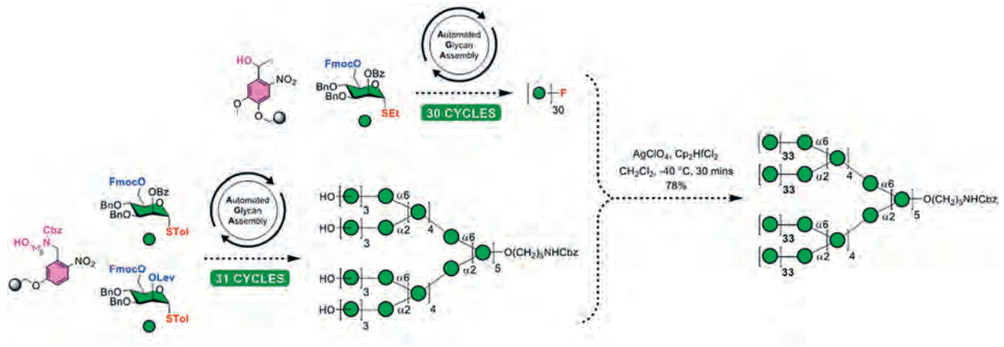
Group Leader since 2018

2017—2018 Research Associate
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

2013—2017 Research Associate
YSBL, The University of York (UK)

2013 Research Associate
Leipzig University (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs



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The Seeberger group conceived the concept of automated glycan assembly in 1998 and has since then been developing new methods to accelerate and generalize the method systematically.

Instrument Development. A new microwave-assisted AGA synthesizer enables rapid temperature adjustment from −40° C to +100° C to control glycosylations at low temperature and accelerated capping, protecting group removal, and glycan modifications by using elevated temperatures. Thereby, the temporary protecting group portfolio is extended from two to four orthogonal groups, which give rise to oligosaccharides with up to four branches. In addition, sulfated glycans and unprotected glycans can be prepared. The new design reduces the typical coupling cycles from 100 min to 60 min while expanding the range of accessible glycans. The instrument drastically shortens and generalizes the synthesis of carbohydrates for use in biomedical and material science.

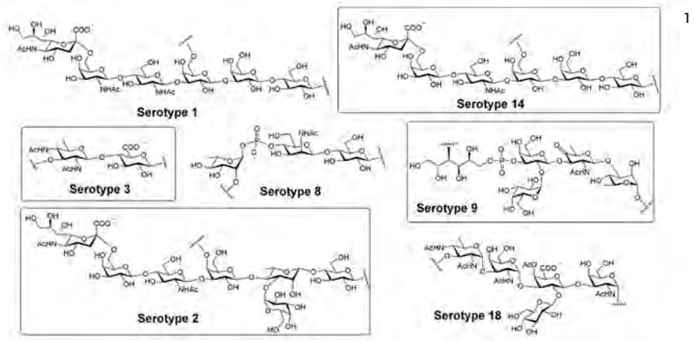
Polysaccharide Synthesis — the Basis for Material Science. Efforts towards the synthesis of ever-larger polysaccharides. In 2020, the systematic improvement of automated glycan assembly, including linker, coupling cycle, and product purification, enabled access to a 100-mer polysaccharide via a 201-step synthesis within 188 hours. Convergent block coupling of 30- and 31-mer polysaccharide fragments, prepared by AGA, yielded a multiple-branched 151-mer polymannoside in 78% yield. Quick access to polysaccharides provides the basis for future material science applications of carbohydrates.

Installation of Difficult Linkages. AGA provides quick access to trans-linked glycans such as cellulose, but the stereoselective installation of multiple cis-glycosidic linkages present in amylose had not been possible. In 2021, we developed thioglycoside building blocks with different protecting group patterns that, in concert with temperature and solvent control, achieve excellent stereoselectivity during the synthesis of linear and branched α-glucan polymers with up to 20 cis-glycosidic linkages. The molecules serve as probes to understand the biosynthesis and the structure of α-glucans.

Fig. 1 Synthesis of a 151-mer polysaccharide prepared by a 31+30+30+30+30 block coupling of polysaccharides prepared by automated glycan assembly.

References: [1] Joseph, A.; Pardo-Vargas, A.; Seeberger, P. H.: Total Synthesis of Polysaccharides by Automated Glycan Assembly. J. Am. Chem. Soc., 2020, 142, 8561—8564.
[2] Danglad-Flores, J.; Leichnitz, S.; Sletten, E. T.; Joseph, A. A.; Bienert, K.; Le Mai Hoang, K.; Seeberger, P. H.: Microwave-assisted Automated Glycan Assembly. J. Am. Chem. Soc., 2021, 143, 8893—8901.
[3] Zhu, Y.; Delbianco, M.; Seeberger, P. H.; Automated Assembly of Starch and Glycogen Polysaccharides. J. Am. Chem. Soc., 2021, 143, 9758—9768.

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs



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The bacterial surface is covered by capsular polysaccharides (CPS). The group uses synthetic oligosaccharide antigens to understand all aspects of the immune response to glycans. The long-term goal is a detailed understanding of the factors that determine glycan immunogenicity and render a protective immune response in mammals. New vaccine carrier concepts, novel delivery systems, different adjuvants, and routes of administration are currently being explored.

Streptococcus suis bacteria are one of the most serious health problems for pigs and an emerging zoonotic agent in humans working in the swine industry. *S. suis* bacteria express CPS, a major bacterial virulence factor that defines the serotypes. We synthesized the oligosaccharides resembling the CPS of *S. suis* serotypes 2, 3, 9, and 14. Lead antigens for the development of semi-synthetic *S. suis* serotype 2 and 9 glycoconjugate veterinary vaccines were identified using glycan microarrays.

Anti-Glycan Antibodies in Multiple Sclerosis. Multiple sclerosis (MS) is an autoimmune relapsing-remitting disease of the central nervous system (CNS) of unknown etiology. Changes in gut microbiota composition and an eminent role of B cells have been implicated in MS pathogenesis. How gut microbiota shape IgA responses and how IgA B cells contribute to neuroinflammation remain unknown. In collaboration with medical groups in Basel and San Francisco, we found that gut microbiota-specific IgA B cells traffic to the inflamed CNS in active MS and other neuroinflammatory diseases. Using glycan microarrays, we showed that antibodies to specific gut bacteria are in the cerebral spinal fluid. This finding is very significant for efforts aiming to diagnose and eventually treat MS.

Fig. 1 Structures of the most common S. suis CPS repeating units. Highlighted structures were prepared in the group.

References: [1] Seeberger, P. H.: Discovery of Semi- and Fully-Synthetic Carbohydrate Vaccines Against Bacterial Infections Using a Medicinal Chemistry Approach. Chem. Rev. 2021, 121, 3598—3626.
[2] Zhang, S.; Sella, M.; Sianturi, J.; Priegue, P.; Shen, D.; Seeberger, P. H.: Discovery of oligosaccharide antigens for semi-synthetic glycoconjugate vaccine leads against Streptococcus suis serotypes 2, 3, 9 and 14. Angew. Chem. Int. Ed. 2021, 60, 14679–14692.
[3] Pröbstel, A.-K.; Zhou, X.; Baumann, R.; Rojas, O. L.; Wischnewski, S.; Kutza, M.; Sellrie, K.; Kim, K.; Ramesh, A.; Dandekar, R.; Greenfield, A. L.; Schubert, R. D.; Bisanz, J. E.; Vistnes, S.; Khalegi, K.; Liesche, F.; Ramaglia, V.; Bischof, A.; Singh, S.; Tran, E. B.; Barba, P.; Zorn, K.; Heijnen, I.; Oechtering, J.; Forsberg, K.; Henry, R.; Helmuth, J.; Shiow, L. R.; Gelfand, J. M.; Graves, J.; Cree, B. A. C.; Hauser, S. L.; Kuhle, J.; Weishaupt, J. H.; Andersen, P. M.; Schlegel, J.; Turnbaugh, P. J.; Seeberger, P. H.; Gommerman, J. L.; Schirmer, L.; Wilson, M. R.; Baranzini, S. E.: Gut microbiota-specific IgA+ B cells 1 traffic to the CNS in active multiple 2 sclerosis. Science Immunology 2020, 5, eabc7191.

Prof. Dr. Peter H. Seeberger

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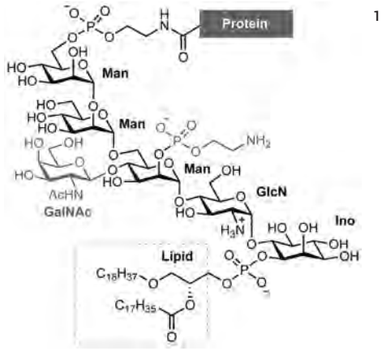
↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs



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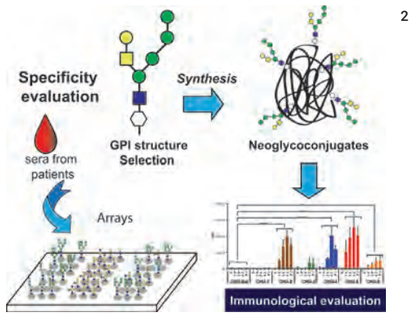

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Fig. 1 General structure of mammalian GPIs. (Black) Core structure.
Fig. 2 Steps for GPI-activity determination in diagnostics using arrays.

CHEMISTRY AND BIOLOGY OF GLYCOSYLPHOSPHATIDYLINOSITOLS

GPI and Glycoproteins

The attachment of Glycosylphosphatidylinositols (GPIs) to proteins (glypiation) is a posttranslational modification (PTM) in eukaryotes. GPIs are glycolipids, having a conserved core structure with cell-specific phosphorylations, acylations, and glycosylations (Fig. 1). Glypiated proteins (GPI-APs) and free GPIs are present in the outer leaflet of the plasma membrane (PM). Studies on the functions of GPIs established the glycolipid role in attaching proteins to the PM; however, GPIs specific role in infections, the activity of glypiated proteins, and other processes is still unknown.

To study GPIs biologically and overcome the difficulties in isolating them from natural sources, the group has in recent years developed and applied two strategies to synthesize parasitic and mammalian GPIs. We established the serodiagnosis of toxoplasmosis using microarrays, beads, and electrochemical-based assays (Fig. 2). [1] The determination of Anti-GPI IgG and IgM responses allowed differentiation of acute and chronic infections with high sensitivity and specificity, showing high potential for detecting other parasitic diseases. In addition, GPI-glycoconjugates showed immunogenic activity in vivo and induced anti-GPI antibody production, T cell activation and protection of mice from a challenge with Plasmodium parasites.

We used synthetic structures to develop a strategy to get GPI-APs and get glypiated parasitic proteins with enhanced proinflammatory activity in vitro, [2] suggesting that GPIs are potential structures for therapeutics and vaccines development. Further studies include the application of GPI derivatives for understanding the biophysical behavior of GPIs in model systems, disclosing the effect of GPI modifications in the formation of microdomains in monolayers, and rescuing the GPI biosynthesis in vitro.[3]

References: **[1]** Garg, M.; Stern, D.; Gross, U.; Seeberger, P. H.; Seeber, F.; and Varón Silva, D.: Detection of Anti-Toxoplasma gondii Antibodies in Human Sera using Synthetic Glycosylphosphatidylinositol Glycans on a Bead-Based Multiplex Assay, Anal. Chem. 2019, 91, 17, 11215—11222.
[2] Roller, R. F.; Malik, A.; Carillo, M. A.; Garg, M.; Rella, A.; Raulf, M. K.; Lepenies, B.; Seeberger, P. H.; and Varón Silva, D.: Semi-Synthesis of Functional Glycosylphosphatidylinositol-Anchored Proteins, Angew. Chem. Int. Ed. 2020, 59, 12035—12040.
[3] Guerrero, P. A.; Murakami, Y.; Malik, A.; Seeberger, P. H.; Kinoshita, T.; Varón Silva, D.: Rescue of glycosylphosphatidylinositol-anchored protein biosynthesis using synthetic glycosylphosphatidylinositol oligosaccharides. ACS Chem. Biol. 2021 16 (11), 2297—2306 (2021).

Prof. Dr. Daniel Varón Silva

Group Leader 2011—2021

Since 2021 Professor of Organic and Bioorganic Chemistry
Institute for Chemistry and Bioanalytics, School of Life Sciences, University of Applied Sciences and Arts Northwestern Switzerland (Muttenz, Switzerland)

2020 Deputy Professor of Organic Chemistry
Department of Chemistry, Humboldt University of Berlin (Germany)

2009—2010 Postdoctoral Fellow
MPICI, Department of Biomolecular Systems (Potsdam, Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/bs

Department of Colloid Chemistry

Department of Colloid Chemistry

General Structure

The department is organized along "project structure" lines, the content of which are substantiated below. Each "project" is led by a senior scientist or a young "project leader", the latter—with a temporary contract of 4—6 years, use their partial independence to complete their habilitation. With promotion to professorship, it is the arrangement with the director that the young people can take their projects, topics, but also third-party funding with them to continue their path in science. For some years now, the academic market situation, however, has been moving so much into our field of research that it is turning into a threat: the department is losing so many young people and topics that continuity is hard to maintain.

From the previous line-up of project leaders, Dr. Majd Al-Nadj will continue at TU Berlin in a Start Up Environment, Dr. Baris Kumru has accepted an assistant professorship with tenure track at Delft, and Dr. Nieves López-Salas is moving to the University of Paderborn as an assistant professor with tenure option. It is good news that the head of the Electron Microscopy lab, Dr. Nadja Tarakina, has returned from her twin maternity leave, and also two new TEM microscopes could be negotiated. They are currently being completed and will soon bring back full support function to the institute. Dr. Paolo Giusto has started a new group on "covalent 2D-materials", filling at least one gap and helping as a junior member with our big ERC Synergy Grant.

The other group leader vacancies are currently temporarily being used by a number of rather independent postdoctoral fellows with clear academic ambitions. Dr. Mateusz Odziomek is an Alexander von Humboldt fellow who is taking over the projects of Nieves López-Salas' Carbon group, Dr. Roza Bouchal is a (female) EU Curie fellow who is currently developing a Sustainable Batteries portfolio, and Dr. Lu Peng is a (female) H2020 project leader who is working on new "Carbocatalysts" for the new catalytic conversions to come (also financed by METHASOL, a big EU FP7 project). A Joint Group with the Agricultural University of Harbin was created in 2019, making a 5th female scientist (external) group leader in my department: Prof. Dr. Fan Yang. Dr. Yang is working on "Soil Inspired Materials" and developed "Artifical Humic Acids" to bring back fertility to depleted soils and for sustainable agriculture. She has already received a number of distinctions, among them the listing as an "IUPAC breakthrough innovation 2022".

With five female and five male leading scientists, colloid chemistry is gender balanced, a state we had already reached at PhD level about five years ago.

Speaking as the director of this department, I am very happy with the new personalities and the profile I was able to establish, although it is more and more difficult to fill the junior executive vacancies at such a high level. The department now covers very actual topics, which are mostly new fields developed in the last 10 years.

Scientific fields

Due to the restricted space of this introduction, I can highlight only a few of the most recent accomplishments of the department (after 2018).

Sustainable Chemistry, Biobased Materials, Biorefinery

Based on previous work on "pasta catalysis", we were able to present a new generation of heterogeneous carbon catalysts with acidic or base properties (Dr. Al-Naji). The catalyst was used in the chemical recycling of real yellow-bag plastic waste, and a patent was granted. The base catalyst on the other hand could recycle a number of polyesters into the monomers.

Department of Colloid Chemistry

Dr. Filonenko developed a bio-based deep eutectic solvent system enabling the dissolution of cellulose directly as nanofibers, a significant processing advantage in making and processing nanocellulose. In cooperation with a Finnish group, 3D printing with such nanocellulose dispersions was perfected.

Optimizing the artificial humic acid process (Prof. Dr. Yang), we could show that doses as low as 0.3 per mill bring soil fertility and an increase of crop yields of up to 20 percent. The technology is already being applied in field experiments. The process turned out to be suitable to cover a number of fertilizer and biowaste problems. Analyzing the metagenome of soil, it was shown that the AHA mostly operates via establishing a performing soil microbial system, i.e. we are entering the "living materials" domain.

Carbon Nitride and Photosynthesis

Dr. Savateev and his group continued to explore photoredox-catalysis for new organic reactions and remarkably widened application space. Dr. Giusto used his CVD process for transparent layers of carbon nitride to also coat battery materials and found SEI properties and ion permeation. Dr. Teixeira, an AvH visitor, optimized photochemical water splitting with polyheptazineimides and the cocatalyst chain and transport to exceed an apparent quantum yield of 80 percent, the remainders to get most presumably been based by imperfect light management and engineering. Carbon nitride species were also used to deposit Fe(IV)=O species for photochemical alkane and methane-monooxidation.

PHIs were also decorated with diverse common transition metals (single atom, Dr. Lu Peng) and analyzed for oxygen evolution reaction (EU Project Methasol). The carbon nitride principle is extended to similar heterocycle chemistry.

Noble Carbons, Sorption, Electrocatalysis

Dr. López-Salas developed noble carbons from nucleobases and optimized them for CO_2 and water sorption. Water sorption in particular has reached a level where "chillers" (desorption cooling) are now to be discussed. In (electro)catalysis, such carbons decorated with common metal ions turned out to bring unexpected activity-stability profiles, for instance in sustainable oxygen-to-hydrogenperoxide reduction.

Low temperature carbonization schemes were explored, where we were able to lower the temperature below 200 degrees under otherwise regular conditions, making carbon synthesis compatible to ordinary materials (Dr. Odziomek).

Dr. Volker Strauss is analyzing flash laser carbonization and is developing "printable gas sensors" based on this technology.

A new crystalline carbon (potential allotrope) was synthesized and used as a synthetic peroxidase. Previously unknown reactivities for deep oxidation of water could be realized (Tingting Lian).

Energy Materials

Following the MPG-FHG project (Clusterbatt, Dr. Oschatz), Dr. Giusto developed special sulfur-doped carbons, which enable a new anode generation of sodium batteries. Dr. Bouchal developed hypersaline aqueous solvent systems, which allow stable and cyclable zinc batteries for large-scale commodity applications. Porous carbons with high N,O content were found to be effective cathode materials for metal-air batteries.

The ERC Synergy project (Antonietti, together with P. Simon/Toulouse) MOMASTOR was launched and explores the future modes of energy storage for the forthcoming all-green electricity system.

Independent Junior Group

Dr. Lukas Zeininger is a DFG Emmy Noether fellow, and his Complex Emulsion group is hosted by the department. His report is found below.

A General Outlook

As judged by the successful careers of the young scientists of the department and many distinctions (e.g. the Premio internazionale Lombardia è Ricerca 2020; the 3 prize winners shared 1,000,000 euros overall), the reception of the department's research is in general very positive. This is also reflected in very favorable international rankings from leading science journals (e.g. ↘ https://research.com/u/markus-antonietti).

Also, the Scientific Advisory Board (SAB) of the institute gave the Department of Colloid Chemistry strong support to continue on the path of using the tools of materials chemistry to address the three changes modern society is facing: the energy change, the raw materials change, and climate change. Currently, practically all of our projects are located within this triad. Synthetic soil brought us into the context of "Living Materials", and this is a topic we will try to grow, together with the new department and also external microbiologists.

My directorship will be ending in a happy retirement in five years' time, but I am very glad that a great many exciting research projects are already scheduled for the intervening period. Additionally, I am particularly pleased to have the chance to work with so many talented young scientists.

Prof. Dr. Dr. h.c. Markus Antonietti

Publication selection

Ghosh, I.; Khamrai, J.; Savateev, A.; Shlapakov, N.; Antonietti, M.; König, B.: Organic semiconductor photocatalyst can bifunctionalize arenes and heteroarenes. Science 365 (6451), 360—366 (2019).

Chen, L.; Yan, R.; Oschatz, M.; Jiang, L.; Antonietti, M.; Xiao, K.: Ultrathin 2D Graphitic Carbon Nitride on Metal Films: Underpotential Sodium Deposition in Adlayers for Sodium-Ion Batteries. Angewandte Chemie International Edition 59 (23), 9067—9073 (2020).

Wang, H.; Shao, Y.; Mei, S.; Lu, Y.; Zhang, M.; Sun, J.; Matyjaszewski, K.; Antonietti, M.; Yuan, J.: Polymer-derived heteroatom-doped porous carbon materials. Chemical Reviews 120 (17), 9363—9419 (2020).

Yang, F.; Tang, C.; Antonietti, M.: Natural and artificial humic substances to manage minerals, ions, water, and soil microorganisms. Chemical Society Reviews 50 (10), 6221—6239 (2021).

↘ Further information can be found at www.mpikg.mpg.de/kc

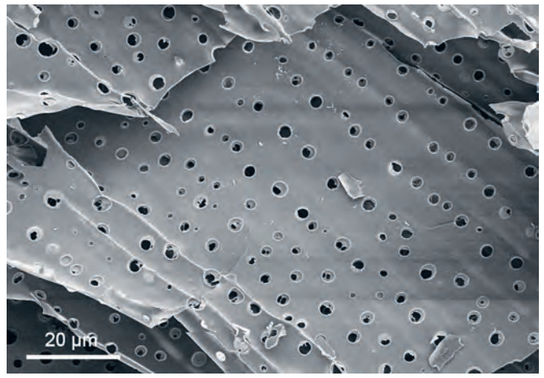

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Fig. 1 Hemicellulose is one of the three main components of plant biomass, and one of the most abundant biopolymers. Mild conditions of extraction preserve its native structure.

Nature collects solar energy and transforms it into a vast variety of compounds with unique and advantageous properties. Utilizing the abundance of natural compounds to develop functional materials is one route available to modern sustainable chemistry. The materials originated from natural sources have the advantage of biodegradability and biocompatibility, under the condition of minimal chemical modification, and high performance in many specific applications.

In our group, we develop new sustainable methods for the isolation of natural polymers, aiming to preserve their biodegradability and unique natural advantages in order to facilitate their valorization into novel advanced materials. This is done with novel eutectic solvents—a physical mixture of ionic compounds, similar to highly concentrated metabolic media found in living cells. Substituting toxic organic solvents with safer alternatives is of high necessity due to the excessive use of solvents in synthetic chemistry. The reactive eutectic solvents developed in our group shift the paradigm of a restricted role of solvents solely as a media for reaction and extends it to use them as reagents [1]. Using this atom- and energy-saving approach, we valorize natural molecules (saccharides, citric acid), turning them into flavoring agents with antibacterial properties or dyes.

High activity of the reactive eutectics towards saccharides caused by the presence of ammonium formate paved the way to use it for isolation of nanocrystalline cellulose—nanocellulose [2]. The nanocellulose is interesting due to its high mechanical strength compatible with Kevlar fibers and its ability to form transparent and gas tight films and effectively stabilize emulsions (Pickering emulsions). This affords a wide spectrum of applications for the nanocellulose, among which we investigate its role in reinforcing natural polymer matrixes, gas tight and gas permeable films and coatings, and bioprinting. The advantage of the method for nanocellulose isolation developed in our group is that the product has less distortion of native structure of crystals (thus higher thermal stability and better mechanical properties), the mild charge is optimal for Pickering emulsions, and amino groups are present.

Reactions at high concentrations are an efficient pathway to mimic natural transformations of lignocellulose into humic matter—a fundamental of high soil quality and fertility and a long-term CO_2 deposit [3].

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[3] Yang, F. and Antonietti, M.: Artificial humic acids: sustainable materials against climate change. Advanced Science (2020).

Dr. Svitlana Filonenko

Group Leader since 2019

2018 Postdoc
MPICI, Department of Colloid Chemistry (Potsdam, Germany)

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Aalto University (Finland)

2012—2017 Research Fellow
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↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc

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Fig. 1 Carbon nitride thin films coated by chemical vapor deposition over a quartz shaped flower under ambient illumination (left) and UV (right).

In our group, we are driven by the vision to expand the horizon of common materials. We design and synthesize 2D-covalent thin film materials with controlled chemical composition, structural motifs, morphology, and electronic properties for applications in electrochemical energy devices such as batteries and supercapacitors. Within the framework of the ERC Synergy project MoMaSTOR (ID: 951513), we focus particularly on the synthesis of thin films as artificial solid electrolyte interfaces (a-SEI) in sodium-ion battery anodes.

Thin films are usually defined as materials with one dimension (i.e. the thickness, usually in the 1—1,000 nanometer range) much smaller than the other two. In a world where devices are required to be smaller and more efficient than ever before, thin films and interfaces are playing an extremely important role. On the one hand, the choice/synthesis of the precursor enables the introduction of specific functionalities in the thin film materials according to the application requirements. On the other hand, the design and optimization of the deposition process enables us to achieve different thicknesses, structures, and chemical composition to improve device performance with a negligible change of size and weight.

In our group, we recently developed methods for the synthesis of carbon-based materials such as carbon nitride [1], boron carbon nitride [2], and red carbon thin films in a one-step, bottom-up approach using vapor-based methods, such as chemical vapor deposition. The latter technique is particularly promising as it enables the homogeneous deposition of nanometer-sized thin films with controllable thickness on target substrates, regardless of their shape. Indeed, the deposition of carbon nitrides thin films over a porous carbon-based anode material was successfully tested and shown to increase the performance of the electrode in sodium-ion batteries, improving storage capacity, efficiency, and long-term stability. Eventually, the thin film materials developed in our group have also found very promising applications beyond energy storage, such as in optics, sensing, photocatalysis, polymer synthesis, and membranes for ion transport. [3]

References: [1] Giusto, P.; Cruz, D.; Heil, T.; Arazoe, H.; Lova, P.; Aida, T.; Comoretto, D.; Patrini, M.; Antonietti, M.: Shine Bright Like a Diamond: New Light on an Old Polymeric Semiconductor. Advanced Materials 2020, 32, 1908140.
[2] Giusto, P.; Arazoe, H.; Cruz, D.; Lova, P.; Heil, T.; Aida, T.; Antonietti, M.: Boron Carbon Nitride Thin Films: From Disordered to Ordered Conjugated Ternary Materials. Journal of the American Chemical Society 2020 142 (49), 20883—20891.
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2D-COVALENT THIN FILMS
FOR ENERGY STORAGE

Dr. Paolo Giusto

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2021—2023 Master in Business and Administration
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2017—2020 PhD Student, Polymer Chemistry
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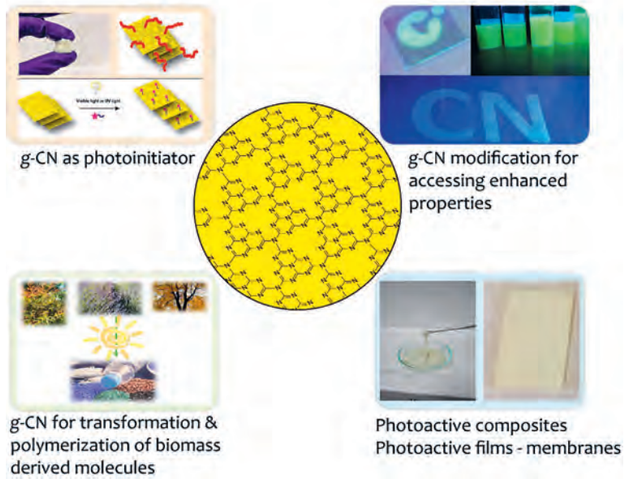

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Fig. 1 Main interest areas of the research group based on photochemistry.

Our group is inspired by the basic principles of polymer and colloid chemistry. The material that is in focus is called graphitic carbon nitride (referred as CN), a metal-free semiconductor with tunable synthesis from cheap and abundant molecules. Heating up nitrogen rich molecules to around 550° C results in the formation of photoactive material that has the ideal C_3N_4 structure (as seen in the middle of Fig. 1). Carbon nitride represents a diverse group of materials, and the literature is expanding rapidly based on the synthesis and application of this class. The main interest for CN comes from heterogeneous catalysis, where CN powder can be applied for a variety of applications that can be conducted under visible light. On the other hand, due to strong aromatic interactions of CN sheets, dispersibility is highly hindered. Yet, CN dispersions hold great promise for the sculpting of novel architectures.

Merging CN dispersions with polymer and colloid chemistry granted access for photoactive hybrid materials. [1] In terms of aqueous dispersibility, CN can enhance the mechanical properties of soft materials while at the same time it can be employed as a polymerization photoinitiator. Due to the amphiphilic properties of CN, we can access heterophasic systems where CN is located at the interface. Hence, many heterophase photopolymerization techniques were demonstrated. Alternatively, CN nanoparticles strengthen the interface due to electrostatic jamming. Based on that, liquid-liquid printing principles were shown and the photoactivity of liquid soft matter was harnessed. For organic dispersions, a special type of CN was formulated in our lab. This giant leap allowed access to organic polymers for the first time, and photoactive organic polymers were synthesized. [2] Additionally, we demonstrated the usage of CN as a heterogeneous photoinitiator to form commodity polymers and non-doped conducting oligomers.[3] Finally, the synthesis of band gap widened metal doped novel CN hybrids was elucidated.

References: [1] Kumru, B.; Antonietti, M.: Adv. Colloid Interface Sci., (2020), 283, 102229.
[2] Esen, C.; Antonietti, M.; Kumru, B.: J. Appl. Polym. Sci., (2021), 138(35), 50879.
[3] Esen, C.; Antonietti, M.; Kumru, B.: ChemPhotoChem, (2021), 5(9), 857—862.

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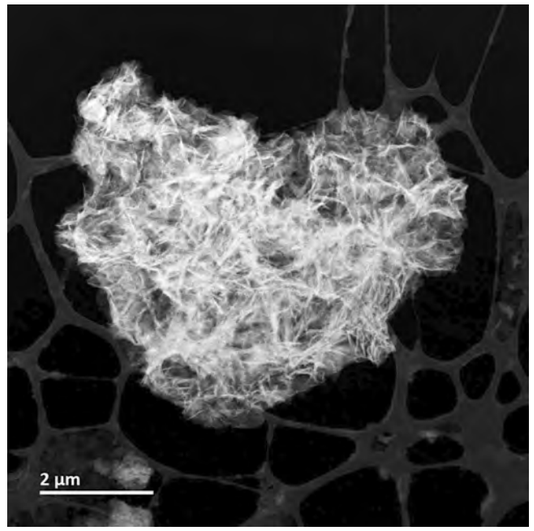

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Fig. 1 TEM picture of a carbonaceous material prepared from heat treatment of carbon suboxide at low temperatures.

Carbon materials can be processed as dense and hard 2D or 3D very porous solids, like diamond, graphene, or active carbon. Introducing other lightweight elements in the carbon chemical backbone (for example, nitrogen or boron) changes carbons conductivity and introduces surface terminating functionalities, transforming the materials into semiconductors or semimetals with collective electron properties. In other words, carbon materials' physicochemical properties can be widely tuned. Because of that, they are usually "winning horses" for very different applications including catalysis, environmental remediation, energy storage, and conversion technologies, among many others.

Surprisingly, carbonization as such is still considered a "black box" process. Over the last two years, our group has focused on studying carbon condensation mechanisms using two strategies: 1) precoding of chemical information in molecular precursors and 2) using precursors that would undergo simplified condensation pathways to prepare carbon materials at low temperatures.

The possibility of using molecules as carbon precursors opens the path to exploring the introduction of large amounts of heteroatoms with precoded structures. When introducing very large amounts of heteroatoms, chemical and polar pores are generated in carbonaceous networks. We focused especially on the preparation of highly nitrogen-doped carbonaceous materials and studied the ability of the formed pores to 1) selectively adsorb greenhouse gases [1], 2) interact with and adsorb water [2], 3) their catalytic activity, and 4) their ability to stabilize metal single sites for their use as electrocatalysis [3].

On the other hand, we also aimed to synthesize carbon-based materials using novel predefined oligomeric and polymeric carbon suboxide derived precursors (i.e. poly carbon suboxide), which allow the synthesis of carbon materials at low temperatures and fine-tuning of their chemical composition and pore structure (Fig. 1). The release of only CO or CO_2 upon condensation facilitates understanding the condensation mechanisms. The resulting materials are also comprising polar pores but, comprising oxygen heteroatoms.

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[3] Lepre, E.; Heske, J.; Nowakowski, M.; Scoppola, E.; Zizak, I.; Heil, T.; Kühne, T. D.; Antonietti, M.; López-Salas, N.; Albero, J.: Ni-Based Electrocatalysts for Unconventional CO_2 Reduction Reaction to Formic Acid, Nano Ener. (2022), 97, 107191.

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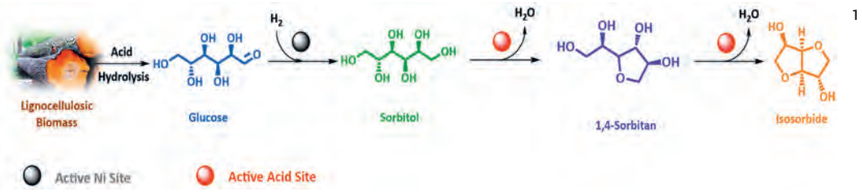
Materials Science Institute of Madrid (ICMM-CSIC) and the Autonomous University of Madrid (Spain)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc



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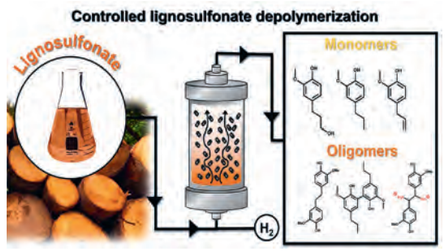

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Fig. 1 Synthesis of isosorbide by hydrogenation of glucose to sorbitol over 35Ni/NDC, followed by sorbitol dehydration to isosorbide over β zeolite.
Fig. 2 Controlled lignosulfonate depolymerization via reductive catalytic fractionation in flow system.

The current environmental challenge drives the transition towards a more sustainable society, including a circular bio-economy. Among renewable resources, waste lignocellulosic biomass (LCB) consisting of cellulose, hemicellulose, and lignin represents the most abundant and low-cost one. Additionally, the multi-functionalities of LCB gives it the potential to be used in a wide range of applications. For this goal, biorefinery as an engineering concept for producing valuable bio-based building blocks from wet waste LCB was proposed. The biorefinery concept links the field of heterogeneous catalyst design and sustainable chemical processes engineering.

Continuous Flow Valorization of Lignocellulosic Biomass with Sustainable Heterogenous Catalyst

For the integrated continuous flow process to upgrade LCB towards fine chemicals, a pelletized catalyst was developed. This catalyst contains a non-noble metal and is able to work under hydrothermal conditions for a long time, on stream at a temperature above 100° C. For this purpose, we have designed a Ni catalyst supported on nitrogen-doped carbon (NDC) via an innovative "kitchen-lab" approach. [1] This catalyst was used for converting cellulosic biomass fraction such as sugars, furanics, and levulinics to a wide range of bio-based chemicals in continuous flow processes. As an example, we have developed an integrated process for conversion of glucose to isosobide via sorbitol in two consecutive reactors (Fig. 1). [2] Furthermore, it was used with high efficiency in two approaches for continuous flow valorization of lignin (native and waste lignin, i.e. lignosulfonate) to monomers and low molecular weight fractions via reductive catalytic fractionation (Fig. 2). [3]

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[3] Brandi, F.; Antonietti, M.; Al-Naji, M.: Controlled lignosulfonate depolymerization via solvothermal fragmentation coupled with catalytic hydrogenolysis/hydrogenation in continuous flow reactor. Green Chemistry 23 (24), p. 9894—9905 (2021).

Dr. Majd Al-Naji

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Foto: David Ausserhofer

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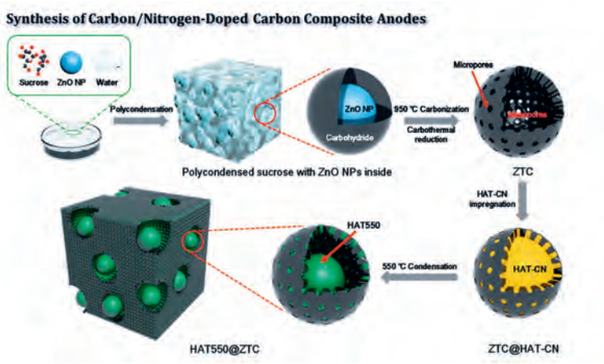
Institute of Chemical Technology, Leipzig University (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc



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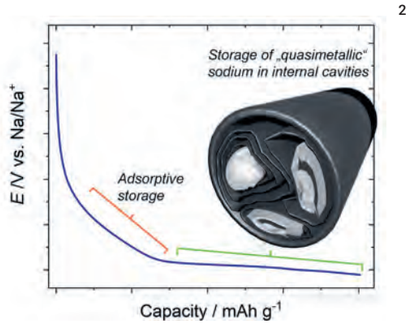

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Nanoporous carbon-based materials are attractive compounds for various energy and environmental applications. This includes but is not limited to their use as electrode materials in electrochemical energy storage, in catalysis, or for adsorptive separation processes. Research in the Energy and Environmental Utilization of Carbon Nanomaterials group is focused on the design of nanocarbon materials from molecular precursors and by using templating approaches. The fundamental operating principles of these applications are investigated based on the use of model substances with precisely defined pore sizes and chemical architectures. A central synthetic approach of our group is the combination of heteroatom-rich carbons with a certain chemical functionality (e.g. intrinsic catalytic activity or a high adsorption potential for polar substances such as water or metal ions) with electrically conductive carbon compounds into all-carbon nanohybrid materials to combine their individual advantages (Fig. 1) [1].

One particular field of interest in the years 2019 and 2020 was the development of carbon-based materials for the negative electrodes of sodium batteries (SBs). SBs are promising future alternatives to lithium-based batteries due to the higher abundance of sodium in comparison to lithium. Our group has contributed to a profound understanding of the influence of "closed pores" on the metal storage capabilities of the electrode materials based on a series of model compounds (Fig. 2) [2]. With this approach, the energy storage capability of SBs can be significantly enhanced without sacrificing their operating safety and cycling stability. Based on the developed knowledge, we have applied a chemical-vapor deposition process to achieve synthetic control over the formation of such internal volume in carbon materials that can be used for storage of quasi-metallic at electrochemical potentials close to Na/Na^+ [3]. Other fields of major interest are the electrochemical fixation of dinitrogen and the structures of carbon-water and carbon-ionic liquid interfaces.

References: [1] Yan, R.; Leus, K.; Hofmann, J. P.; Antonietti, M.; Oschatz, M.: Porous nitrogen-doped carbon/carbon nanocomposite electrodes enable sodium ion capacitors with high capacity and rate capability. Nano Energy 67, 104240 (2020).
[2] Schutjajew, K.; Pampel, J.; Zhang, W.; Antonietti, M.; Oschatz, M.: Influence of pore architecture and chemical structure on the sodium storage in nitrogen-doped hard carbons. Small 17 (48), 2006767 (2021).
[3] Schutjajew, K.; Giusto, P.; Härk, E.; Oschatz, M.: Preparation of hard carbon/carbon nitride nanocomposites by chemical vapor deposition to reveal the impact of open and closed porosity on sodium storage. Carbon 185, p. 697—708 (2021).

Fig. 1 Principle of the synthesis of an all-carbon nanohybrid material composed of a conductive matrix ("ZTC") and an embedded functional carbon ("HAT550").
Fig. 2 Typical sodiation curve of a carbon-based negative electrode of a sodium-ion battery. Closed pores can lead to "plateau capacity" needed for high energy.

Prof. Dr. Martin Oschatz

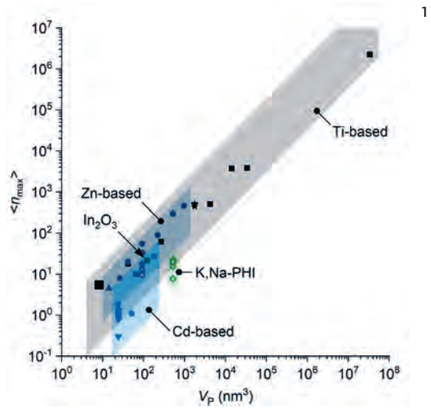
Group Leader 2016—2020

2020 Call from the Friedrich Schiller University Jena (1st ranked) to accept the full Professorship (W3)
for the Chemistry of Materials for Energy Applications (Germany)

2019—2020 Covering the position of a University Professor
for Inorganic Chemistry at the University of Potsdam (Germany)

2019—2020 Board Member and Principal Investigator in the Cluster of Excellence Unifying Systems in Catalysis ("UniSysCat")

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc



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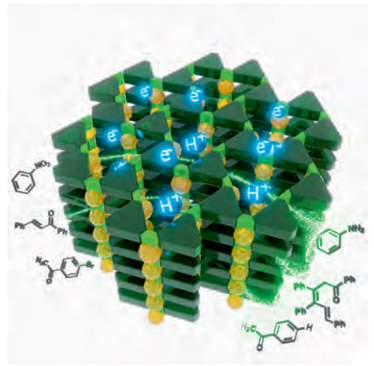

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Photocharging is a process of electron accumulation in a semiconductor material that is triggered by visible light illumination. The photocharging of a semiconductor is similar to charging an electric battery, except that energy is provided directly by photons rather than an electric power source. This phenomenon allows the integration of the light harvester and the energy storage device into one nano object—a semiconductor nanoparticle. The photocharging of semiconductors has been studied since 1980. Rich experimental data have been accumulated. However, a rational approach in designing photo-chargeable semiconductor materials is underdeveloped.

In the past two years, the group has summarized and quantified experimental data that was accumulated over many years and created an online database. [1] Using the database, we correlated ability of several classes of materials, namely those based on Ti, Zn, Cd, In, W, and graphitic carbon nitrides, to undergo photocharging with their structure. We found that the maximum number of electrons that a certain semiconductor particle can store ($<n_{max}>$) scales with its volume (Fig. 1). More comprehensive analysis led to the conclusion that microporous structure, high ionic conductivity, and highly positive valence band potential are the three most important parameters that allow a semiconductor to accumulate greater numbers of electrons—in other words, to be a more capacious battery.

For this reason, we applied potassium poly(heptazine imide), a carbon nitride-type microporous ion semiconductor, as a photo rechargeable reductant in several classes of organic reactions (Fig. 2). [2] The database will facilitate the rational design of photo-rechargeable materials to enable unprecedented chemical transformations and to construct devices for solar energy harvesting, conversion, and storage.

References: [1] Savateev, A.: Photocharging of Semiconductor Materials: Database, Quantitative Data Analysis and Application in Organic Synthesis. Advanced Energy Materials (2022) https://public.tableau.com/app/profile/oleksandr.savatieiev https://pcmat.mpikg.mpg.de/
[2] Mazzanti, S.; Schritt, C.; ten Brummelhuis, K.; Antonietti, M.; Savateev, A.: Multisite PCET with photocharged carbon nitride in dark. Exploration (2021).

Fig. 1 Dependence of maximum number of electrons stored in a single semiconductor particle ($<n_{max}>$) vs. its volume. Data points that belong to the same class of materials are highlighted with shaded area. Data were obtained from the Database of Photocharged Materials.
Fig. 2 A scope of reactions enabled by photocharged K-PHI.

Dr. Aleksandr Savateev

Group Leader since 2017

2020 First PhD Student
Dr. Yevheniia Markushyna graduated in 2020 with the grade "magna cum laude"

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"Functionalization of Organic Molecules by Visible Light Photocatalysis", Potsdam University (Germany)

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↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc

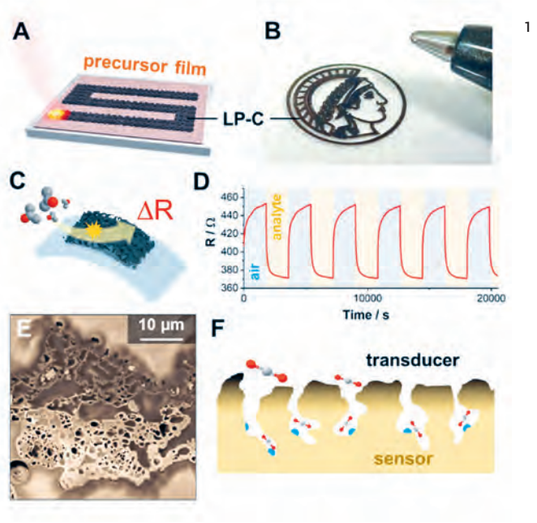

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Fig. 1 A) Laser-patterning process; B) Laser-patterned carbon; C) LP-C chemiresistor; D) Typical sensor response; E)/F) Inverted sensor architecture

Functional carbons are among the most promising materials for a range of future applications in flexible transient electronics. In particular, bio-based carbonized materials emerge as inexpensive and potentially bio-degradable alternatives. Their application, however, is inhibited by difficult processing and lack of control over the material properties. Therefore, we are exploring new concepts for the fabrication and utilization of carbonized materials in flexible electronic applications.

In the past three years, we have developed an *integrated approach* for on-the-spot laser-induced synthesis of flexible, carbonized films with specific functionalities. To this end, we design versatile precursor links made from naturally occurring organic starting materials and reactants, which are carbonized with an infrared laser to obtain functional patterns of conductive porous carbon networks.

In our studies, we obtained deep mechanistic insights into the *formation process* and the *microstructure* of laser-patterned carbons (LP-C).[1] We shed light on the kinetic reaction mechanism based on the interplay between the precursor properties and the reaction conditions. Furthermore, we investigated the use of *porogens*, *additives*, and *reactants* to provide a toolbox for the chemical and physical fine-tuning of the electronic and surface properties and the targeted integration of functional sites into the carbon network.

Based on this knowledge, we developed *prototype resistive chemical and mechanical sensors*. For example, the electronic response (ΔR) towards adsorption of gaseous analytes was significantly increased by integration of metallic molybdenum carbide nanoparticles, which decrease the charge carrier density.[2]

Moreover, by selection of abundant nitrogen-rich precursors, we designed *nitrogen-doped carbon sensors* with a specific response to *gaseous* CO_2.[3] The unidirectional laser impact leads to a unique "inverted" sensor architecture with a graphitized, porous transducer layer on top of the film while preserving the CO_2-sensitive nitrogen functionalities in the sensor layer underneath.

In further studies, we show the general applicability of LP-C as electrodes in *electrocatalytic applications*.

References: **[1]** Hepp, M.; Wang, H.; Derr, K.; Delacroix, S.; Ronneberger, S.; Loeffler, F. F.; Butz, B.; Strauss, V.: Trained laser-patterned carbon as high-performance mechanical sensors. npj Flex. Electron. 6 (2022) 3.
[2] Wang, H.; Delacroix, S.; Zieleniewska, A.; Hou, J.; Tarakina, N. V.; Cruz, D.; Lauermann, I.; Ferguson, A. J.; Blackburn, J. L.; Strauss, V: In Situ Synthesis of Molybdenum Carbide Nanoparticles Incorporated into Laser-Patterned Nitrogen-Doped Carbon for Room Temperature VOC Sensing. Adv. Funct. Mater. 31 (2021), 2104061.
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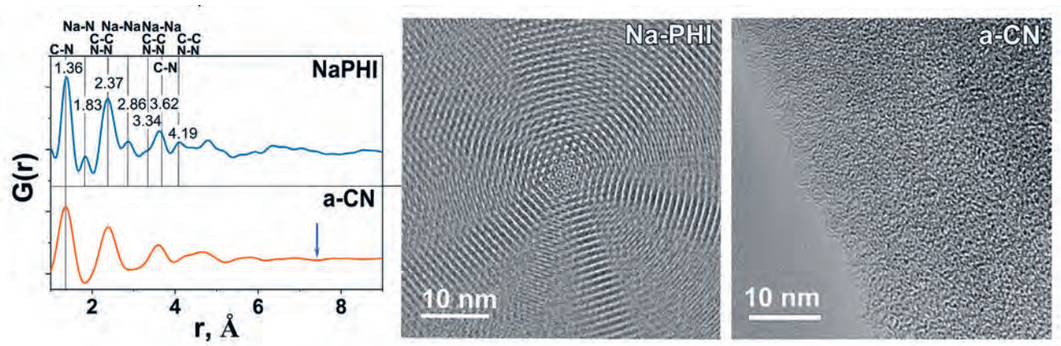

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Fig. 1 eRDF of Na-PHI and a-CN, for which the average coherence length (ACL) is marked by a blue arrow; ARL of Na-PHI reaches 4.7 nm (not shown). HRTEM images of Na-PHI and a-CN.

Two main topics are currently in development in the Electron Microscopy group: (1) understanding of important processes in chemistry and materials science (materials formation, condensation, electrochemical reactions, etc.) at the nanoscale and (2) nanoscale characterization of organic-inorganic interfaces.

In the past two years, we have applied energy-filtered electron radial distribution function (EF-eRDF) analysis to study the structure of poorly crystalline, nano-, and amorphous materials. Zero-loss energy filtering improves the signal-to-noise ratio 5 times, considerably enhancing the quality of the electron total scattering data, especially in the case of amorphous materials. Using this technique, we were able to characterize bonding, coordination, and the average coherence length, for example, in carbon-nitride materials with different degrees of crystallinity such as polyheptazine imides, amorphous CN covalent networks (Fig.1.) [1-2]. The fact that eRDF can be collected within a few seconds on any standard transmission electron microscope and that it is normally recorded at very low electron doses in comparison to TEM imaging techniques makes eRDF analysis not only easily accessible to many users but also ideal for characterizing beam-sensitive and poorly crystalline materials. EF-eRDF in combination with HR-(S)TEM gives a unique set of information at the nanoscale, which is extremely useful to study processes. Using this approach, we performed a time-dependent study of the formation of CeO2 mesocrystals in water solution. [3] We showed that, in the absence of additives, CeO2 mesocrystal growth is guided by amorphous hydrated Ce(IV)-hydroxides formed at the very early stages of the reaction and serving as an intermediate in the liquid-to-solid phase transformation. Primary particles nucleate, grow, and align inside the amorphous hydroxide. We also studied the process of the condensation of CN frameworks from molecular precursors in-situ in the microscope. Combining this with EF-eRDF analysis, we were not only able to distinguish several stages of molecular precursor condensation but also to directly link it to the developing of porous structures and sorption properties.

References: [1] Kossmann, J. et al.: Carbon, 172, (2021) pp. 497—505.
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[3] Li, Z. et al.: Angew Chem Internat Edit 61 (6), (2022) e202112204.

Dr. Nadja Tarakina

Group Leader since 2017

2020 Habilitation in Experimental Physics
Institute of Physics, University of Würzburg (Germany)

2014—2017 Experimental Officer in Microscopy
The NanoVision Centre, Queen Mary University of London (UK)

2011—2014 Academic Fellow
University of Würzburg (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc

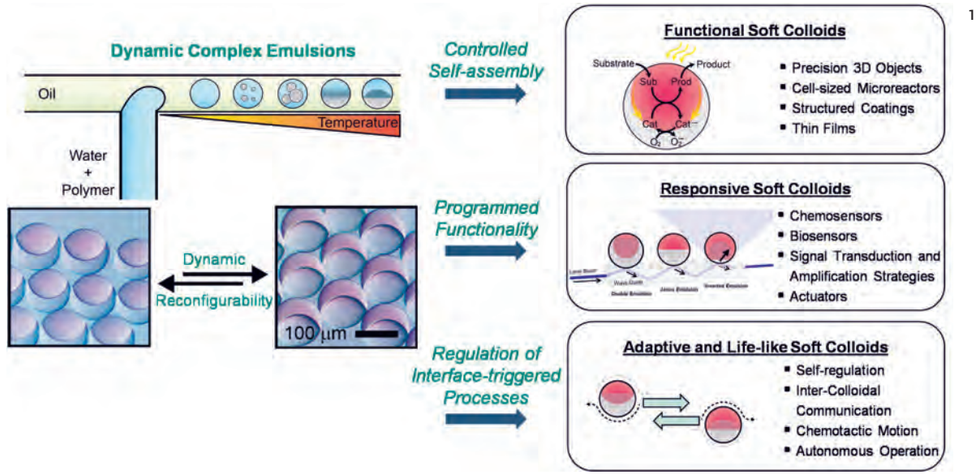

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Fig. 1 Dynamic multiphase emulsion droplets as colloidal tectons for the generation of functional, responsive, and adaptive soft materials.

The autonomous regulation of chemical reactivity represents a fundamental ability of living organisms. In nature, chemical information can be processed with high fidelity and the highest substrate specificities are achieved as multiple individual or combinations of independent chemical equilibrium-driven transformations are translated into a specific response. This cross-check capability and self-regulation behavior forms the basis for the high complexity and specificity achieved within biological systems and is further fundamental for the complex emergent behavior observed in multibody systems, for instance their self-regulated ability to communicate, move, evolve, and self-organize into patterns or networks.

In our group, we are interested in the bio-inspired generation of artificial soft materials that exhibit chemo-intelligence in that they are capable of autonomously interacting with their environment and operate in response to (bio)chemical cues. More specifically, we seek to dissect and emulate individual autonomous capabilities of biological colloids by using our own, synthetically minimal, and structurally highly defined complex soft colloids, based on both active complex emulsions and responsive polymers. It is our mission to explore the basic mechanisms that govern interactions between natural and artificial soft materials and to gain a basic physicochemical understanding of the thermodynamics and dynamics of these new types of active soft matter. Our findings help to unravel fundamental mechanisms of inter-colloidal communication in nature, and we use our discoveries to create new, transformative application concepts, e.g. in biomimicry, solar energy conversion and catalysis, dynamic optical coatings, environmental remediation and monitoring, as well as in chemo- and biosensing platforms.

References: **[1]** Frank, B. D.; Djalali, S.; Baryzewska, A. W.; Giusto, P.; Seeberger, P. H.: Reversible morphology-resolved chemotactic actuation and motion of Janus emulsion droplets. Nat. Commun. 2022, 13, 2562.
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[3] Pavlovic, M.; Antonietti, M.; Schmidt, B. V. K. J.; Zeininger, L.: Responsive Janus and Cerberus Emulsions via Temperature-induced Phase Separation in Aqueous Polymer Mixtures. J. Colloid Interf. Sci. 2020, 575, 88.

Dr. Lukas Zeininger
Emmy-Noether Group Leader since 2019

2020 VW Experiment! Research Grant
Volkswagen Foundation, Solar Paint: Janus Emulsion-based Solar Concentrators

2019 Acceptance to the DFG Emmy Noether Program (Dynamic Liquid Colloids: Principles & Applications)
MPICI, Department of Colloid Chemistry (Potsdam, Germany)

2016–2018 Postdoctoral Fellow
Department of Chemistry, Massachusetts Institute of Technology (MIT) (Cambridge, USA)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/kc

Department of Theory & Bio-Systems

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Founding Director
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Dr. rer. nat., summa cum laude,
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Physics Diploma
at the University of Heidelberg

2017 Wolfgang Ostwald Prize

Publication selection

Lipowsky, R.: Remodeling of Membrane Shape and Topology by Curvature Elasticity and Membrane Tension. Adv. Biology, 6:2101020, 2022.

Steinkühler, J.; Knorr, R. L.; Zhao, Z.; Bhatia, T.; Bartelt, S.; Wegner, S.; Dimova, R.; Lipowsky, R.: Controlled division of cell-sized vesicles by low densities of membrane-bound proteins. Nature Commun., 11:905, 2020.

Ghosh, R.; Satarifard, V.; Grafmüller, A.; Lipowsky, R.: Spherical Nanovesicles Transform into a Multitude of Nonspherical Shapes. Nano Lett., 19:7703—7711, 2019.

“Life is motion”
ARISTOTLE

Our body consists of trillions of individual cells. When we look at tissues and organs with the naked eye, corresponding to millimeter resolution, most tissues appear to be rather immobile. However, this view changes drastically when we increase the resolution by a factor of 1,000 to obtain micrometer resolution and to explore the interior of single cells. Indeed, each cell is enclosed by its plasma membrane and contains a large number of intracellular membranes that partition space into many different subcompartments. These subcompartments are very dynamic and undergo frequent remodeling processes via membrane fusion and fission. In addition, on the nanometer scale, we find directed movements by biomolecular machines such as molecular motors, protein filaments, and ribosomes which are coupled to ATP or GTP hydrolysis. One long-term challenge is to build synthetic biosystems that mimic this intracellular activity. In order to do so, we need to improve our understanding of the hidden dimensions of self-organization at the nanoscale.

Research in the Department of Theory & Bio-Systems

From 2019 to 2021, the department hosted eight research groups, led by Rumiana Dimova, Andrea Grafmüller, Reinhard Lipowsky, Markus Miettinen, Tom Robinson, Sophia Rudorf, Angelo Valleriani, and Thomas Weikl. The details about the research in these groups are described in separate reports by the group leaders. In the following, the main focus will be summarized and a few results will be highlighted.

Molecular Modeling. The research groups of Andrea Grafmüller, Markus Miettinen, and Reinhard Lipowsky studied the molecular dynamics of polysaccharides and lipids. The Grafmüller group focused on long polysaccharide chains and optimized the corresponding force fields in order to obtain a reliable description for the interactions between sugars and water. The Miettinen group was active within the network NMRlipids, a collaborative effort of several groups to understand lipid bilayers on the atomistic scale. Using data-driven calibration, the network improved the force fields for the simulations of lipid bilayers. A collaboration between Miettinen and Lipowsky revealed that frequent flip-flops between the two leaflets of a bilayer membrane can lead to tensionless leaflets. [Miettinen and Lipowsky: Nano Letters 2019] The Lipowsky group used coarse-grained molecular dynamics simulations to explore the shape transformations and division of nanovesicles. [Ghosh et al.: Nano Letters 2019; ASC Nano 2021]

Biomolecular Processes. The research groups of Sophia Rudorf, Angelo Valleriani, and Reinhard Lipowsky used stochastic modeling to study biomolecular processes. The Rudorf group worked on the dependence of protein translation on EF-Tu concentration and codon optimization via synonymous substitution. One doctoral project of the Rudorf group addressed the post- and co-translational assembly of proteins in vitro and in vivo. The in-vitro study was performed in collaboration with the lab of Roy Bar-Ziv at the Weizmann Institute. [Vonshak et al.: Nature Nanotechnology 2020] The Valleriani group collaborated with several experimental groups on bacteriophages and on malaria parasites. The Lipowsky group further developed the modeling of cooperative cargo transport by teams of molecular motors. [Ucar and Lipowsky, Nano Letters 2020] Another study addressed the force-dependent unbinding rate of molecular motors in optical traps. [Berger et al., Nano Letters 2019]

Proteins and Membranes. Thomas Weikl’s group studied the interactions of proteins and other biomolecules. Using multiscale modeling, the group analyzed the bonds between membrane-anchored receptors and ligands that are relevant for phagocytosis by macrophages. The simulations addressed experimental data obtained by Jan Steinkühler during his visit to the lab of Dennis Discher at UPenn. The study revealed the cooperative nature of the receptor-ligand bond arising from nanoscale membrane fluctuations. [Steinkühler et al., J. Cell Sci. 2019]

Membranes and Giant Vesicles. The behavior of biomembranes and giant unilamellar vesicles (GUVs) has been addressed by the groups of Rumiana Dimova, Tom Robinson, and Reinhard Lipowsky. The Dimova group used superresolution microscopy to characterize highly curved membrane segments. [Roy et al., Nano Letters 2020; Zhao et al., Advanced Materials 2021] The Robinson group has further developed microfluidic methods to produce giant unilamellar vesicles and designed microfluidic chips that can be used to manipulate vesicles and cells. The Lipowsky group has created multispherical shapes of giant vesicles [Bhatia et al., Soft Matter 2020], achieved unprecedented control over the division of such vesicles [Steinkühler et al., Nature Communications 2020], and developed a quantitative description for active shape oscillations as observed in the lab of Petra Schwille at the MPI of Biochemistry. [Christ et al., Soft Matter, 2021]

International Max Planck Research Schools. During 2019—2021, the department remained in charge of the International Max Planck Research School on “Multiscale Biosystems”, which started its operation in 2013.

↘ Further information can be found at www.mpikg.mpg.de/th

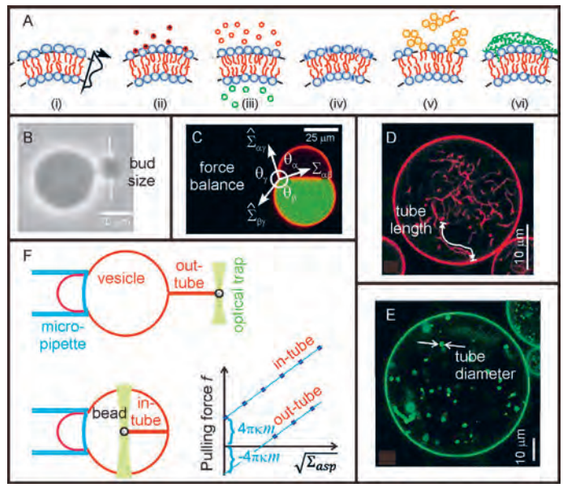

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Fig. 1 Examples for sources of membrane remodeling via the generation of nonzero membrane spontaneous curvature via different molecular mechanisms (A), and experimental approaches for assessing this curvature (B—E) based on measuring the size of buds (B), membrane nanotubes (D, E), and contact angles (C), and from pulling tubes from vesicles held by a micropipette at tension Σ_{asp} (F). Reproduced from [2].

Giant vesicles are a model membrane system that has been initially established and used as a workbench for studying basic properties of simple lipid bilayers. Nowadays, they are increasingly employed by biophysicists to unravel the mechanisms driving various biological processes occurring at the level of the cell membrane. They represent a promising and extremely useful biomembrane system because they provide the possibility for systematic and direct measurements of the membrane mechanics as a function of composition, surrounding media, and environmental factors and perturbations, as summarized in a recent book [1]. Giant vesicles are employed not only in the field of biophysics and biology but also in physical chemistry, in quests to understand the origin of life, as simple artificial cells for reconstructing essential cellular processes, and in application-oriented directions such as drug delivery and synthesis of materials where the vesicles are used as microreactors.

Presumably, the most important advantage of giant unilamellar vesicles (GUVs) over other model membrane systems is their cell-size dimensions and that the membrane response to external factors such as ions, (macro)molecules, hydrodynamic flows, or electromagnetic fields can be directly observed under the microscope. In the last couple of years, our group has dedicated significant effort to understanding the mechanism of membrane reshaping and developing assays for the quantitative assessment of curvature generation using GUVs as a model membrane system [2], see Fig. 1.

Apart from synthetic GUVs made by the bottom-up self-assembly of lipids, we also employ a top-down approach for constructing vesicles, namely by deriving them directly from cells (a process called blebbing). These plasma membrane-derived vesicles store significant area in the form of nanotubes in their lumen. We found that these nanotubes can be recruited by mechanical tension applied to the outer vesicle membrane. They ascribe to the membrane a “super-elastic” response, which emerges from the interplay of membrane heterogeneity and spontaneous curvature [3]. This finding allows for bottom-up engineering of synthetic biomaterials that appear one magnitude softer and with much larger deformability than conventional lipid vesicles. These results open a path towards designing super-elastic synthetic cells possessing the inherent mechanics of biological cells.

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Dr. Rumiana Dimova

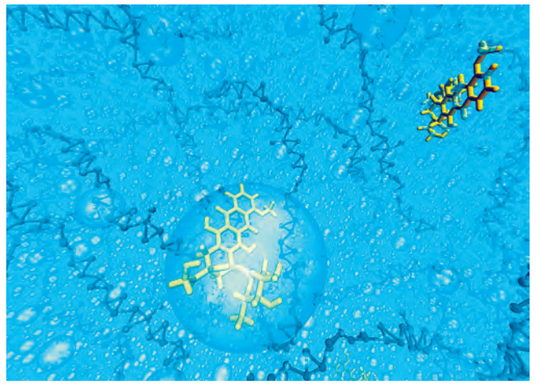
Group Leader since 2001

2021 Liesegang Prize of the German Colloid Society
in recognition of Rumiana Dimova’s work on lipid bilayers and biomembranes

2014 Emmy Noether Distinction for Women in Physics
(European Physical Society)

2012 Habilitation in Biophysics
Potsdam University (Germany)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/th



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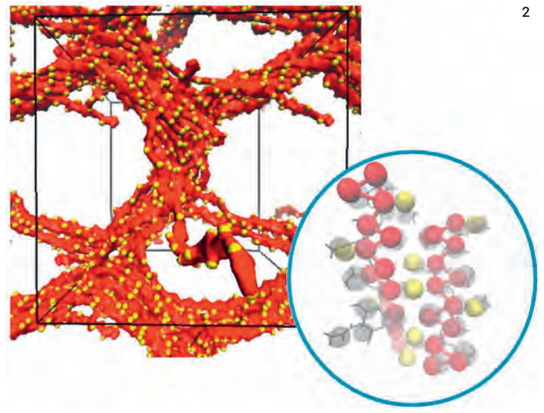

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Fig. 1 Small molecules (yellow) diffusing through chitosan (gray) hydrogel.
Fig. 2 Network of self-assembled chitin-like fibrils in a coarse-grained model locally resemble the chitin crystal structure (inset).

Carbohydrates are important for a large variety of biomolecular functions and form the basis of bio-materials with highly optimized material properties. Their many OH groups can form hydrogen bonds, both within supramolecular aggregates and with water. Which of these interactions dominates is highly dependent on the molecular details, giving rise to a broad spectrum of material structures and properties. As a result, natural polysaccharides are of great interest for a multitude of applications.

The Multiscale Modeling group develops computational tools to understand the structure-function relations of carbohydrates. To predict properties at the material scale, models need to be able to both capture details at the scale of individual atoms and to propagate those to the level of the supramolecular aggregates.

The predictive power of molecular simulations depends heavily on their ability to capture the balance of molecular interactions. The osmotic pressure is a sensitive measure to quantify this balance and is increasingly used in the development of simulation models. We have shown that precise results for the computationally expensive osmotic pressure calculations can be obtained using a bottom-up coarse graining procedure at a fraction of the cost [1].

Extending the setup to include a lipid bilayer allows evaluation of carbohydrate-lipid interactions, showing that, as for other carbohydrate systems, attractive interactions are strongly over-represented in common force fields [2].

Our multiscale modeling strategy has been successfully applied to characterize the physicochemical properties of various polysaccharide systems, including drug transport through functionalized chitosan hydrogels [3] and the aggregate formation of cellulose derivatives.

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Dr. Andrea Grafmüller

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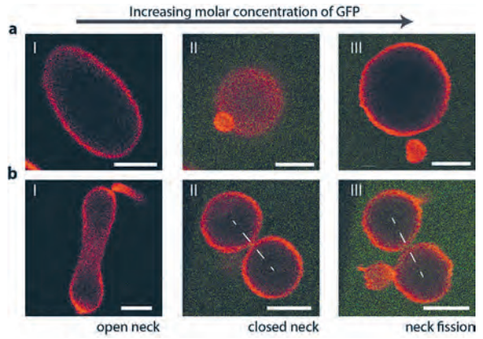
since 2021 Machine Learning Researcher
Nostos Genomics

2010—2011 Postdoctoral Scientist
University of Chicago (USA)

2009—2010 Postdoctoral Scientist
University of Utah (USA)

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/th



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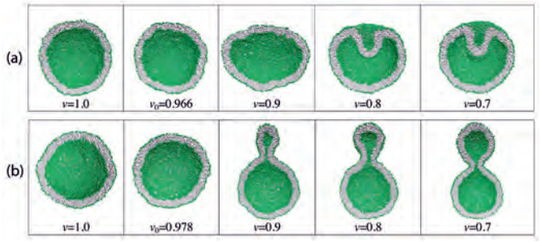

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Fig. 1 Division of GUVs (red) by increasing the molar concentration of green fluorescent protein (GFP, green) in the exterior aqueous solution: (a) Asymmetric division into one large and one small daughter vesicle; and (b) Symmetric division into two daughter vesicles of equal size. The division process starts, in the absence of GFP, from a prolate vesicle shape as displayed in I. Addition of GFP then transforms each GUV into two (punctured) spheres that are connected by a closed membrane neck as in II. A further increase in the GFP concentration leads to the fission of the neck and to the division of the GUV as shown in III. [1]
Fig. 2 Shape transformations of two spherical nanovesicles (NVs) with volume $U = 1.0$ when their volume is reduced to $U = 0.7$ via osmotic deflation. The spherical NVs have the same size and are built up from the same total number of lipids but differ in their leaflet tensions which are controlled by the number of lipids assembled in each leaflet. The spherical NV has a compressed inner leaflet in (a) and a compressed outer leaflet in (b). As a consequence, the spherical NV transforms into a stomatocyte in (a) and into a dumbbell in (b). [5]

In the reporting period from 2019 to 2021, the group focused on the remodeling of biomembranes. Two types of synthetic membrane compartments were studied: giant unilamellar vesicles (GUVs) with a size of tens of micrometers and nanovesicles (NVs) with a size of tens of nanometers. The studies of GUVs were based on the fruitful interplay between the theory of curvature elasticity and experimental observations by optical microscopy. The investigations of NVs were pursued via molecular dynamics simulations.

Remodeling of giant vesicles

For GUVs, fine-tuning of the spontaneous curvature has been achieved by low densities of membrane-bound green fluorescent protein (GFP), which allowed the controlled division of such vesicles, as shown in Fig. 1. [1] This division process represents a milestone for the bottom-up approach to synthetic biology.
Additional studies on GUVs described (i) the creation of multispherical GUV shapes, [2,3] which demonstrated the complex energy landscapes of these vesicles, and (ii) active shape oscillations of GUVs generated by Min proteins [4]. Shreya Pramanik worked on her doctoral project to elucidate the binding of His-tagged molecules to giant vesicles.

Remodeling of nanovesicles

For nanovesicles (NVs), the mechanical tensions, Σ_1 and Σ_2, of the two leaflets have been identified as key parameters that control the NV morphology. To avoid membrane rupture, we focused on bilayer membranes, for which the bilayer tension $\Sigma = \Sigma_1 + \Sigma_2$ is close to zero. For such a tensionless bilayer, the leaflet tensions satisfy $\Sigma_2 = -\Sigma_1$, which implies that one leaflet is stretched by a positive tension whereas the other leaflet is compressed by a negative tension. The leaflet tensions can be directly controlled in simulations by the number of lipids that are initially assembled in each leaflet.
Additional studies of NVs revealed (i) that a multicomponent bilayer with a flip-flopping lipid species can relax towards a reference state in which both leaflet tensions vanish [6] and (ii) that shape transformations, as in Fig. 2, can also be induced by the adsorption of small solutes onto the NV membrane [7]. Miftakh Zamaletdinov worked on his doctoral project to determine how the behavior of NVs depends on their size.

The results for both GUVs and NVs were summarized in a recent review [8].

References: [1] Steinkühler, J.; Knorr, R. L.; Zhao, Z.; Bhatia, T.; Bartelt, S.; Wegner, S.; Dimova, R.; Lipowsky, R.: Controlled division of cell-sized vesicles by low densities of membrane-bound proteins. Nature Commun., 11:905, 2020.
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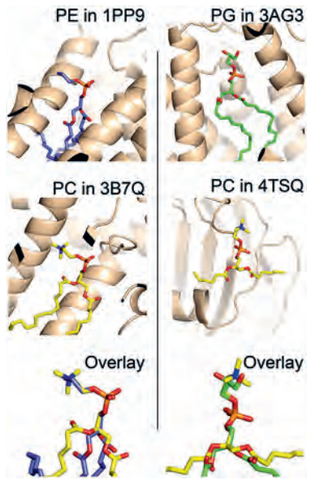
[8] Lipowsky, R.: Remodeling of Membrane Shape and Topology by Curvature Elasticity and Membrane Tension. Adv. Biology, 6:2101020, 2022.

↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/th



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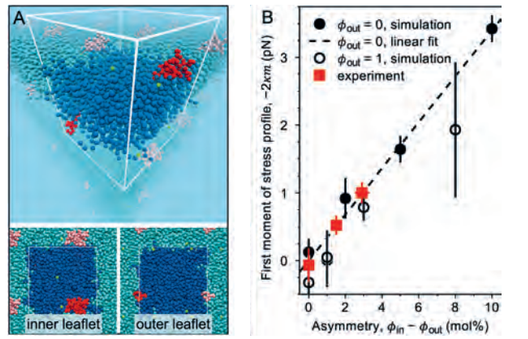

2

Fig. 1 Left: PE headgroup bound to cytochrome (PDB ID: 1PP9) in an identical conformation as PC bound to Sec14 (3B7Q). Right: PG headgroup bound to cytochrome c oxidase (3AG3) in an identical conformation as PC bound to FraC (4TSQ).
Fig. 2 A) Simulation snapshot of a GM1 lipid (red) in a bilayer on POPC lipids (blue). B) As a function of bilayer asymmetry, calculated first moment of lateral stress profile (black) matched the experimental measurement (red) quantitatively.

Many interesting molecular systems from chemistry, physics, and biology can be considered to be classical many-body systems. To describe their behavior, no quantum mechanics is needed; atoms and chemical bonds can be treated as objects of classical mechanics. In molecular dynamics (MD) simulations, the time evolution of such systems is solved numerically. The continuing exponential growth in computing power has made MD a tool that can provide impressive 3D videos on the spatial and temporal functioning of complex biomolecules; however, the usefulness of MD fully depends on the fidelity of the classical approximation, i.e. the underlying "force field". Our group strives towards the ideal of truly faithful biomolecular MD, in which the positions and movements of atoms match reality as precisely as the most structurally sensitive experimental methods (NMR spectroscopy and scattering) can measure. The critical assessment of MD against these experiments is crucial: It not only reveals the limits of applicability of our current force fields, but the critically vetted MD provides the best available intuitive interpretation of these typically hard-to-interpret experimental data. We approach these themes through three topics. 1) The open science collaboration NMRlipids Project (↘ www.nmrlipids.blogspot.fi), which has most recently shown that all current lipid force fields fail to capture the phosphatidyl serine headgroup structure [1]; and that all major lipid headgroup types sample wide ranges of conformations, with little effect from differences in headgroup chemistry, see Fig. 1. [2]; 2) via automated data-driven calibration of biomolecular force fields, and 3) via calculation of nanoscale stress distributions across biomolecular systems from MD data.

References: [1] Antila, H.; Buslaev, P.; Favela-Rosales, F.; Ferreira, T. M.; Gushchin, I.; Javanainen, M.; Kav, B.; Madsen, J. J.; Melcr, J.; Miettinen, M. S.; Määttä, J.; Nencini, R.; Ollila, O. H. S.; Piggot, T. J.: Headgroup Structure and Cation Binding in Phosphatidylserine Lipid Bilayers. Journal of Physical Chemistry B 123 9066 (2019).
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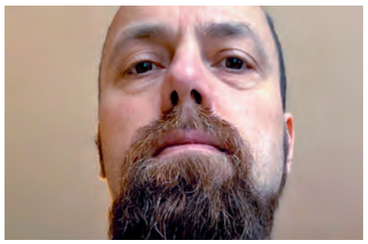
[3] Miettinen, M. S.; Lipowsky, R.: Bilayer membranes with frequent flip-flops have tensionless leaflets. Nano Letters 19 5011 (2019).

Prof. Dr. Markus Miettinen

Group Leader 2017—2022



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Department of Chemistry and Computational Biology Unit, University of Bergen (Norway)

2012—2016 Postdoctoral Scientist
Department of Physics, Freie Universität Berlin (Germany)

2005—2010 Doctor of Science
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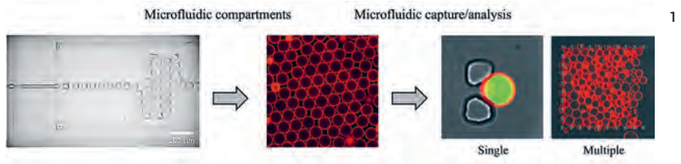
↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/th



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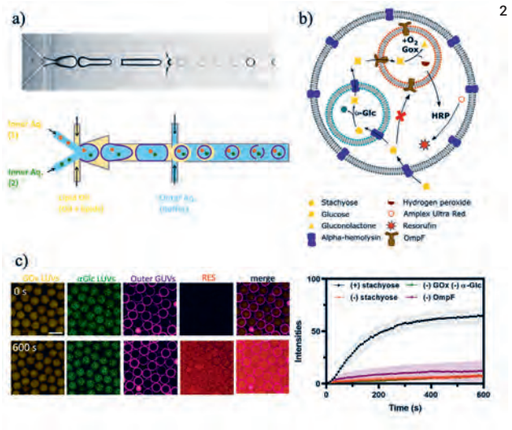

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Fig. 1 Microfluidics is used for synthetic cell research in two major areas. To create monodisperse GUVs and also to capture them for analysis/manipulation.
Fig. 2 Bottom-up creation of a synthetic eukaryotic cell. a) Microfluidics is used to co-encapsulate two populations of nano-size vesicles with enzymes. b) The metabolic pathway with each step confined to its own compartment. c) Monitoring the final fluorescent product inside the synthetic cells.

Bottom-up synthetic biology aims at the de novo construction of synthetic minimal cells using non-living components. Building minimal cells and controlling each aspect of their design not only gives us the opportunity to understand real cells and their origins but also provides alternative routes to novel biotechnologies. In this field, giant unilamellar vesicles (GUVs) are used extensively as scaffolds to construct synthetic cells owing to their compatibility with existing biological components. Our group is interested in using GUVs to create multiple-compartment systems, thus mimicking eukaryotic cells and providing additional functionalities to our synthetic cells.

We use microfluidic technology for two main areas of research (Fig. 1). The first is to create our synthetic cells from GUVs with high monodispersity and with high encapsulation of biomolecules. Our designs are able to produce pure-lipid GUVs at high-throughput rates (3 kHz) without surfactants or residual oils and encapsulating a wide range of materials (e.g. DNA, enzymes, lipid vesicles, microparticles) [1]. We also use microfluidic devices to spatially confine our synthetic cells for high-throughput analysis [2]. The trapped cell-like systems can then be used for a variety of applications from membrane biophysics to ligand-membrane interactions.

Recently, we have focused on setting up reaction-diffusion systems inside synthetic cells as a first step towards complex eukaryotic mimics [3]. Microfluidics is used to encapsulate two populations of nano-sized vesicles for the purpose of establishing enzymatic cascade reactions between subcompartments (Fig. 2). The final system comprises three coupled enzymatic reactions, which propagate in a specific spatial direction due to selective membranes pores. Not only does microfluidics provide a high degree of control over conditions such as enzyme concentrations, buffers, and numbers of compartments but the GUV monodispersity allows us to directly compare the effects that compartmentalization has on the biochemical reaction rates.

References: [1] Yandrapalli, N.; Petit, J.; Bäumchen, O.; and Robinson, T.: Surfactant-free production of biomimetic artificial cells using PDMS-based microfluidics. Communications Chemistry 4, 100 (2021).
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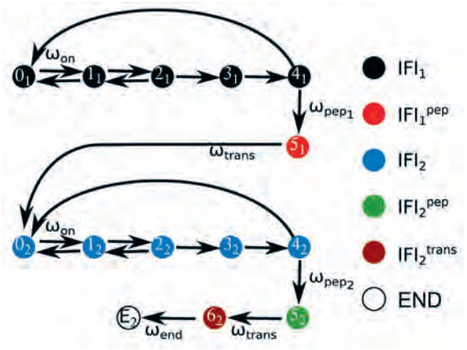
1



2

Fig. 1 Screenshot of our OCTOPOS software. OCTOPOS can be used to optimize mRNA sequences for enhanced protein synthesis [2].
Fig. 2 Typical representation of a translation process with states (•) corresponding to different biochemical configurations of the involved molecules.

Cells have to fulfill many different tasks during their lifetime—they move, divide, communicate, change their function, and much more. To perform all of these tasks, cells rely on one of the most important classes of biomolecules: proteins. Each cell contains thousands of different proteins, and every single one of them has a specific purpose. Although proteins differ a lot in their functionality, they are all linear chains of amino acids made from the same building blocks. The huge variety of protein structures and functions arises from the choice and order of the individual amino acids in these chains.

The information about which amino acid needs to go where to make a specific protein is encoded in the DNA. To synthesize a new protein, the corresponding part of the DNA is transcribed to messenger RNA (mRNA). A molecular machine called ribosome binds to the mRNA and decodes it step by step, thereby catalyzing the synthesis of the corresponding amino acid chain until the new protein is finished. This process is called translation.

Our group builds theoretical frameworks that help to investigate and understand the biophysical and biochemical details of translation. In our projects, we combine tools and methods from mathematics, bioinformatics, and data science to create in silico models of translation in different systems and organisms. We work in close collaboration with experimental groups from bio-related fields such as plant physiology, biostatistics, biotechnology, or biophysics. We use our computational models of translation for many different applications. For example, our work helps to explain the efficiency of antibiotics [1], create new mRNA sequences for maximal protein yield [2], or design biochips for the assembly of biomolecular machines [3].

References: [1] Rudorf, S.: Efficiency of protein synthesis inhibition depends on tRNA and codon compositions. PLOS Computational Biology (2019).
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[3] Vonshak, O.; Divon, Y.; Förste, S.; Garenne, D.; Noireaux, V.; Lipowsky, R.; Rudorf, S.; Daube, S. S.; Bar-Ziv, R. H.: Programming multi-protein assembly by gene-brush patterns and two-dimensional compartment geometry. Nature Nanotechnology (2020).

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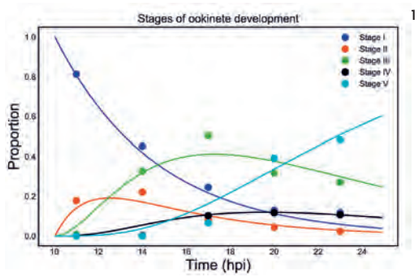

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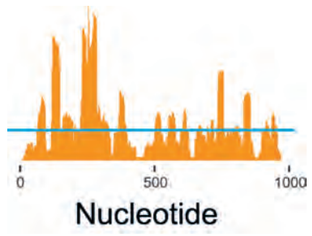

2

Fig. 1 Experimental data and model fitting. Experimental data out of several independent experiments have provided the changing proportions over time of the traditional five ookinete stages (dots) [1]. A simple chemical kinetics model associates a state to each stage and produces a fit (lines) from which the timescales associated to each stage can be determined. Moreover, more refined models in the same class have shown a better fit when stage II and stage III ookinetes are expanded to accommodate for one extra stage. The experimental validation of this prediction will lead to a new classification of the morphologies of ookinetes.
Fig. 2 Example of a ribosome profile in E. coli. By means of an experimental technique called Ribo-seq, it is possible to determine the regions in each translated mRNA in which the ribosomes are slower (peaks) or faster (valleys). Their identification is obtained by comparing the profiles from independent experiments [2].

A new stage in P. falciparum ookinete maturation

Plasmodium falciparum is a deadly parasite responsible for most of the malaria cases worldwide. This parasite requires a mosquito vector in order to infect humans. Inside the mosquito, the parasite goes through several life stages that are subject to intense investigations. The ookinete stage is the focus of this project. Here I developed a mathematical model that recapitulates the known experimental kinetic steps [1] of the parasite in this stage, during which the cells take several distinguishable morphologies (Fig. 1). The model predicts the existence of an additional intermediate morphology that is currently the subject of experimental investigation. This project is an experimental and theoretical collaboration with Elena A. Levashina's group at the Max Planck Institute for Infection Biology in Berlin. The results of this project may help uncover variations in the development of the parasite under different conditions. This knowledge could be exploited in the fight against the disease.

Uncovering slow and fast translated regions in E. coli transcriptome

When ribosome translate a messenger RNA, they don't do it at a uniform speed. This fact is well-known in molecular biology. Many studies looking into this phenomenon have tried to uncover both the mechanisms responsible for local slow-downs and its possible consequences for the expression of the genes. Together with Davide Chiarugi, currently at the Max Planck Institute for Human Cognitive and Brain Sciences in Leipzig, we developed a method to look for those sub-sequences in the transcriptome of Escherichia coli where ribosomes are slow (or fast) in a reproducible manner by comparing many independent experimental studies under the same growth conditions (Fig. 2). One big challenge in this analysis is the low signal-to-noise ratio, which requires ad-hoc tools to harvest a few sequences. In this project, we are taking the data available in published research papers and developing a computer program to dig into the data following an initial pilot study [2]. This analysis tool will produce a list of highly reliable and reproducible sequences from which we will learn the patterns that make up a fast versus a slow translated region. Experiments planned in collaboration with Prof. Silke Leimkühler at the University of Potsdam and Prof. Zoya Ignatova at Hamburg University will finally exploit this knowledge by unveiling the effect of tRNA modifications on the speed and efficiency of translation.

References: [1] Siciliano, G.; Costa, G.; Suárez-Cortés, P.; Valleriani, A.; Alano, P.; Levashina, E. A.: Critical steps of Plasmodium falciparum ookinete maturation. Frontiers in Microbiology 11, 269 (2020).
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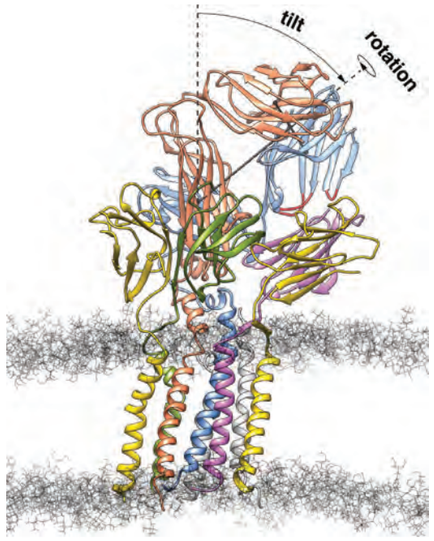

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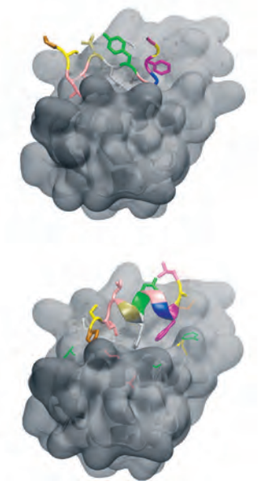

2

Fig. 1 Illustration of large orientational variations of the TCR extracellular domain in the membrane-embedded TCR-CD3 complex.
Fig. 2 A metastable binding intermediate (top) and the native bound state (bottom) of PMI (colored) and MDM2 (gray).

References: [1] Pandey, P. R.; Rozycki, B.; Lipowsky, R.; Weikl, T. R.: Structural variability and concerted motions of the T cell receptor—CD3 complex. eLife (2021).
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Biomolecular recognition typically involves conformational changes. Our group explores the interactions, conformations, and function of biomolecules with simulations and modeling. In the past three years, we have used atomistic molecular dynamics (MD) simulations and Markov state modeling of protein interactions to gain insights on the coupling of conformational changes to binding and function.

We have investigated the structural and orientational variability of the membrane-embedded T cell receptor (TCR)-CD3 complex in extensive MD simulations based on a recent cryo-EM structure of the complex. We have found that the TCR extracellular domain is highly variable in its orientation by attaining tilt angles relative to the membrane normal that range from 15° to 55°. These large orientational variations are coupled to conformational changes throughout the TCR-CD3 complex and may play a role in the signal transmission from extracellular antigen-binding sites to intracellular activation motifs.

Unstructured proteins and peptides typically fold during binding to ligand proteins. The inhibitor peptide PMI folds into a helix during binding to the oncoprotein Mdm2. Our atomistic simulations and Markov state modeling indicate that the binding-induced folding of PMI is highly parallel and can occur along a variety of pathways. Binding occurs prior to helix formation on some pathways and after helix formation on other pathways. On the majority of pathways, however, binding is intricately coupled to folding, without clear temporal ordering of binding and folding.

In addition, we have investigated how membrane proteins cooperate in the shaping and adhesion of biomembranes. Our simulations of carbohydrate–carbohydrate interactions of glycolipids in membrane adhesion revealed weakly attractive, "fuzzy" interactions that result from a large variety of short-lived, bound conformations.

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↘ Further information on the research group as well as on the publications can be found at www.mpikg.mpg.de/th

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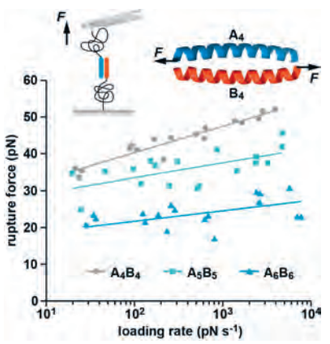
Proteins are essential building blocks of biogenic materials. In addition to purely protein-based materials, a wide range of composite materials are formed in nature, where proteins mediate specific interactions with insoluble organic structures or mineral surfaces. In all cases, the thermodynamic, kinetic, and mechanical stability of protein-protein or protein-surface interactions crucially determines material assembly, structure, and function. Our goal is to elucidate the molecular mechanisms (i) to obtain a fundamental understanding of the underlying interactions and (ii) to utilize the discovered principles towards the controlled bottom-up synthesis of bio-inspired mechanoresponsive materials. Protein building blocks of interest are extracellular matrix-inspired α-helical coiled coils (CCs) and collagen-mimetic peptides (CMPs). In addition, chitin- and magnetite-binding proteins are investigated. The following examples highlight key findings obtained in this reporting period.

In collaboration with A. Vila Verde (U Duisburg-Essen) and A. Valleriani, we have tested CC length as one possible parameter for tuning CC interactions. Increasing length leads to a higher thermodynamic and kinetic stability. At the same time, longer CCs can access a larger number of conformational states when experiencing a shear force *F*. As a consequence of this entropic contribution, long CCs are mechanically weaker than short CCs when measured at high loading rates *(dF/dt)* with dynamic single-molecule force spectroscopy (Fig. 1). Future experiments aim to increase CC length further to mimic natural CC-containing proteins that undergo a force-induced transition from α-helices to β-sheets. In collaboration with L. Bertinetti (TU Dresden), E. Schneck (TU Darmstadt), and P. Fratzl, we have utilized CMPs to probe structural changes in response to alterations in osmotic pressure. We observed a sequence-specific elongation or contraction, which suggests that collagen biochemistry and mechanics are fine-tuned at the amino acid level [1].

Sequence-controlled CCs and CMPs are versatile physical crosslinks for the synthesis of peptide-polymer hybrid hydrogels. CMPs and CCs have similar thermodynamic stability; however, the association and dissociation rates of CMPs can be extremely slow (timescales of days). Whereas CC-crosslinked hydrogels were rapidly self-healing [2], out-of-equilibrium properties were observed for CMP-crosslinked hydrogels with the slowest dissociation rates. These include aging and compressed exponential stress relaxation, which may indicate that material relaxation requires unjamming of trapped configurations (collaboration with W. Ellenbroek, TU Eindhoven). These results highlight how knowledge of the molecular crosslink properties allows for understanding and controlling the resulting materials.

Moving from dynamically crosslinked hydrogels towards hierarchically structured composites, as they frequently occur in nature, is still a major challenge. In collaboration with D. Faivre (U Marseille), we have identified and characterized new magnetite-binding proteins from the magnetotactic bacterium *Desulfamplus magnetovallimorits* [3] (Fig. 2). In addition to providing new insights into the biomineralization of biogenic magnetite nanoparticles (MNPs), these proteins can now be utilized for the synthesis of composite materials that are crosslinked via the protein-MNP interaction or that allow for *in situ* MNP biomineralization. In a related project (collaboration with Y. Politi, TU Dresden), we are characterizing chitin-binding proteins, which are derived from spiders. Preliminary results show that the chitin-binding proteins possess dissociation rates on the second timescale, suggesting a contribution to stress relaxation and self-healing in spider cuticles. Future goals include the use of mutant proteins with different binding strength to synthesize molecularly controlled chitin-protein composites.



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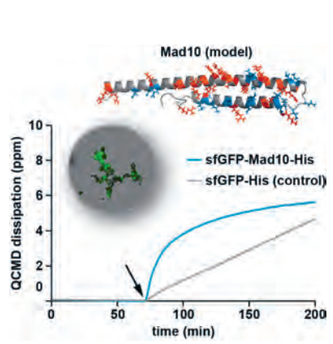

2

Fig. 1 Single-molecule force spectroscopy of coiled coils of different length (A_4B_4—8 helical turns; A_5B_5—10 helical turns; A_6B_6—12 helical turns).
Fig. 2 Qualitative (fluorescence) and quantitative (quartz-crystal microbalance with dissipation, QCMD) analysis of magnetite-binding proteins [3].

References: [1] Ruiz-Rodriguez, L.; Loche, P.; Thornfeldt Hansen, L.; Netz, R. R.; Fratzl, P.; Schneck, E.; Blank, K. G.; Bertinetti, L.: Sequence-specific response of collagen-mimetic peptides to osmotic pressure. (2021) MRS Bulletin 46, 889.
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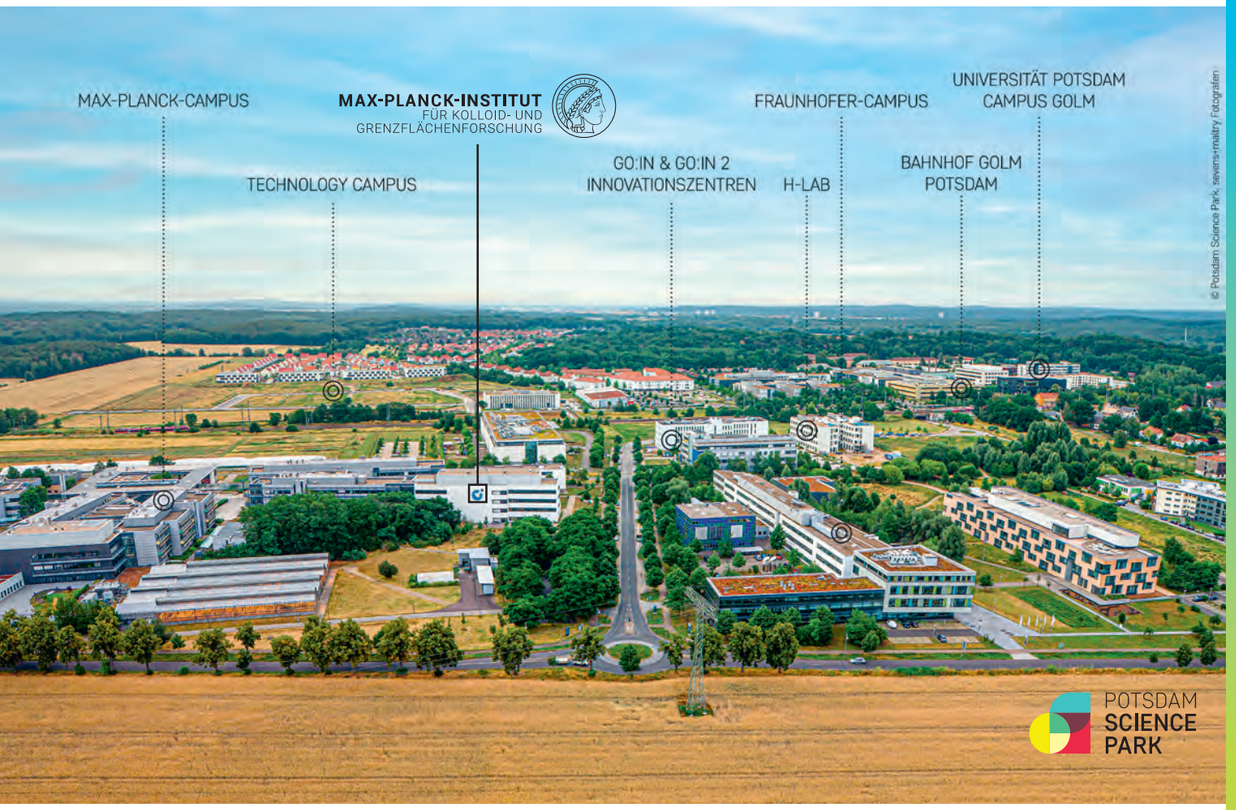

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Potsdam, Juni 2022

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Potsdam, June 2022

Dem Anwenden muss das Erkennen vorausgehen.
Insight must precede application. MAX PLANCK

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