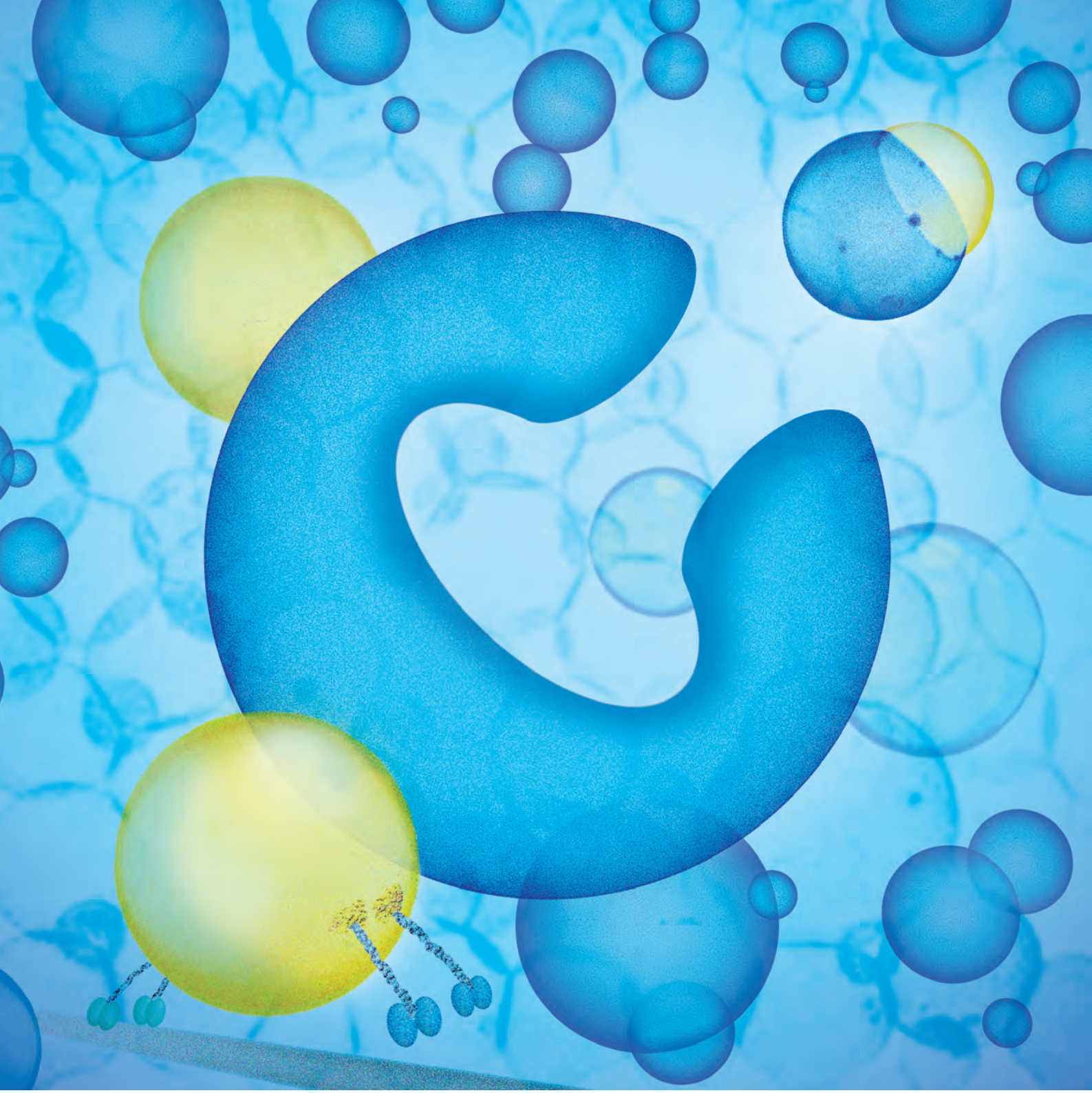

Max Planck Institute of Colloids and Interfaces

REPORT 2015-2016

MAX-PLANCK-GESELLSCHAFT

Lipidvesikel mit
Membrandomänen

Lipid vesicles
with membrane domains

Max Planck Institute of Colloids and Interfaces

RESEARCH REPORT 2015-2016

Imprint

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von links: Peter H. Seeberger, Markus Antonietti, Peter Fratzl, Helmuth Möhwald, Kerstin Blank, Reinhard Lipowsky

„Die beste Methode die Zukunft vorherzusagen besteht darin, sie zu erfinden."
(Alan Kay)

Das Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPI-KG) wurde 1992 als eines der ersten Max-Planck-Institute in den neuen Bundesländern gegründet und hat sich seitdem zu einer weltweit führenden Forschungsinstitution entwickelt. Das Institut bezog 1999 ein neues Gebäude im Wissenschaftspark Golm, der seit 2003 zu Potsdam gehört.

Die Kolloid- und Grenzflächenforschung beschäftigt sich mit sehr kleinen Strukturen im Nano- und Mikrometerbereich. Einerseits handelt es sich dabei um eine „Welt der versteckten Dimensionen", andererseits bestimmen diese winzigen Strukturen die Eigenschaften von Materialien und Biosystemen auf mesoskopischen und makroskopischen Skalen. Ein quantitatives Verständnis der Nanostrukturen bildet deshalb die Grundlage, um neuartige Impfstoffe, intelligente Wirkstoffträger und Mikrokompartimente sowie adaptive Biomaterialien zu entwickeln. Dazu ist ein interdisziplinärer Zugang notwendig, der (bio)chemische Synthese und biomimetische Materialwissenschaften mit physikalisch-chemischer Analyse und Charakterisierung sowie theoretischer Modellierung verknüpft.

Das MPI-KG wird kollegial geleitet und gliedert sich seit der Emeritierung von Helmuth Möhwald im Jahre 2016 in die vier Abteilungen „Biomolekulare Systeme" (Peter Seeberger), „Kolloidchemie" (Markus Antonietti), „Biomaterialien" (Peter Fratzl) und „Theorie & Bio-Systeme" (Reinhard Lipowsky) sowie die Max-Planck-Forschungsgruppe „Mechano(bio)chemie" (Kerstin Blank). Das Institut hat zur Zeit etwa 350 Mitarbeiter mit einem Frauenanteil von 45 %.

Die Mission des Instituts besteht darin, mit wissenschaftlicher Exzellenz eine Brücke von Molekülen zu vielskaligen Materialien und Biosystemen zu schlagen und dabei den wissenschaftlichen Nachwuchs bestmöglichst zu fördern. Tatsächlich sind inzwischen mehr als 50 ehemalige Mitarbeiter/innen auf Professuren an in- und ausländische Universitäten berufen worden.

Forschungsschwerpunkte

Die Nano- und Mikrostrukturen, die am MPI-KG erforscht werden, sind aus noch kleineren atomaren und molekularen Bausteinen aufgebaut. Die Synthese und der Zusammenbau dieser Bausteine nutzt das Prinzip der Selbstorganisation aus: Man stellt die äusseren Bedingungen so ein, dass sich die Bausteine „von selbst" miteinander verbinden und größere Strukturen aufbauen. Die beiden Abteilungen „Biomolekulare Systeme" und „Kolloidchemie" beschäftigen sich schwerpunktmäßig mit diesem Systemaufbau.

In der Abteilung „Biomolekulare Systeme" werden maßgeschneiderte Zuckermoleküle mit einer vorgegebenen Sequenz synthetisiert und mit anderen molekularen Gruppen verknüpft. Diese komplexen Kohlehydrate können andere Kohlehydrate sowie Proteine und Antikörper an ihrem molekularen Aufbau erkennen und diskriminieren, ein Prozess, der mit Hilfe sogenannter Glyco-Chips systematisch untersucht wird. Ein langfristiges Ziel ist dabei die Entwicklung von Impfstoffen auf Zuckerbasis.

Die Abteilung „Kolloidchemie" setzt verschiedenartige Makromoleküle ein, um daraus mesoskopische Verbundsysteme und Hybridmaterialien mit unterschiedlicher Architektur aufzubauen. Der Schwerpunkt liegt dabei auf der gezielten Kodierung von Strukturbildung und Selbstorganisation, d. h. die Moleküle enthalten bestimmte Muster, die die Strukturbildung steuern und die Zielstruktur weitgehend festlegen. Ein langfristiges Thema ist die Spaltung von Wasser mit Hilfe von Sonnenlicht. Für diesen Prozess wurde mit einem neuartigen Kohlenstoffnitrit-Polymer ein vielversprechender Katalysator gefunden.

Nano- und Mikrostrukturen sind hierarchisch aufgebaut. Besonders eindrucksvolle Beispiele für diesen „verschachtelten" Systemaufbau finden sich in mineralisierten Geweben, wie Knochen, Zähnen oder Muschelschalen, sowie in Pflanzen und deren Zellwänden. Diese Systeme werden in der Abteilung „Biomaterialien" mit physikalischen Methoden erforscht. Dabei wird auch die Methode der fokusierten Synchrotronstrahlung eingesetzt, die es erlaubt, die Struktur von Mikrodomänen des Materials mit atomarer Auflösung sichtbar zu machen. Im Zentrum des Interesses stehen die Struktur-Funktions-Beziehungen dieser natürlichen Materialien, insbesondere ihre außergewöhnlichen mechanischen Eigenschaften, die sich ständig wechselnden äußeren Bedingungen anpassen.

Das vielskalige Verhalten von biomimetischen und biologischen Systemen wird auch in der Abteilung „Theorie & Bio-Systeme" untersucht. Aktuelle Schwerpunkte sind biomolekulare Maschinen sowie biomimetische Membranen und deren Wechselwirkung mit Nanopartikeln. Zur Abteilung gehören auch mehrere experimentelle Arbeitsgruppen, die Lipid-Vesikel und deren „multiresponsive" Verhalten untersuchen. Die theoretischen und experimentellen Aktivitäten verfolgen das langfristige Ziel, die grundlegenden Mechanismen und generellen Prinzipien aufzuklären, die die Selbstorganisation von Bio-Systemen im Nanobereich bestimmen.

Die Max-Planck-Forschungsgruppe „Mechano(bio)chemie" untersucht den Einfluss von Kräften auf die Struktur und Funktion von Molekülen und Materialien. Aktuelle Schwerpunkte sind molekulare Kraftsensoren, Kräfte in polymeren Materialien sowie die Integration von Kraftmessung und Fluoreszenzdetektion.

Diese verschiedenen Forschungsaktivitäten werden im Hauptteil dieses Berichts sehr viel ausführlicher beschrieben. Dieser Hauptteil ist nach den Abteilungen des Instituts gegliedert und setzt sich aus den Forschungsberichten der einzelnen Arbeitsgruppen zusammen.

Aktuelle Entwicklungen

Unser Erweiterungsgebäude mit etwa 2300 qm Nutzfläche wurde 2015 nach einer längeren Planungsphase und einer relativ kurzen Bauphase fertiggestellt. Der überwiegende Teil der neuen Fläche dient der Unterbringung der Abteilung See-

berger, die von 2008 bis 2015 provisorisch in angemieteten Räumen an der FU Berlin untergebracht war. Außerdem haben wir mit dem Erweiterungsgebäude zusätzliche Laborflächen für weitere unabhängige Nachwuchsgruppen erhalten, sowie für die Inbetriebnahme moderner Großgeräte (Elektonenmikroskopie, NMR, Hochleistungsrechner).

Unser Doktorandenprogramm, die „International Max Planck Research School (IMPRS)" über „Multiscale Bio-Systems", an der auch die Universität Potsdam, die Freie Universität Berlin und die Humboldt-Universität zu Berlin beteiligt sind, hat sich in den letzten beiden Jahren kontinuierlich und erfolgreich weiterentwickelt: Seit 2013 haben wir vier Kohorten von Doktoranden in die Schule aufgenommen. Dabei wurden insgesamt 36 Doktoranden aus mehr als 1400 Bewerbern ausgewählt. Wir möchten das Doktorandenprogramm für sechs weitere Jahre fortsetzen und haben einen Antrag auf eine zweite Förderperiode gestellt, der vor im Mai 2017 sehr positiv begutachtet wurde.

Eine Herausforderung der letzten beiden Jahre war die Entscheidung unseres Präsidiums, die Bezahlung von neuen Doktoranden und Postdoktoranden aus Nicht-EU-Staaten von Stipendien auf Verträge umzustellen. Diese Umstellung ist inzwischen weitgehend abgeschlossen.

Im letzten Jahr haben wir Joanna Aizenberg von der Harvard-Universität sowie Ulrich S. Schubert von der Universität Jena als auswärtige wissenschaftliche Mitglieder des MPI-KG vorgeschlagen, um unsere Forschungsaktivitäten auf den Gebieten der adaptiven Materialien und der grünen Polymerchemie zu verstärken. Dieser Vorschlag wurde inzwischen von den entsprechenden Gremien der Max-Planck-Gesellschaft bestätigt.

Vor kurzem hat unser Institut, zusammen mit dem MPI für Molekulare Pflanzenphysiologie und der Universität Groningen, ein "Artist-in-Residence" Programm gestartet. Das Projekt „Knowlegde Link through Art and Science", kurz KLAS, bringt mit Hilfe eines internationalen Wettbewerbs innovative Künstler/innen in den Wissenschaftspark Potsdam-Golm, die dort Seite an Seite mit Forscher/innen der Gastinstitutionen arbeiten werden.

Weitere Informationen über das MPI-KG finden Sie unter *http://www.mpikg.mpg.de*

Ich danke allen Kollegen/innen und Mitarbeiter/innen des MPI-KGs, unserem wissenschaftlichen Beirat, unserem Kuratorium sowie der Leitung der Max-Planck-Gesellschaft für ihre tatkräftige Unterstützung während der letzten beiden Jahre.

Reinhard Lipowsky
Geschäftsführender Direktor 2015-2016

Fotos: G. Gnaudschun

Preface

„The best way to predict the future is to invent it."
(Alan Kay)

The Max Planck Institute of Colloids and Interfaces (MPI-CI) was founded in 1992 as one of the first Max Planck Institutes in the new states of Germany and soon became a world-wide leading research institution. In 1999, the MPI-CI moved to a new building in the Science Park Golm, which belongs to Potsdam since 2003.

Colloids and interfaces consist of very small and ultra-thin structures with linear dimensions between nanometers and micrometers. On the one hand, these nanostructures represent a „world of hidden dimensions". On the other hand, these small structures determine the properties and functions of much larger systems and materials. Therefore, a quantitative understanding of these structures provides the knowledge base to develop novel vaccines, intelligent drug delivery systems and microcompartments as well as adaptive materials. Such a deeper understanding can only arise from an interdisciplinary approach that combines (bio)chemical synthesis and biomimetic materials with physical analysis and characterization as well as theoretical modelling.

After the retirement of Helmuth Möhwald in 2016, the MPI-CI consists of the four Departments „Biomolecular Systems" (Peter Seeberger), „Colloid Chemistry" (Markus Antonietti), „Biomaterials" (Peter Fratzl) and „Theory & Bio-Systems" (Reinhard Lipowsky) as well as of the Max Planck Reserch Group „Mechano(bio)chemistry" (Kerstin Blank). The institute has currently about 350 associates with a 45 percentage of women.

The mission of the MPI-CI is to bridge the gap between molecules and multiscale materials and biosystems through excellence in science and via the support of young scientists. In fact, more than 50 former associates have taken up professorships at universities in Germany and Europe.

Focus Areas of Research

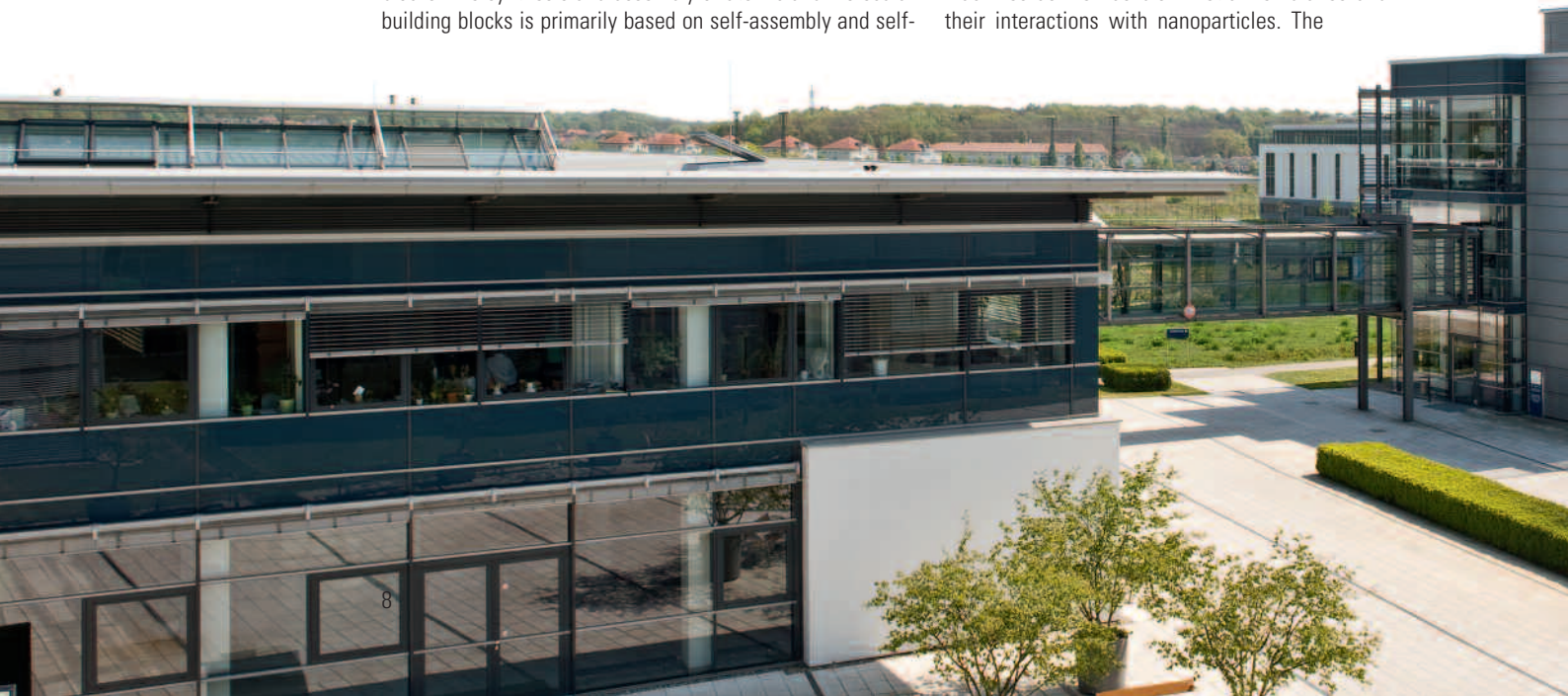
The nano- and microstructures investigated at the MPI-CI are built up from even smaller atomic and molecular building blocks. The synthesis and assembly of atomic and molecular building blocks is primarily based on self-assembly and self-organization. When placed into an appropriate environment, the building blocks assemble „by themselves" into well-defined larger structures. These structure formation processes represent the focus areas of the two Departments „Biomolecular Systems" and „Colloid Chemistry".

The Department „Biomolecular Systems" synthesizes and designs sugar molecules and carbohydrates with well-defined and fine-tuned architectures. These complex macromolecules are able to specifically recognize and distinguish other macromolecules such as proteins and antibodies, a process that is studied by immobilizing the molecules on so-called glycochips. A long-term goal of this research is to develop new vaccines based on the fine-tuned sugar molecules.

In the Department „Colloid Chemistry", a variety of macromolecules is used in order to construct mesoscopic compound systems and hybrid materials. One important aspect of this activity is the molecular encoding of self-assembly and self-organization by specific molecular groups that guide these processes towards a certain target structure. A long-term target is water cleavage by sunlight, which can be achieved by polymeric carbon nitride, a promising new catalyst.

Nano- and microstructures are built up in a hierarchical fashion. Particularly impressive examples for this „nested" system architecture is found in mineralized tissues such as bone, teeth, and seashells as well as in plants and their cell walls. These systems are studied in the Department „Biomaterials" using a variety of experimental characterization methods. One particularly powerful method is microfocussed synchrotron radiation, by which one can determine the structure of micrometer domains with atomic resolution and determine the structure-function relationships of these natural materials. One important aspect are their extraordinary mechanical properties, which can adapt to changing environmental conditions.

The multiscale behavior of biomimetic and biological systems is also investigated in the Department „Theory & Bio-Systems". Current focus areas are biomolecular machines as well as biomimetic membranes and their interactions with nanoparticles. The



The extension of our building, completed 2015.

department includes several experimental research groups that study lipid vesicles and their multiresponsive behavior. The long-term goal of these theoretical and experimental activities is to elucidate the fundamental principles and generic mechanisms, that govern the selforganization of biomimetic and biological systems in the nanoregime.

The Max Planck Research Group „Mechano(bio)chemistry" investigates the influence of mechanical forces on the structure and function of molecules and materials. Current focus areas are molecular force sensors, forces in polymeric networks, as well as the integration of force spectroscopy with fluorescence detection.

The different research activities mentioned above will be described in much more detail in the main body of this report, which is organized according to the departments of the MPI-CI. Each department consists of several research groups, which will present the research results obtained during the past two years.

Recent Developments

After a relatively long planning and a relatively short construction phase, the extension of our building was completed in 2015. Most of the additional space was used to relocate the Seeberger Department that had been temporarily accommodated, from 2008 to 2015, at the Free University of Berlin. In addition, the extension provided us with additional lab space for independent junior research groups as well as for the installment of large equipment such as electron microscopy, nuclear magnetic resonance, and high performance computing.

Our graduate program, the International Max Planck Research School (IMPRS) on „Multiscale Bio-Systems", which includes faculty members from the University of Potsdam, the Free University of Berlin and the Humboldt University of Berlin, continued to attract a large number of students. Starting in 2013, we have now admitted four cohorts of doctoral students, selecting 36 students out of about 1400 applicants. We want to continue this graduate program for another six years and have recently submitted a proposal for a second funding period.

One challenge during the last two years was the decision of the Max Planck Society to use contracts rather than stipends for the employment of doctoral and postdoctoral associates even when they come from non-European countries. This readjustment has now been completed to a large extent.

In 2016, we proposed Joanna Aizenberg, Harvard University, and Ulrich S. Schubert, University of Jena, to become External Scientific Members of the MPI-CI in order to intensify our research activities on adaptive materials and green polymer chemistry. This proposal has now been approved by the corresponding committees of the Max Planck Society.

Recently, our institute has launched, together with the MPI of Molecular Plant Physiology and the University of Groningen, a new artist-in-residence program. The corresponding project „Knowledge Link through Art and Science" (KLAS) will bring innovative artists to the Science Park Potsdam-Golm. The artists will work for four weeks side by side with the researchers of the participating institutes.

More information about the MPI-CI can be found at http://www.mpikg.mpg.de/en

I take this opportunity to thank all of my colleagues and associates at the MPI-CI, our scientific advisory board and our board of trustees for their active support during the past two years. Last not least, I am grateful to our president and to our vice-president for their continuous support of our institute.

Reinhard Lipowsky
Managing Director 2015-2016

Das Institut in Zahlen

Haushalt

Die Jahre 2015/2016 waren durch die Erweiterung um 2300 qm Labor- und Bürofläche des Instituts gekennzeichnet. Dadurch konnten auch dringend notwendige Investitionen vorwiegend in hochauflösender Elektronenmikroskopie, optischer und Raman-Mikroskopie sowie Kernresonanzspektroskopie getätigt werden. Der Haushalt **(Abb. 1)** weist daher einen ungewöhnlichen Zuwachs auf. Bereinigt um diese außerordentlichen Ausgaben kann man erkennen, dass die institutionelle Förderung etwa konstant geblieben ist, der Anteil der Drittmittel aber signifikant schrumpfte **(Abb. 2)**. Dies liegt vor allem daran, dass mehrere Projekte, gefördert durch den European Research Council (ERC) und auch normale EU-Projekte, ausliefen und sich zudem der Anteil der Förderung durch das Bundesministerium für Bildung und Forschung (BMBF) reduzierte. Dies konnte nicht vollständig durch die erhöhte Förderung durch die Deutsche Forschungsgemeinschaft (DFG) kompensiert werden. Hier macht sich offenbar die Schließung der relativ drittmittelstarken Abteilung Grenzflächen im Jahr 2014 bemerkbar. Außerdem wurden anwendungsnahe Projekte nicht mit entsprechender Förderung durch EU oder BMBF weitergeführt, sondern bevorzugt in Ausgründungen übernommen. Im Gegensatz zu Fraunhofer-Instituten ist der Anteil direkter Industrieförderung mit <1% vernachlässigbar gering, typisch für ein Institut der Grundlagenforschung.

Wenn man also den um die erhöhten Investitionen bereinigten Institutshaushalt von etwa 20 Mio. Euro als Maßstab nimmt, hat sich der Drittmittelanteil am Haushalt auf 18.5% (3.75 Mio Euro) erniedrigt. Der erniedrigte Drittmittelanteil schlägt sich auch in der Struktur der Ausgaben nieder **(Abb. 3)**, wo ein Rückgang der Personalausgaben für jüngere Wissenschaftler um 10% zu verzeichnen ist. Teilweise ist dieser Rückgang aber auch buchungstechnisch bedingt, da mehrere jüngere Wissenschaftler/innen auf institutsfinanzierte Stellen transferiert wurden. Der Anteil letzterer erhöhte sich daher und wegen verschiedener Gehaltserhöhungen auf etwa 45%.

Fig. 1

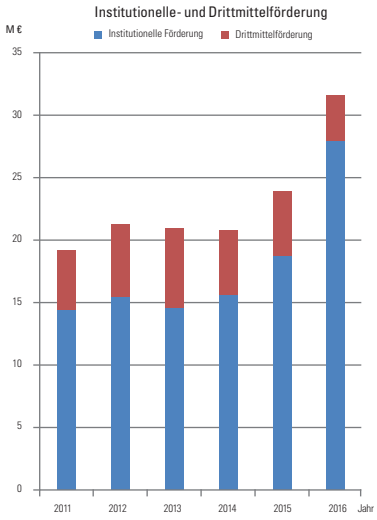


Fig. 3

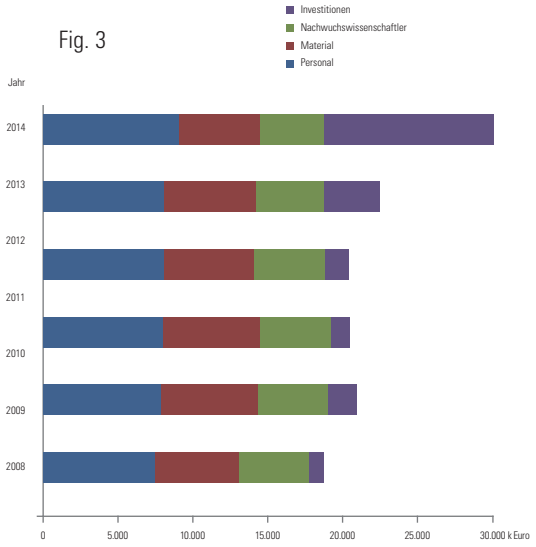


Fig. 2

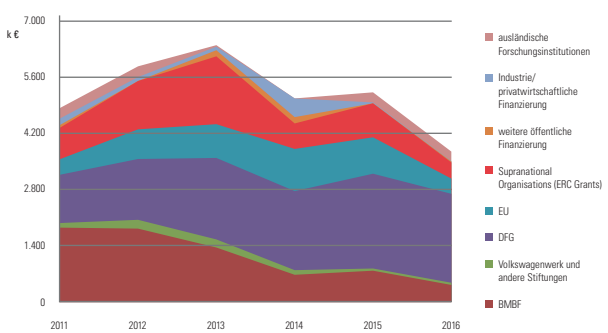
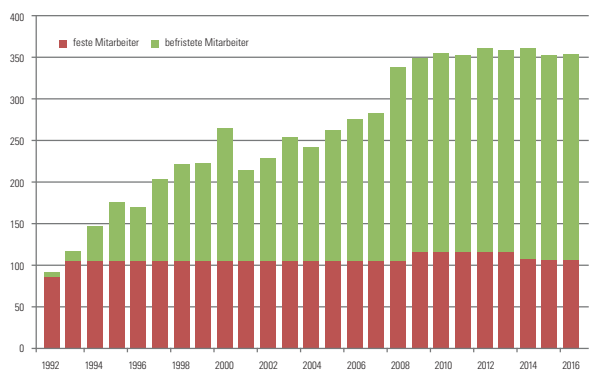


Fig. 4



Personal

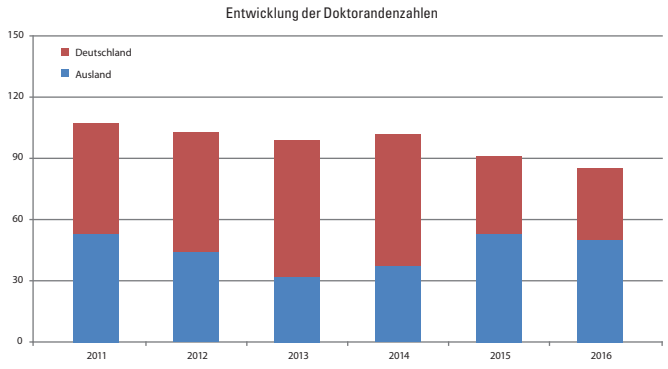
Die Anzahl am Institut beschäftigter Personen blieb in den letzten Jahren etwa konstant wie auch die Zahl der Mitarbeiter auf Haushaltsstellen **(Abb. 4)**. Während die administrativen und technischen Mitarbeiter fast ausschließlich permanente Stellen besitzen, ist es bei den Wissenschaftlern umgekehrt. Neben den Direktoren sind weniger als zehn Wissenschaftler permanent beschäftigt. Dieses zeichnet die gewünschte hohe Fluktuation im Wissenschaftsbereich aus, da sich das Institut als Brutstätte erfolgreicher Forscher versteht, die ein neues Gebiet aufgreifen und dann ihre Arbeit an anderer Stelle in Forschung oder Industrie fortsetzen.

Bei den Postdoktoranden blieb die Zahl mit etwa 90 in den letzten Jahren konstant mit einem weit überwiegenden Anteil an Ausländern **(Abb. 5)**. Die Zahl der Doktoranden aus dem Inland reduzierte sich jedoch signifikant, so dass die Gesamtzahl an Doktoranden auf etwa 85 sank. Hier befinden sich nun die ausländischen Gäste leicht in der Mehrzahl. Insgesamt liegt der Anteil ausländischer Gäste bei etwa 48% mit einer Mehrheit im Wissenschaftlichen und einer sehr kleinen Minderheit im technischen und administrativen Bereich.

Die Nationalitätenverteilung hat sich in den letzten Jahren nur gering verschoben. Der Anteil der Gäste aus dem europäischen Ausland beträgt annähernd 50%, wobei der Anteil Westeuropäer sich im Vergleich zu dem der Osteuropäer etwas erhöhte. Der Anteil der Inder und der Chinesen blieb etwa gleich, der der Amerikaner sank etwas, und der Anteil von Wissenschaftlern aus dem Nahen Osten erhöhte sich. Letzterer besteht zu etwa gleichen Teilen aus Gästen aus Iran (9) und aus Israel (8), gefolgt von Wissenschaftlern aus der Türkei (5) **(Abb.6)**.

Die Geschlechterverteilung spiegelt leider eine allgemeine Situation wieder: Während bei den Doktoranden die Geschlechter etwa gleich vertreten sind, befinden sich die promovierten Wissenschaftler in einer deutlichen Mehrzahl **(Abb. 6 und 7)**. Der unterschiedliche Anteil unter den Stipendiaten sollte dabei nicht besonders gewertet werden, da an Max-Planck-Instituten seit 2015 nur in Ausnahmefällen

Fig. 5



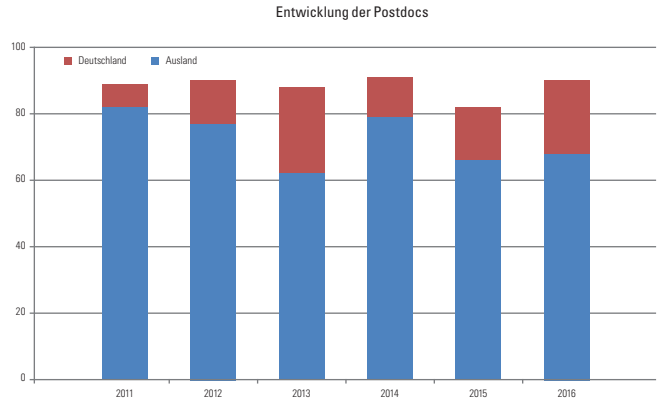
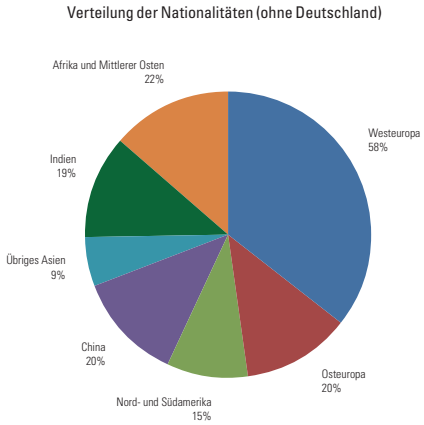


Fig. 6



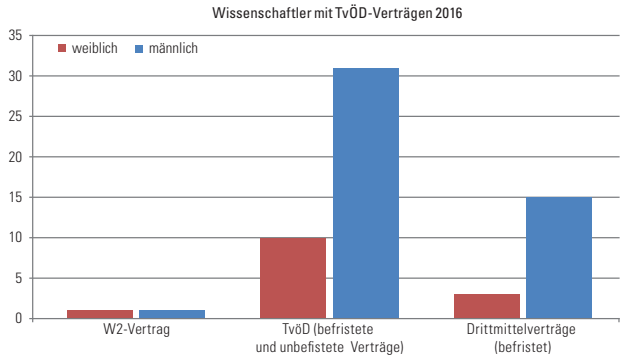
Stipendien vergeben werden, deren Anteil also in Zukunft fast verschwinden wird.

Wissenschaftliche Ergebnisse und deren Einfluss

Naturwissenschaftler, nicht nur Administratoren, messen gern, und dazu wurden bibliometrische Analysen immer mehr verfeinert. So zeigt **Abb. 8**, dass die Zahl der Publikationen nach dem Aufbau seit etwa 10 Jahren etwa konstant 350 beträgt. Dies ist durchschnittlich für ein Forschungsinstitut mit etwa 350 Mitarbeitern, außerordentlich ist dagegen, dass diese Publikationen im Durchschnitt mehr als 40mal zitiert werden. Dieses ist hervorragend, und das MPIKG muss keinen Vergleich mit einer Einheit ähnlicher Größe weltweit scheuen. Es beweist, dass das MPIKG, das mit Absicht nicht den klassischen Trends der Kolloid- und Grenzflächenforschung folgte, viele Trends in diesem Gebiet erst etabliert hat. Dieses sehen offenbar auch viele junge Wissenschaftler so, die gern am MPIKG forschen und die sich auch gern an ihre erfolgreiche Zeit in Golm erinnern. Dieses schlägt sich auch in den jährliche Rankings der Humboldt-Stiftung nieder, bei denen das MPIKG in den letzten Jahren einen Podestplatz einnahm, weit vor erheblich größeren MPI oder Forschungszentren.

Wichtiger als Zitationen und Publikationen ist jedoch der Wissenstransfer durch Köpfe, und dies geschieht durch die Ausbildung junger Wissenschaftler auf verschiedenen Stufen ihrer Karriere. Deren Qualität ist nur mit großer Verzögerung anhand ihrer Karrieren zu erfassen und kaum zu quantifizieren. Die Zahl der ehemaligen Mitarbeiter auf Professorenstellen oder äquivalenten Stellen im akademischen Bereich dürfte mittlerweile bei etwa 300 liegen. Wenn man bedenkt, dass etwa 25 Doktoranden und 50 Postdoktoranden jährlich das MPIKG verlassen, kann man davon ausgehen, dass dieser Wissenstransfer erheblich zur Weiterentwicklung des Gebiets beiträgt. Dies ist insbesondere dann der Fall, wenn es gelang, diese Wissenschaftler für die Kolloid- und Grenzflächenforschung zu begeistern, und wir erhielten viele Rückmeldungen, dass dies gelungen ist.

Fig. 7



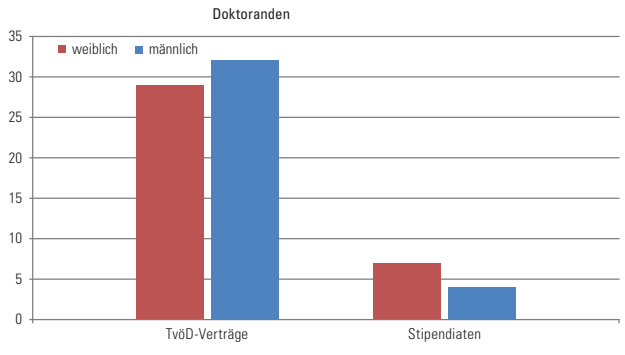
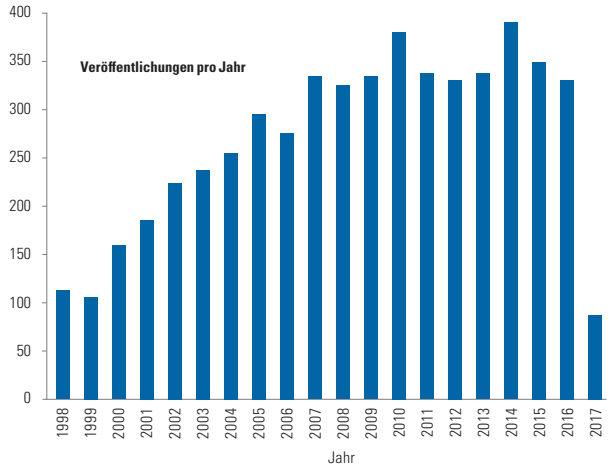
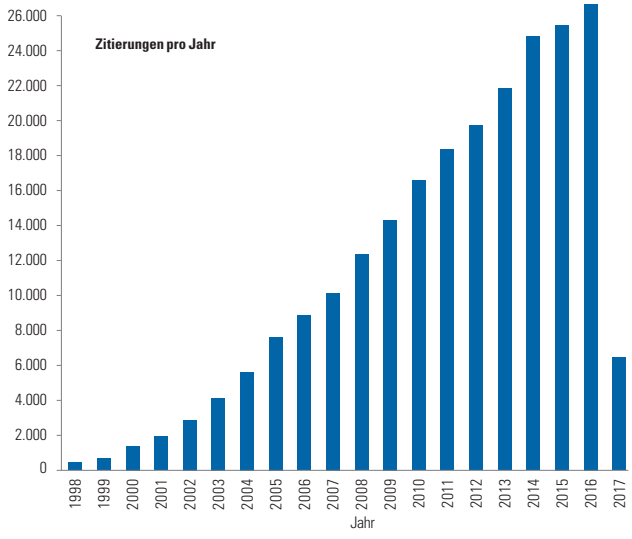


Fig. 8





The Institute in Numbers

Budget

The total budget of the MPIKG has increased from about 19.1 Million Euro in 2011, 23.8 Million Euro in 2015, to peak at 31.4 Million Euro in 2016 **(Fig. 1)**. The 2016 values included significant one-time infrastructure investments to establish the Department for Biomolecular Systems in the new extension building here in Golm, as well as the set-up of the new electron microscopy lab. In addition, beginning in 2014, external funding mainly via EU and BMBF decreased remarkably, which was due to the finalization of the two ERC Senior Grants of Seeberger and Antonietti, but also the leave of the Möhwald group. This development of lower external allocations continued until 2016, and currently only about 12 percent of the budget are covered by external funds („Drittmittel"). The budget in 2015 and 2016 is almost equally distributed along the budget positions staff (blue), junior scientists (green), and materials (red) with a peak on investments in 2016.

External Funds

In 2016, around 12 percent of the total budget was raised from external sources. The sources of these funds have changed over the last five years **(Fig. 2)**.

The funds obtained from the BMBF (Federal Ministry of Education and Research) have increased remarkably, because the institute is well positioned to participate in different funding initiatives, such as nanomaterials, sustainable energy, and bio-economy. Funding from the DFG (German

Fig. 1

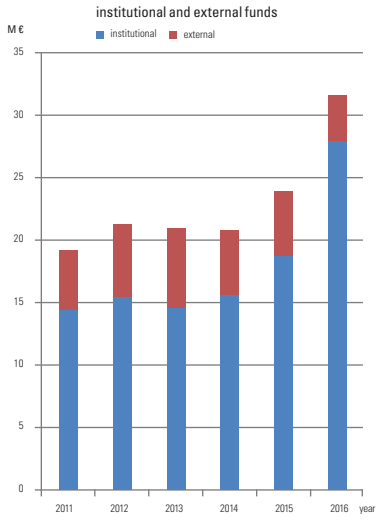


Fig. 3

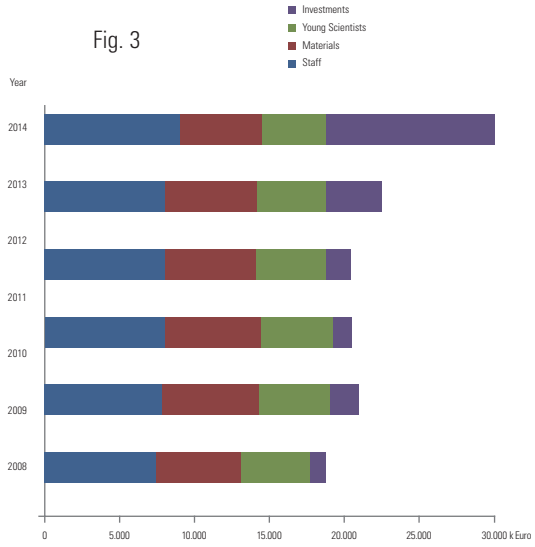


Fig. 2

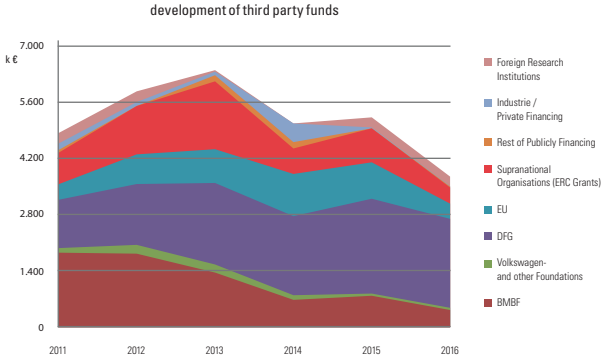
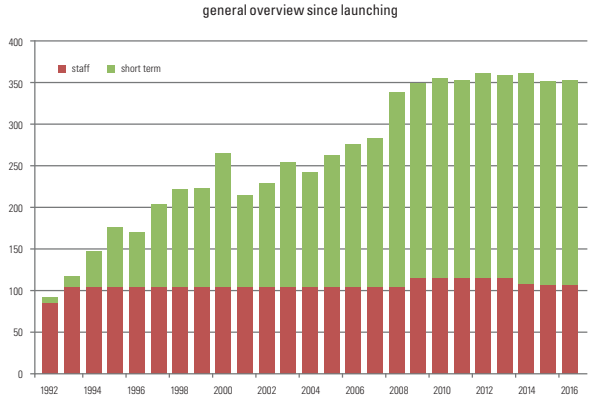


Fig. 4



Research Foundation) increased mainly due to the activity at the level of group leaders. Industrial and private funds have further decreased. In many cases, this is reflecting terms set by companies more and more interested in working with the institute that are departing from fundamental research to an "extended work bench" approach that is often not attractive for us. Another clear reason is that especially the Seeberger department directly attracts venture capital to a huge extend, which- as not devoted to the institute- does not show up in these statistics. However, we are looking forward to strengthening our ties again with the industry and to gaining more funding from this side.

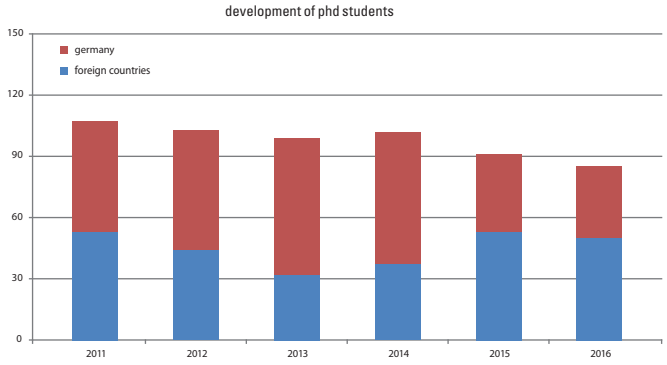
The MPIKG is participating in the International Max Planck Center program with RIKEN (2011-2016). In this context, one research group in the Department of Biomolecular Systems (Dr. Varon Silva) is funded by additional moneys from the Max Planck Society. The MPIKG is also part of the "MaxNet Energy", and Dr. Nina Fechler in Colloid Chemistry is paid from those resources.

Personnel

At present, the MPIKG consists of 4 departments with a total number of 353 employees. About one third (106) of these employees are centrally paid staff including group leaders, technicians, and the employees of our administration, whereas two thirds (247) are employed on soft money and temporary contracts: Those are mainly doctoral students, junior scientists, and foreign visitors **(Fig. 4)**. The overall growth in the number of employees in 2008 reflects the addition of the Seeberger department, ever since the head-count is rather constant.

Since 2011, the number of postdocs at the institute has remained constant **(Fig 5)**. However, the number of PhD students has significantly decreased due to the MPS-wide obligate conversion of stipend to contracts with social security coverage **(Fig 5)**. i.e. a slightly increased amount of money is good for less PhD contracts. It is to be expected that this shrinking process may continue until 2019.

Fig. 5



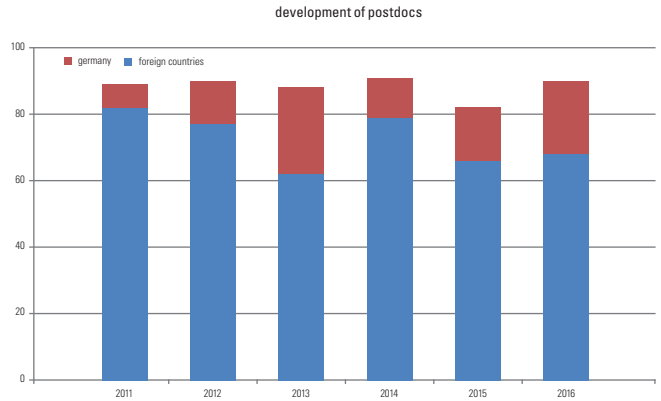
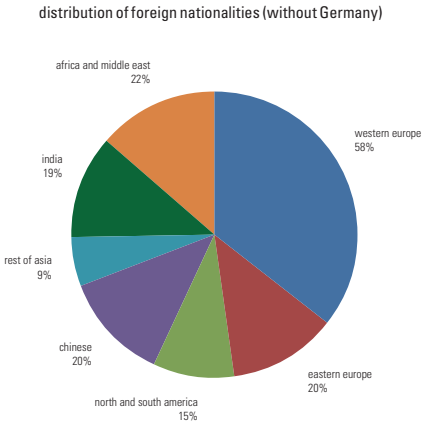


Fig. 6



The MPIKG is a truly international institution that attracts researchers and students from all over the world. The global distribution of nationalities for all employed scientists, i.e., staff scientists, postdocs, and students and guests is shown in **Fig. 6**.

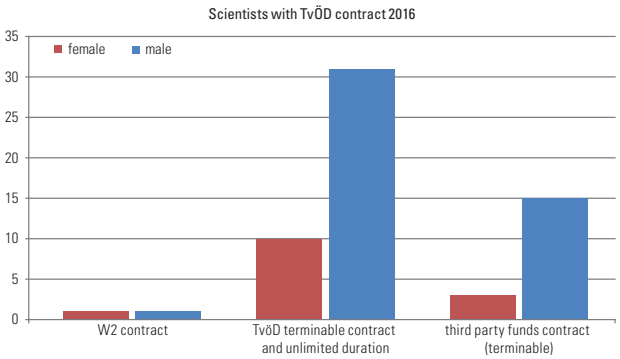
The gender distribution **(Fig.7)** reflects a general problem of higher academia in our research field: Throughout studies and PhD-work, the gender distribution is meanwhile balanced, while for Post Docs and Group leaders, the distribution is clearly not to our satisfaction. This problem was discussed also with gender representatives, but is to be seen as the consequence of a conglomerate of reasons. In spite of a whole spectrum of family friendly measures onto the campus, it is very difficult to convince talented women for the academic career, as temporal contracts are regarded as unsave. In addition, due to the need for women in leading positions also at other places, our best own coworkers get quickly further promoted and leave the institute for better positions. We are working on these problems in every single case, but interdependencies to the overall science system cannot be neglected.

Scientific Output and Impact

The main output of our research activities at the MPIKG is provided by scientific publications. The numbers of publications per year of the whole MPIKG and of the associated citations per year are displayed in **Fig. 8** for the time period between 1993 and 2017 (partial). This citation analysis is based on those 5,160 articles that were found in the ISI Web of Science. Up to 2005, the number of publications per year increased roughly linearly and then leveled off at an average number of about 320. The latter saturation reflects the constant number of researchers and students during the last years (compare **Fig. 4**). The number of citations, on the other hand, has grown much faster. In fact, the relative citation rate is still increasing. This clearly demonstrates the growing impact of the institute within the scientific community being far from saturated.

The citation analysis also reveals that the research performed at the Institute is truly multidisciplinary and covers a large number of subject categories.

Fig. 7



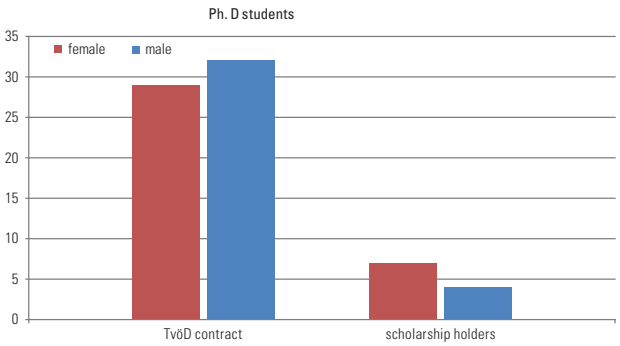
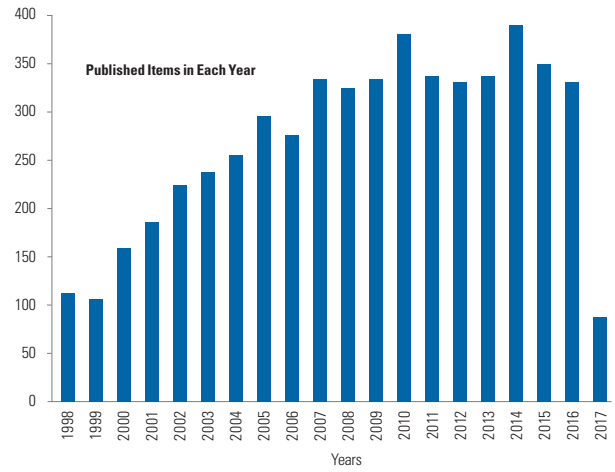
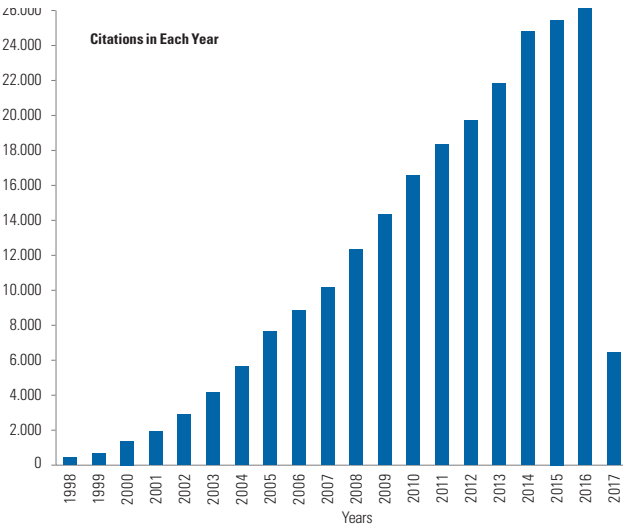


Fig.8





Das Forschungsprogramm des Max-Planck-Instituts für Kolloid- und Grenzflächenforschung (MPIKG)

Vision und Mission

Kolloide sind winzige Bausteine, die grundlegende Einheiten von lebenden Organismen und vielen nützlichen Materialien darstellen. Das Verständnis ihres Aufbaus sowie ihre erfolgreiche Synthese, erlaubt die Lösung drängender Probleme u.a. in den Bereichen Gesundheit, Energie und Werkstoffe.

Das Forschungsprogramm des MPIKG beschäftigt sich deshalb primär mit den fundamentalen wissenschaftlichen Problemen von Kolloiden und deren Grenzflächen. Die wissenschaftliche Vision des Instituts ist auf zwei Kernbereiche ausgelegt: Zum einen auf das Herstellen, Visualisieren, Messen und das Verständnis dieser Bausteine und zum anderen auf deren vielfältige Wechselwirkungen und Anordnungen **(Abb.1)**. Unsere Forschung umfasst daher sowohl biologische und medizinische Fragestellungen als auch Materialien und deren verschiedenste Anwendungen. Die bioinspirierte Materialforschung schlägt dabei die Brücke zwischen den beiden Ausrichtungen, indem sie Materialstrukturen, die in der Natur vorkommen, in Konzepte für technische Materialien übersetzt.

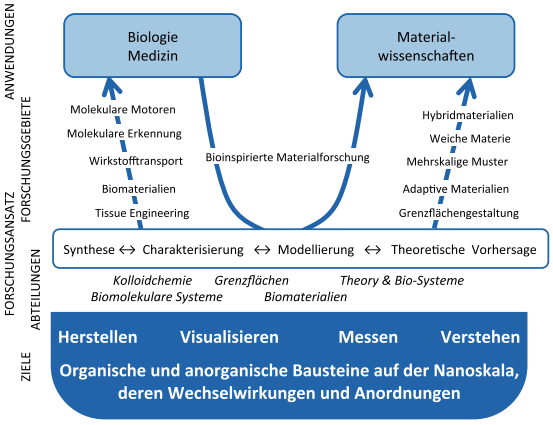


Abb. 1: Wissenschaftliche Strategie des MPIKG

Wir wollen dabei wissenschaftliche Exzellenz mit außergewöhnlichem Engagement in der Betreuung und Unterstützung von jungen WissenschaftlerInnen kombinieren. Unsere Mission ist es, eine Brücke von Molekülen zu mehrskaligen Materialien und Biosystemen zu schlagen und dabei Nachwuchswissenschaftlerlnnen bestmöglich zu fördern.

Das MPI für Kolloid- und Grenzflächenforschung nimmt, 25 Jahre nach seiner Gründung, eine führende Rolle in verschiedenen innovativen Wissenschaftsfeldern ein. Diese Forschungsgebiete - geordnet von kleinen zu größer werdenden Objekten – reichen von der Synthese, Charakterisierung und theoretischen Beschreibung von Kohlehydraten, Proteinen und Lipiden über funktionalisierte Nanopartikel und Hybridmaterialien, Polyelektrolyt-Multischichten, der Selbstorganisation von komplexen Grenzflächen und Mehrkomponentenmembranen bis hin zu hierarchischen Biomaterialien basierend auf Polysacchariden, Proteinen oder mineralisierten Geweben, wie Knochen und Zähnen. In all diesen Bereichen bürgt der Name des MPIKG für Exzellenz in der Grundlagenforschung.

Das Institut verfolgt zwei generelle Strategien, um seine Spitzenposition in diesem Bereich zu etablieren und weiter auszubauen: (i) Es identifiziert und wählt fortwährend neue interdisziplinäre Forschungsthemen, die eine höchstmögliche Relevanz für die Wissenschaft und Gesellschaft aufweisen; (ii) es ist sehr aktiv in der Ausbildung von DoktorandInnen und der Förderung junger WissenschaftlerInnen. So wird das MPIKG zum idealen Ausgangspunkt für erfolgreiche akademische Karrieren.

In den letzten Jahren wurden insbesondere Themen, welche unmittelbar mit biomimetischen und biologischen Systemen verknüpft sind, in die Forschungsarbeit aufgenommen. So gibt es vier neue Schwerpunktgebiete: Molekulare Erkennung von Kohlehydraten, fotoinduzierte molekulare Prozesse, Transportprozesse und Informationsverarbeitung durch molekulare Maschinen und biomimetische Bewegungssysteme. Diese Forschungsbereiche finden sich auch als Themen-Schwerpunkte in der neuen Internationalen Max Planck Research School über „Multiscale Bio-Systems: Von der molekularen Erkennung zum mesoskopischen Transport“. Das Graduiertenprogramm startete 2013 und wird in einer zweiten Förderperiode bis zum Jahr 2019 gefördert. Ein besseres Verständnis von vielskaligen Biosystemen ist dabei Grundlage für eine Vielzahl möglicher Anwendungen wie z.B. der Entwicklung von intelligenten Wirkstoffträgern und Biomaterialien.

Interdisziplinäre Expertise

Die komplexe und vielfältige Welt der Kolloide und Grenzflächen bietet eine große Anzahl an räumlichen und zeitlichen Organisationseinheiten, welche von molekularen bis hin zu mesoskopischen Skalen reichen. Für eine umfassende Untersuchung dieser Systeme und Prozesse bieten die einzelnen Abteilungen des Instituts eine komplementäre Methodik und Fachkenntnis in den Bereichen Chemie, Biochemie, Physik, Materialwissenschaften und Theorie. Die Abteilungen „Biomolekulare Systeme“ (Seeberger) und „Kolloidchemie“ (Antonietti) besitzen spezielle Expertise bei der chemischen Synthese von Molekülen und Materialien. Die Abteilung

„Biomaterialien“ (Fratzl) und die Emeritusgruppe „Grenzflächen“ (Möhwald) fokussieren ihre Arbeit dagegen auf die strukturelle Analyse und physikalische Charakterisierung dieser Systeme. Wenn es um das Verständnis und die Modellierung geht, ist die Abteilung „Theorie & Bio-Systeme“ federführend.

Nach der Gründung der Abteilung „Biomaterialien“ unter Peter Fratzl im Jahr 2003 und der Abteilung „Biomolekulare Systeme“ unter Peter H. Seeberger im Jahr 2008 wurde 2014 eine neue unabhängige Max-Planck-Forschungsgruppe zum Thema „Mechano(bio)chemie“ (Kerstin Blank) etabliert, um die Aktivitäten im Bereich der Biosysteme zu stärken.

Langfristige Ziele

Jede Abteilung des MPIKG hat sich langfristig anspruchsvolle Ziele gesetzt: Die Abteilung von Peter Seeberger untersucht die Rolle von kompexen Kohlehydraten, die fast alle Zellen umhüllen. Grundlegende Einsichten haben auf Kohlehydrate basierende Impfstoffkandidaten hervorgebracht. Die ForscherInnen um Markus Antonietti sind auf dem Weg enzymähnliche Nanokatalysatoren und die künstliche Photosynthese zu entwickeln und so grüne Energiegewinnung und -speicherung zu ermöglichen. Im Mittelpunkt der Abteilung von Peter Fratzl stehen das Verständnis und die Nachahmung von natürlichen auf Proteinen oder Polysacchariden basierenden Materialen, von Pflanzenbewegung und sowie von Knochenwachstum und -heilung. Das Verständnis und die Überwindung der Komplexitäts-Lücke zwischen künstlichen und natürlichen Systemen ist ein langfristiges Thema in der Abteilung von Reinhard Lipowsky. Schließlich beschäftigt sich die Gruppe um Kerstin Blank mit dem Einfluss mechanischer Kräfte auf Moleküle und Materialien.

Neue Forschungsperspektiven

Während der letzten Jahre haben sich einige neue zukunftsweisende Forschungsgebiete herauskristallisiert. Bei der molekularen Erkennung von Kohlehydraten handelt es sich um ein Arbeitsgebiet aus der Abteilung Seeberger, welches aber mit aktuellen Untersuchungen aus den Abteilungen Antonietti und Lipowsky Schnittmengen aufweist. Die Forschung in diesem Kernbereich basiert im Wesentlichen auf der Synthese von Polysacchariden und Kohlehydraten, die eine sehr definierte molekulare Architektur besitzen (Abt. Seeberger). Diese Kohlehydrate werden sowohl an Nanopartikeln (Abt. Antonietti) als auch an Lipid-Doppelschichten (Abt. Lipowsky) verankert. Diese Systeme können mit verschiedenen experimentellen und theoretischen Methoden untersucht werden, wobei eine hohe räumliche und zeitliche Auflösung angestrebt wird.

Fotoinduzierte molekulare Prozesse sind ein Fokus der Abteilung Antonietti, wobei es hier gemeinsame Interessen mit den Abteilungen Seeberger und Lipowsky gibt. Ein neuer Katalysator auf der Basis von Kohlenstoff und Stickstoff wurde 2007 vorgestellt und wird nun weiter entwickelt bzw. optimiert (Abt. Antonietti). Andere fotoinduzierte Prozesse beinhalten die Entwicklung total neuartiger organisch-chemischer Reaktionskaskaden mit höchster Einfachheit und Ausbeuten (Abt. Seeberger, Abt. Antonietti), und fotoinduzierte konformative Änderungen von supramolekularen Strukturen (Abt. Lipowsky).

Biomolekulare Maschinen, die molekulare Lasten transportieren oder Informationen verarbeiten, sind ein Schwerpunkt der Abteilung Lipowsky. Aktuelle Themenbereiche sind dabei der kooperative Lastentransport durch Teams von molekularen Motoren, die Krafterzeugung durch Filamente und die Proteinsynthese durch Ribosomen. Verwandte Thematiken werden in der Abteilung Fratzl und der Blank-Gruppe bearbeitet, wie z.B. die molekulare mechanische Wechselwirkung von Zellen mit ihrer extrazellulären Umgebung. Ein weiteres aktuelles Thema der Abteilung Lipowsky sind asymmetrische Doppelschicht-Membranen sowie der Einschluss von Nanoteilchen durch derartige Membranen.

Biomimetische Bewegung und Gewebewachstum sind Kernthemen innerhalb der Abteilung Fratzl. Formänderungen in Geweben werden durch die Erzeugung von ungleichmäßigen, internen Belastungen ausgelöst. Diese werden durch die Wasseraufnahme in Zellwänden und durch Zellproliferation in Knochen und Hautgewebe erzeugt (Abt. Fratzl). Weiterführende Studien dieser belastungsauslösenden Prozesse werden mittels mehrskaligen Computersimulationen durchgeführt (Abt. Lipowsky). Auf diese Weise wird das Ziel verfolgt, die zu Grunde liegenden molekularen Mechanismen aufzudecken. Auch dies steht in einem engen Zusammenhang mit Untersuchungen in der Blank-Gruppe, die sich mit mechanischen Struktur-Funktions-Beziehungen von protein-basierten Materialbausteinen beschäftigt.

Programme für Doktorandinnen und Doktoranden

Ein starkes Engagement für die Ausbildung von DoktorandInnen ist Markenzeichen unseres Instituts. Die erste Max Planck Research School (IMPRS) über „Biomimetische Systeme“ wurde über zwölf Jahre erfolgreich betrieben und beendete ihre Arbeit im Herbst 2012. Die zweite IMPRS über „Multiscale Bio-Systems“ begann ihre Arbeit 2013 und ist in einer ersten Förderperiode bis 2019 bewilligt. Hauptziel der IMPRS ist es, dass die teilnehmenden DoktorandInnen effi-

zient und erfolgreich an einem zukunftsweisenden Forschungsprojekt arbeiten können, und das unter Erlernen verschiedener Disziplinen. Darüber hinaus ist das MPIKG auch noch in weiteren Graduiertenschulen aktiv: Diese sind das DFG-Graduiertenkolleg "Self-Assembled Soft Matter Nano-Structures at Interfaces", koordiniert von der TU Berlin, die Berlin-Brandenburg School for Regenerative Therapies (BSRT), koordiniert von der Charité - Universitätsmedizin Berlin, die SALSA, School of Analytical Sciences Adlershof, koordiniert von der Humboldt-Universität zu Berlin und das ZIBI, Zentrum für Infektionsbiologie und Immunologie, koordiniert von der FU Berlin.

Förderung von jungen WissenschaftlerInnen

Das Institut ist und war schon immer ein guter Nährboden für junge WissenschaftlerInnen, die eine akademische Karriere anstreben. Viele der früheren MitarbeiterInnen und Postdocs sind jetzt ProfessorInnen an deutschen oder ausländischen Universitäten. Während der letzten zehn Jahre haben etwa 40 frühere ArbeitsgruppenleiterInnen, Doktoranden und Wissenschaftler Spitzenpositionen eingenommen, die vergleichbar mit den deutschen W3 oder W2 Professuren sind. In der neuen IMPRS über „Multiscale Bio-Systems“ sind alle ArbeitsgruppenleiterInnen des MPIKG, die an verwandten Themen arbeiten, Mitglieder der erweiterten Fakultät der Schule und nehmen an der Auswahl und Zulassung der StudentInnen teil.

Gesellschaftliche Relevanz

Viele Forschungsaktivitäten am MPIKG haben -als Grundlagenforschung- potentielle Anwendungen in verschiedenen Technologie-Feldern und haben das Potenzial die Lebensqualität der Menschheit nachhaltig zu verbessern. Die Entwicklung von Impfstoffen auf der Basis von Kohlenhydraten und die Möglichkeit große Mengen dieser Moleküle zu produzieren, ist vielversprechend und wegweisend für die Prävention von bakteriellen Infektionen wie Krankenhauskeimen aber auch Parasitenerkrankungen wie Malaria. Diese Impfstoffe sind speziell für Entwicklungsländer sehr bedeutsam. Funktionelle Nanopartikel und Materialien können für die Erzeugung und Speicherung von Energie und für neue Methoden der CO_2-Bindung eingesetzt werden. Darüber hinaus besitzen diese Systeme ein breites Anwendungsspektrum in Bezug auf den intelligenten Wirkstofftransport, da sie die molekulare Erkennung und Bewegung mit der gezielten Wirkstofffreigabe kombinieren. Am Institut werden Biosysteme untersucht, die in Zukunft zu neuen Materialkonzepten führen werden, die auf bioinspirierten Designs basieren oder zur Organregeneration beitragen. Schließlich wird unsere Gesellschaft sehr stark von den jungen WissenschaftlerInnen profitieren, die ihre breite interdisziplinäre Ausbildung am MPIKG erhalten haben und das Institut verlassen, um ihr Wissen in anderen Wissenschafts- und Ingenieurbereichen anzuwenden.

Markus Antonietti, Peter Fratzl, Reinhard Lipowsky, Peter H. Seeberger

Picture: © Lutz Hannemann

The Research Program of the Max Planck Institute of Colloids and Interfaces (MPICI)

Vision and Mission

Colloids are small building blocks which can be basic units of living organisms and of many useful materials. Mastering their synthesis and assembly will solve urgent problems in health, energy, materials, and many other important areas. The research program of the MPICI is to address fundamental scientific problems of such colloids and of the interfaces between them. Thus the scientific vision of the institute is in two areas: to lead the effort in making, visualizing, measuring and understanding these nanoscale building blocks, as well as to control their interactions and assembly (**see Fig. 1**). Our research includes biological or medical questions, as well as materials with their very diverse applications. Bio-inspired materials research is therein bridging between the two directions by translating materials structures found in nature into design concepts for engineering materials.

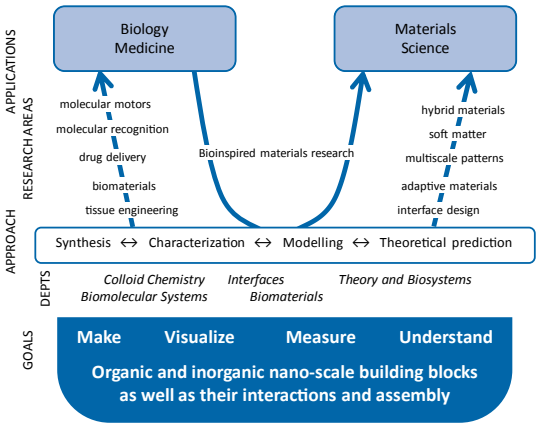


Fig. 1: Scientific strategy of the MPICI

We therefore intend to combine scientific excellence with exceptional commitment to mentoring and supporting young scientists. Our mission is: Bridging the gap between molecules and multiscale materials and bio-systems through excellence in science and by the support of young scientists.

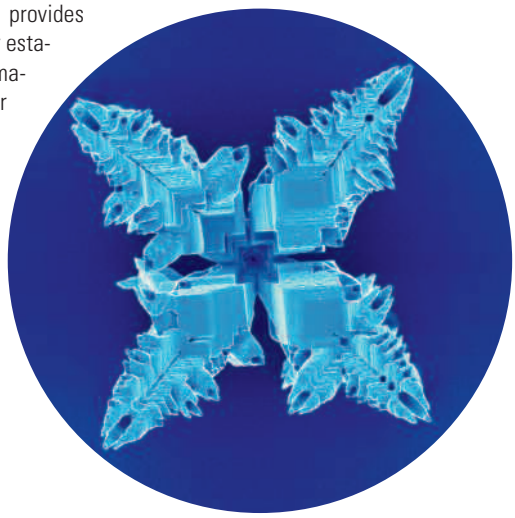
The MPI of Colloids and Interfaces (MPICI), 25 years after its foundation, has attained a leading position in several innovative fields of research. These areas - ordered from smaller to increasingly larger objects - include the synthesis, characterization and theoretical description of carbohydrates, proteins and lipids over functionalized nanoparticles and hybrid materials, polyelectrolyte multilayers, the self-organization of complex interfaces and multi-component membranes up to hierarchical biomaterials based on polysaccharides, proteins or mineralized tissues, such as bone and teeth. In all of these areas, the name of the MPICI serves as a trademark for excellence.

The MPICI pursues two general strategies in order to keep and strengthen its leading role in these field: (i) The MPICI constantly identifies and selects new interdisciplinary research topics with the highest potential impact on science and society; and (ii) the MPICI is very active in the training of graduate students and the support of young scientists and, thus, continues to be a hotbed for academic careers.

In the last few years, especially topics which directly relate to biomimetic and biological systems have been taken up. Four new focus areas are: molecular recognition of carbohydrates, photo-induced molecular processes, transport processes based on molecular motors, and biomimetic actuation and motility. These areas are also pursued in the framework of the International Max Planck Research School on "Multiscale Bio-Systems": From molecular recognition to mesoscopic transport": This graduate program started in 2013 and is funded in its second funding period until 2019. An improved understanding of multiscale bio-systems also provides the knowledge base for many possible applications such as the development of intelligent drug carriers and biomaterials.

Interdisciplinary Expertise

The complex and versatile world of colloids and interfaces provides many levels of spatial and temporal organization, from molecular to mesoscopic scales. In order to address these multiscale systems and processes, the departments at the MPI provide complementary methodology and core expertise from chemistry, biochemistry, physics, materials science, and theory. The departments of "Biomolecular Systems" (Seeberger) and "Colloid Chemistry" (Antonietti) have their core expertise in the chemical synthesis of molecules and materials. The department of "Biomaterials" (Fratzl) and the Emeritus Group on "Interfaces" (Möhwald) focus on structural analysis and physical characterization. The department of "Theory & Bio-Systems" (Lipowsky) provides expertise in theory and modeling. After establishing the Fratzl department on "Biomaterials" in 2003 and the Seeberger department on "Biomolecular Systems" in 2008, a new independent Max Planck Research Group on "Mechano(bio)chemistry" (Kerstin Blank) has been established in 2014 to strengthen the activities in the area of Biosystems.



Long-term Objectives

Each department of the MPICI sets itself its challenging long-term objectives. The Seeberger department characterizes the complex mixture of carbohydrates which surround practically all cells. These fundamental observations have enabled candidates for carbohydrate based vaccines. The Antonietti department wants to establish enzyme-like nanocatalysts and artificial photosynthesis as milestones for green energy production and chemical conversion reactions. The Fratzl department wants to understand and mimic of polysaccharide and protein based materials, analyzes plant motility and understands bone tissue growth and healing. The Lipowsky department wants to understand and bridge the complexity gap between artificial and natural bio-systems. Last but not least, the Blank group elucidates the influence of mechanical forces on molecules and materials.

New Focus Areas

During the last couple of years, several new focus areas have emerged at the MPI: Molecular recognition of carbohydrates is a focus area of the Seeberger department, with overlapping interests of the Antonietti and Lipowsky departments. Research in this core area is based on the synthesis of polysaccharides and carbohydrates with a well-defined molecular architecture (Dept. Seeberger). These carbohydrates are then anchored to nanoparticles (Dept. Antonietti), and lipid bilayers (Dept. Lipowsky). In this way, they become amendable to experimental and computational methods that probe these systems with high spatial and temporal resolution.

Photo-induced molecular processes are a focus area of the Antonietti department, with overlapping interests of the Seeberger and Lipowsky departments. A new type of catalyst based on carbon and nitrogen has been introduced about ten years ago and will be further developed and optimized (Dept. Antonietti). Other photo-induced processes include the development of fundamentally new reaction cascades for organic chemistry (Dept. Seeberger, Dept. Antonietti), photo-induced permeation of polyelectrolyte capsules (Emeritus Group Möhwald), and photoinduced conformational changes of supramolecular assemblies (Dept. Lipowsky).

Biomolecular machines that transport molecular cargo or process nanoscale information is a focus area of the Lipowsky department, with overlapping interests of the Fratzl department and the Blank group. Current topics include the cooperative cargo transport by motor teams, the force generation by filaments and the protein synthesis by ribosomes. A related theme is treated by the groups of Blank and Fratzl where mechanical interactions between cells and the extracellular environment are analyzed. The Lipowsky department puts another focus on asymmetric bilayer membranes and their interactions with nanoparticles.

Biomimetic actuation and growth of tissues are focus areas of the Fratzl department, with overlapping interests of the Lipowsky department. Shape changes in tissues are caused by the generation of non-uniform, internal stresses. These stresses are generated by water absorption in the cell walls of plant tissues and by cell proliferation in bone or skin tissues (Dept. Fratzl). The ongoing experimental studies of these stress-generating processes are also addressed by multiscale computer simulations in order to elucidate the underlying molecular mechanisms (Dept. Lipowsky). These observations are also in context with examinations of the Blank group, which deal with the structure-function relationships of protein-based materials components.

Graduate Programs

The MPICI will continue its strong commitment to the training of graduate students. The first International Max Planck Research School (IMPRS) on "Biomimetic Systems" has been successfully operated for twelve years until fall 2012. The second IMPRS on "Multiscale Bio-Systems" has started in 2013, and its first funding period will last until 2019. The new school covers the new focus areas of the MPICI as described above. The main objective of the IMPRS curriculum is to enable the participating doctoral students to work on their research projects, which are at the forefront of current research, in an efficient and fruitful manner. In addition, the MPICI participates in the following graduate schools: International Research Training Group on “Self-assembled Soft Matter Nano-Structures at Interfaces (coordinated by the TU Berlin), the "Berlin-Brandenburg School of Regenerative Therapies" (coordinated by the Charité Hospital, Berlin), SALSA, the Graduate School of Analytical Sciences Adlershof (coordinated by the Humboldt University Berlin), as well as the Center of Infection Biology and Immunity (ZIBI) (coordinated by the FU Berlin).

Support of Young Scientists

The MPICI will continue to be a hotbed for young scientists who pursue a higher career in academia. A large number of former associates, graduate students and postdocs are now professors at German or foreign universities. In particular, during the last ten years, about 40 former junior scientists of the MPICI have taken up offers for professorships that are equivalent to German W3 or W2 positions. Many of these research group leaders were teaching in the framework of the old IMPRS on "Biomimetic Systems". In the new IMPRS on "Multiscale Bio-Systems", all research group leaders, who work on topics related to the school, are members of the school's associate faculty and take part in the recruitment and admission of the students.

Potential Applications and Impact on Society as a Whole

Many research activities at the MPICI have applications that will be useful and beneficial for research in other disciplines and for society as a whole. The development of vaccines based on carbohydrates, in connection with the possibility to produce large amounts of these molecules, are very promising for the prevention of bacterial infections as against hospital germs or parasitical diseases as Malaria. These vaccines would be particularly beneficial for developing countries. Functionalized nanoparticles and materials can be used for improved photoinduced cleavage of water and for new methods of CO_2 fixation. Likewise, these systems have a wide range of applications in the context of smart drug delivery systems, which combine molecular recognition and activation with triggered drug release.

In the latter context, the interactions of nanoparticles with cell membranes play a decisive role. The bio-systems studied at the MPICI are also likely to lead to new materials concepts based on bio-inspired designs as well as new concepts for material-supported organ regeneration. Finally, the society as a whole will strongly benefit from the many young scientists that have received a broad interdisciplinary training at the MPICI and leave the institute in order to apply their knowledge in other branches of science and engineering.

Markus Antonietti, Peter Fratzl, Reinhard Lipowsky, Peter H. Seeberger

Wissenschaftliche Beziehungen

Das Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG) unterhält intensive Kooperationen mit Universitäten, Forschungsinstituten und der Industrie auf regionaler, nationaler und internationaler Ebene.

Regionale Kooperationen

Zwischen dem Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG) und der Universität Potsdam besteht seit Institutsgründung eine intensive und gute Zusammenarbeit. Alle vier aktiven Direktoren und der Direktor (em.) sind Honorarprofessoren an der Universität Potsdam. Dies spiegelt sich in einer intensiven Lehrtätigkeit sowohl in Bereichen des Grundstudiums als auch in den Wahlpflichtfächern wieder. Prof. Fratzl und Prof. Lipowsky sind zudem Honorarprofessoren an der Humboldt Universität zu Berlin und Prof. Seeberger an der Freien Universität Berlin. Darüber hinaus wurden 2005 Prof. Jürgen Rabe vom Institut für Physik der Humboldt-Universität und 2017 Prof. Joanna Aizenberg, Amy Smith Berylson Professor of Materials Science at Harvard's School of Engineering and Applied Sciences sowie Prof. Dr. Ulrich S. Schubert von der Friedrich-Schiller-Universität Jena (FSU) als Auswärtige Wissenschaftliche Mitglieder an das MPI für Kolloid- und Grenzflächenforschung berufen.

Zusätzlich dazu gibt es Kooperationsvereinbarungen mit dem Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) über die gemeinsame Nutzung von Neutronenstreuinstumenten und Synchrotron-Beamlines sowie mit der Bundesanstalt für Materialforschung und -prüfung (BAM) über die Betreibung einer Mikrofokus-Beamline.

Das MPIKG, die Universität Potsdam, die Humboldt-Universität zu Berlin, Freie Universität Berlin und die Fraunhofer-Institute für Angewandte Polymerforschung IAP sowie für Zelltherapie und Immunologie IZI arbeiten eng im Rahmen der International Max-Planck Research School (IMPRS) on „Multiscale Bio-Systems" zusammen. Die Aktivitäten über biomimetische Systeme wurden zunächst durch die gemeinsam vom Institut und der Universität Potsdam im Jahr 2000 ins Leben gerufene International Max Planck Research School (IMPRS) on „Biomimetic Systems" komplettiert, entscheidend gestärkt und unterstützt. Im Oktober 2012 lief die zwölfjährige Förderung für die Schule aus. Ab Juni 2013 hat die neue International Max-Planck Research School (IMPRS) on „Multiscale Bio-Systems" ihre Arbeit aufgenommen. Diese befasst sich mit dem hierarchischen Aufbau von Biosystemen im Nanometer- und Mikrometerbereich. Sprecher ist Professor Lipowsky.

Darüber hinaus beteiligt sich das Institut an weiteren Graduiertenschulen:
International Research Training Group on "Self-assembled Soft Matter Nano-Structures at Interfaces (koordiniert von der TU Berlin)

- „Berlin-Brandenburg School of Regenerative Therapies" (koordiniert von der Charité, Berlin)
- SALSA, the Graduate School of Analytical Sciences Adlershof (koordiniert von der Humboldt-Universität zu Berlin)
- ZIBI Graduate School, Center of Infection Biology and Immunity (koordiniert von der FU Berlin)

Das MPIKG ist ebenfalls involviert in von der Deutschen Forschungsgemeinschaft (DFG) geförderten „Sonderforschungsbereichen" (SFB):

- Collaborative Research Centre 760 - „Biomechanics and Biology of Musculoskeletal Regeneration" koordiniert von der Charité Medical School, Berlin
- "Multivalenz als chemisches Organisations- und Wirkprinzip: Neue Architekturen, Funktionen und Anwendungen (SFB 765), koordiniert von der FU Berlin.

Zudem koordinierte Prof. Fratzl von 2009 bis 2016 das DFG-Schwerpunktprogramm SPP 1420 „Biomimetische Materialforschung", an dem mehr als zehn Universitäten so - wie Max-Planck-Institute beteiligt waren. Untersucht wurden Bauprinzipien und Herstellung von neuartigen, hierarchisch strukturierten Materialien, die auf natürlichen Vorbildern basieren.

Das Institut ist aber auch Teil des Forschungsnetzwerks MaxSynBio. Die Max-Planck-Gesellschaft bündelt hier ihre Kompetenzen im Bereich synthetische Biologie. Insgesamt neun Max-Planck-Institute beteiligen sich daran. MaxSynBio wird vom Bundesministerium für Bildung und Forschung (BMBF) und von der Max-Planck-Gesellschaft über einen Gesamtzeitraum von sechs Jahren gefördert. Ferner beteiligt sich das Institut am Forschungsverbund „Unifying Concepts in Catalysis" (UniCat), welcher im Rahmen der Exzellenzinitiative des Bundes und der Länder 2007 gegründet wurde und von der TU Berlin koordiniert wird. Prof. Antonietti ist hier seit 2009 Principal Investigator (PI). Darüber hinaus ist das MPIKG auch Mitglied des neuen Projektes „Big-Data Driven Materials Science (BDDMS) unter Federführung des Fritz-Haber-Institutes und gefördert durch die Max-Planck-Gesellschaft.

Ebenfalls beteiligt ist es am vom Bundesministerium für Bildung und Forschung (BMBF) finanzierten Berlin-Brandenburger Zentrums für Regenerative Therapien (BCRT) sowie am Exzellenzcluster "Image- Knowledge-Gestaltung" (P. Fratzl ist Co-Sprecher), welches von der Humboldt-Universität durchgeführt wird.

Nationale und Internationale Kooperationen

Im Rahmen von europäischen Förderprogrammen, laufen zurzeit drei EU-Projekte innerhalb des 7. Rahmenprogramms und vier innerhalb des EU-Rahmenprogramms „HORIZONT 2020", davon zwei ERC Starting Grants. Des Weiteren ist das Institut gemeinsam mit dem Max-Planck-Institut für molekulare Physiologie in Dortmund und dem Riken Advanced Science Institute (ASI) in Wako federführend beteiligt am neuen Riken-Max Planck-Joint Research Center. Beide Forschungseinrichtungen schaffen damit eine Plattform, auf der sie Wissen, Erfahrungen und Infrastruktur sowie neue Methoden und Techniken im Bereich der chemischen Systembiologie bündeln. Das Indian Institute of Science and Education Research (IISER), Pune und das MPIKG haben zudem 2011 eine Max-Planck Partnergruppe ins Leben gerufen. In diesem Gemeinschaftsprojekt sollen innovative Nanosysteme entwickelt und hergestellt werden, die helfen sollen, Krebs besser behandeln zu können. Darüber hinaus gibt es gemeinsame Labors und internationale Partnergruppen mit dem National Laboratory for Physical Sciences at Microscale (CAS) in Hefei, China; der Fuzhou University, China, der Zheijiang University/ Hangzhou sowie der Jiao Tong University/Shanghai. Intensive Projektkooperationen gibt es im Bereich von molekularen Bio-Systemen insbesondere mit dem Weizmann Institute/Israel, der ETH Zürich, und dem Burnham Institute for Medical Research.

Bilaterale- und Kooperationsprojekte bestehen zurzeit unter der Förderung der European Space Agency (ESA), der NATO, des Deutschen Akademischen Austausch Dienstes (DAAD), der Deutschen Forschungsgemeinschaft (DFG), der German Israel Foundation (GIF) for Scientific Research and Development, des National Institutes of Health (NIH), des Schweizer Nationalfonds, der Schweizerischen Eidgenossenschaft sowie der VW-Stiftung mit China, Frankreich, Griechenland, Großbritannien, Irland, Italien, Israel, Japan, Niederlande, Norwegen, Portugal, Polen, Russland, Schweiz, Schweden und Spanien und den USA. Darüber hinaus wird in enger Zusammenarbeit mit dem Ludwig-Boltzmann Institut für Osteologie in Wien (Österreich) an klinisch orientierter Knochenforschung gearbeitet. Ferner betrieb die Abteilung Grenzflächen seit 2008 ein „Laboratoire Européen Associé über „Sonochemie" mit dem CEA-Institut für Separationschemie in Marcoule, das von der Abteilung Biomaterialien weitergeführt wird.

Industriekooperationen, Verwertungsverträge, Ausgründungen

The MPIKG kooperiert mit vielen industriellen Partnern wie z.B. BASF-AG, Firmenich, Merck, Beiersdorf, AstraZeneca UK, Clariant GmbH, Degussa AG, Merck, Procter & Gamble, Servier, Bayer-Schering AG, Nestle, EADS, Daimler, Lam Research und Lion Corporation.

Das Institut hält gegenwärtig 32 Patente. Im Zeitraum von 1993-2017 erfolgten folgende Ausgründungen: Capsulution Nanoscience AG, Colloid GmbH, Nanocraft GmbH, Nanolytics, Optrel, Riegler & Kirstein, Sinterface, Oxidion GmbH, Carbon Solutions GmbH, Glycouniverse, Artemiflow, Vaxxilon, and Fluxpharm.

Wissenschaftliche Beziehungen

Editorial Boards

Unsere Wissenschaftler fungieren als Gutachter und Berater von fachspezifischen Zeitschriften und Journalen. In der folgenden Liste sind nur die Wissenschaftler angeführt, die entweder Herausgeber oder Mitglied eines Editorial Boards sind. Des Weiteren informieren wir Sie über Mitgliedschaften in Fachbeiräten.

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- Advanced Materials Interfaces (H. Möhwald)
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- Physical Chemistry Chemical Physics (H. Möhwald)
- Polymer (M. Antonietti)
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- Science Magazine (P. Fratzl)
- Soft Matter (M. Antonietti)

Fachbeirat:

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- B-Cube Dresden, (P. Fratzl, Scientific Advisory Board, Chair)
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- Berlin-Brandenburg School of Regenerative Therapies, BSRT (P. Fratzl)
- Biofibres Materials Centre, Stockholm (H. Möhwald)
- BWG Excellence Cluster (P. Fratzl, Co-speaker)
- Chinese Academy of Sciences Institute of Nanosciences (M. Antonietti, Scientific Advisory Board)
- CIC biomaGUNE, San Sebastian, Spain (P. H. Seeberger, H. Möhwald)
- DECHEMA Research Group on "Chemical Nanotechnology" (H. Möhwald)
- Dutch Catalysis Excellence Cluster (M. Antonietti, Evaluation Board)
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- WYSS Institute for Bioinspired Engineering at Harvard University (P. Fratzl, Scientific Advisory Board)


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Scientific Relations

The MPKG is collaborating intensively with universities, research institutes, and industry at the regional, national, and international level. In the following subsections, some of these collaborations will be highlighted.

Regional Networks

On the regional level, formal cooperation agreements have been signed with the University of Potsdam in 1995 and with the Humboldt University Berlin in 2005. Markus Antonietti and Peter Seeberger are honorary professors at Potsdam University, Peter Fratzl and Reinhard Lipowsky at both universities, and Peter Seeberger is an honorary professor at the Free University of Berlin. Jürgen Rabe, from the physics department of Humboldt University has been an external scientific member of the MPIKG since 2005, Prof. Joanna Aizenberg, Amy Smith Berylson Professor of Materials Science at Harvard's School of Engineering and Applied Sciences and Ulrich S. Schubert from the Faculty School of Chemistry and Earth Sciences of the Friedrich-Schiller-Universität Jena (FSU) has been an external scientific members since 2017.

Additional cooperation agreements exist with the Helmholtz Center of Materials and Energy (former Hahn Meitner Institute and BESSY) about the joint operation of neutron scattering instruments and synchrotron x-ray beamlines, and with the Federal Institute for Materials Research and Testing (BAM) for running a microfocus beamline.

The MPIKG, the University of Potsdam, the Humboldt University, the Free University Berlin and the two Fraunhofer Institutes on our Campus closely collaborate in the framework of the International Max Planck Research School. The first International Max Planck Research School (IMPRS) on „Biomimetic Systems" has been successfully operated for twelve years until fall 2012. The second IMPRS on „Multiscale Bio-Systems" has started in 2013, and its first funding period will last until 2019. The school is dealing with hierarchical structures of bio-systems on supramolecular and mesoscopic scales between a few nanometers and many micrometers. The speaker of the school is R. Lipowsky.

In addition, the MPICI participates in other graduate schools:

- International Research Training Group on "Self-assembled Soft Matter Nano-Structures at Interfaces (coordinated by the TU Berlin),
- „Berlin-Brandenburg School of Regenerative Therapies" (coordinated by the Charité Hospital, Berlin),
- SALSA, the Graduate School of Analytical Sciences Adlershof (coordinated by the Humboldt University Berlin),
- ZIBI Graduate School, Center of Infection Biology and Immunity (ZIBI) (coordinated by the FU Berlin).

The MPIKG takes part in some priority programs („Sonderforschungsbereiche" SFB) of the German Science Foundation (DFG):

- Collaborative Research Centre 760 - „Biomechanics and Biology of Musculoskeletal Regeneration" coordinated by Charité Medical School
- "Multivalenz als chemisches Organisations- und Wirkprinzip: Neue Architekturen, Funktionen und Anwendungen (SFB 765), coordinated by the Free University

Moreover Prof. Fratzl coordinated from 2009 to 2016 the DFG priority program SPP 1420 „Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials",in which more than ten universities and Max Planck Institutes participated. The program explored the possibility of generating new material classes of great potential by combining the degrees of freedom of hierarchical structuring inspired by nature with the variety of materials offered by engineering. The institute also participated in the network GoFORSys on "Systems Biology", a co-operation with the University of Potsdam and the MPI of Molecular Plant Physiology, which was funded by the Federal Ministry of Education and Research (BMBF).

Furthermore the MPIKG is part of the research project MaxSynBio which is dedicated to Synthetic Biology and is funded by the Max Planck Society and the Federal Ministry of Education and Research. Research groups from nine Max Planck Institutes across Germany, as well as the Department of Theology of the Friedrich Alexander University Erlangen-Nuremberg, are involved. The project started on 1st of August 2014 and will run initially until the end of July 2017 with the option of an extension for additional three years. Our trials to cooperate with the National Excellence Centre on Catalysis of the Technical University Berlin are very promising concerning the development of completely new catalytic schemes and the excellence cluster on "Unifying concepts in catalysis" coordinated by the Technical University, Berlin. Moreover the institute is also a member of the new project „Big-Data Driven Materials Science (BDDMS) in charge of the Fritz Haber Institute and funded by the Max Planck Society.

The MPIKG participate also in the Berlin-Brandenburg Center for Regenerative Therapies (BCRT), in the Excellence Cluster "Image-Knowledge-Gestaltung" (where P. Fratzl is co-spokesperson) coordinated by the Humboldt University and SALSA, the Graduate School of Analytical Sciences Adlershof.

National and International Collaborations

Within the framework of European programs there are three EU projects within the 7th framework program and four within the EU framework program "HORIZON 2020", including two ERC Starting Grants. Furthermore the Institute is together with the Max Planck Institute of Molecular Physiology in Dortmund and the Riken Advanced Science Institute (ASI) in Wako principal partner of the new Riken Max Planck Joint Research Center. The new research center is able to promote the more effective use of research resources as well as information and technology in the field of systems chemical biology. The Indian Institute of Science and Education Research (II SER), Pune and the MPICI have entered 2011 into a research collaboration to design and construct nanodevices to improve treatment of cancer. The Max Planck Partner Group is funded by the Department of Science & Technology, Govt. of India and the Max Planck Society. Furthermore Joint laboratories and international partner groups have been established with the National Laboratory for Physical Sciences at Microscale (CAS) in Hefei, China; with the Fuzhou University, China, with the Zheijiang University/ Hangzhou, as well as with the Jiao Tong University/Shanghai. Project cooperation in the area of molecular biosystems is, among many others, cultivated with the Weizmann Institute/Israel, the ETH Zürich, and the Burnham Institute for Medical Research.

Beyond the collaborations described there exist bilateral and co-operation projects under assistance of the European Space Agency (ESA), the NATO, the German Academic Exchange Service (DAAD), the German Research Foundation (DFG), German Israel Foundation (GIF) for Scientific Research and Development, the National Institutes of Health (NIH), Swiss National Science Foundation (SNSF) and the VW-Foundation with Commonwealth of Independent States (CIS), China, France, Greece, Ireland, Italy, Israel, Japan, the Netherlands, Norway, Poland, Portugal, Switzerland, Sweden, UK and the USA. Clinically oriented bone research is carried out in close collaboration with the Ludwig Boltzmann Institute of Osteology in Vienna (Austria). Moreover the former Department of Interfaces has established a Laboratoire Européen Associé about „Sonochemistry". It is run since 2008 together with the CEA Institute of Separation Chemistry in Marcoule and continued with the Department Biomaterials

Industrial Cooperations, Patents and Spin-Offs

The MPIKG cooperates with many industrial partners such as BASF-AG, Firmenich, Merck, Beiersdorf, AstraZeneca UK, Clariant GmbH, Degussa AG, Merck, Procter & Gamble, Servier, and Bayer-Schering AG, Nestle, EADS, Daimler, and Lam Research, Lion Corporation.

At present the MPIKG maintains 32 patents. In the time period from 1993 to 2017 following spin-offs have been launched: Capsulution Nanoscience AG, Colloid GmbH, Nanocraft GmbH, Nanolytics, Optrel, Riegler & Kirstein, Sinterface, Oxidion GmbH, Carbon Solutions GmbH, Glycouniverse, Artemiflow, Vaxxilon, and Fluxpharm

Editorial and Advisory Boards

Scientists serve as reviewers and advisors for many journals. Therefore listed are only activities as editor and member of an editorial board. Moreover you will find a list where you can find memberships in advisory boards.

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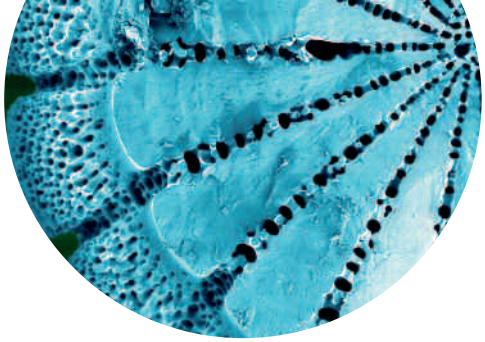
- Science Magazine (P. Fratzl)
- Soft Matter (M. Antonietti)



Advisory Boards:

- Alberta Ingenuity Centre for Carbohydrate Science, Canada (P. H. Seeberger)
- Bayreuther Zentrum für Kolloid- und Grenzflächenforschung (H. Möhwald)
- B-Cube Dresden, (P. Fratzl, Scientific Advisory Board, Chair)
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- Biofibres Materials Centre, Stockholm (H. Möhwald)
- BWG Excellence Cluster (P. Fratzl, Co-speaker)
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- Chinese Academy of Sciences Institute of Nanosciences (M.Antonietti, Scientific Advisory Board)
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- PolyMat San Sebastian (M. Antonietti, Scientific Advisory Board)
- Projekthaus NanoBioMater, University Stuttgart (P. Fratzl, Advisory Board)
- Ray Jaime I Committee (M. Antonietti, Advisory Board)
- WYSS Institute for Bioinspired Engeneering at Harvard University (P. Fratzl, Scientific Advisory Board)

Internationale Max Planck Research School (IMPRS) on Multiscale Bio-Systems

In Zusammenarbeit mit der Universität Potsdam, der Freien Universität Berlin, der Humboldt Universität Berlin und dem Fraunhofer Institut für Zelltherapie und Immunologie IZI hat das MPIKG im Jahr 2013 eine neue IMPRS zum Thema „Multiscale Bio-Systems" etabliert. Der Sprecher der Schule ist Prof R. Lipowsky, der Vize-Sprecher ist Prof R. Seckler und der Koordinator ist Dr. A. Valleriani. Das Graduiertenprogramm vermittelt grundlegende Kenntnisse über Biosysteme in Makromolekülen und wässrigen Lösungen, über molekulare Erkennung zwischen den Grundbausteinen, freie Energieübertragung bei molekularen Maschinen sowie Strukturbildung und Transport in Zellen und Gewebe. Diese Forschungsaktivitäten konzentrieren sich auf vier Kernbereiche: molekulare Erkennung von Kohlehydraten, Interaktion von Biomolekülen mit Licht, gerichtete intrazelluläre Prozesse und gerichtete Formveränderung von Geweben. Ein Hauptziel der IMPRS ist ein quantitatives Verständnis der Prozesse auf supramolekularer und mesoskopischer Ebene im Größenbereich zwischen einigen Nanometern und vielen Mikrometern. Der interdisziplinäre Ansatz verbindet bottom-up und top-down Ansätze, die von verschiedenen Gruppen in Theorie und experimenteller Biophysik, in Physik und Kolloidchemie sowie in Biochemie und Molekularbiologie verfolgt werden.

Rahmenbedingungen

Das englischsprachige Doktorandenprogramm bietet aktuelle Themen interdisziplinärer Forschung und wurde für sechs Jahre genehmigt mit der Aussicht auf Verlängerung um weitere sechs Jahre. Hauptverantwortlicher der Schule ist das Max-Planck-Institut für Kolloid- und Grenzflächenforschung. Im Einklang mit den allgemeinen Regeln der IMPRS kommt weniger als die Hälfte der zugelassenen Studenten aus Deutschland. In den Jahren von 2013 bis 2016 sind circa 1400 Bewerbungen eingegangen, aus denen 36 Doktoranden ausgewählt wurden, elf von ihnen aus Deutschland, der Rest aus 13 anderen Ländern. Die Auswahl der Studenten findet in einem dreistufigen Verfahren statt, bei dem die Kandidaten sich zuerst auf ein Projekt bewerben, das von zwei oder mehr Fakultätsmitgliedern angeboten wird. In der zweiten Stufe wird eine Auswahl von Bewerbern zu Interviews mit den Fakultätsmitgliedern eingeladen. In einem dritten Schritt müssen die besten Bewerber den IMPRS-Lenkungsausschuss und ihre Betreuer überzeugen, um einen Doktorandenvertrag zu bekommen.

Lehrprogramm

Jeder Doktorand arbeitet an einem Projekt unter Aufsicht eines „Dissertationskommitees", das aus mindestens drei Betreuern besteht, welche sich regelmäßig mit dem Doktoranden treffen, um seine Fortschritte und eventuelle Änderungen des Projekts zu besprechen. Die IMPRS organisiert zwei Workshops im Jahr, zu denen sich alle Gruppen treffen um über ihre jeweiligen Projekte zu diskutieren und sich auszutauschen. Vorträge der Doktoranden und viel Zeit während der Poster-Präsentationen erlauben es jedem, persönlich mit den Doktoranden und ihren Betreuern zu sprechen. Zusätzlich dazu organisiert die IMPRS eine Ringvorlesung, in der Fakultätsmitglieder der Schule und eingeladene Sprecher pädagogisch orientierte Vorlesungen halten, die alle vier Kernbereiche der Schule abdecken. Bisher hat die Schule 43 solche Vorlesungen organisiert. Sie bietet auch eine Vielzahl von Veranstaltungen zu Soft Skills – von Workshops zum wissenschaftlichen Schreiben, über Übungen zu Präsentationstechniken bis hin zu Deutschkursen und Vorträgen zu Karriereperspektiven. Das Graduiertenprogramm bietet auch Semesterkurse an, wo einzelne Themengebiete vertieft werden. Bis zum Sommersemester 2017 gab es 42 solcher Kurse, in denen Themengebiete von Biochemie bis statistischer Physik behandelt wurden, um die Kluft zwischen den einzelnen Teildisziplinen zu überbrücken. Gruppenleiter, Nachwuchsgruppenleiter und Professoren des MPIKG, der Universität Potsdam, der FU Berlin, der HU Berlin und des Fraunhofer Instituts für Zelltherapie und Immunologie IZI nehmen an dem Programm teil und bieten Training und Mentoring an.

Weitere Informationen finden Sie unter:
imprs.mpikg.mpg.de

Reinhard Lipowsky und Angelo Valleriani
International Max Planck Research School (IMPRS)
on Multiscale Bio-Systems

International Max Planck Research School(IMPRS) on Multiscale Bio-Systems

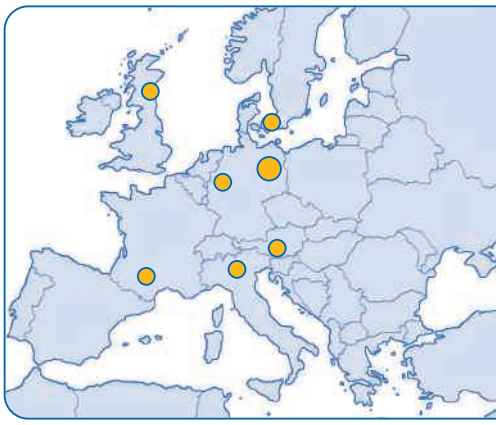
In collaboration with the University of Potsdam, the Free University Berlin, the Humboldt University Berlin, and the Fraunhofer Institute for Cell Therapy and Immunology IZI, the MPI-CI now offers a new IMPRS on "Multiscale Bio-Systems". The speaker of the school is R. Lipowsky, the vice-speaker is R. Seckler, and the coordinator is A. Valleriani. The new IMPRS started its training activities in the winter semester 2013/2014. The IMPRS addresses the fundamental levels of Biosystems as provided by macromolecules in aqueous solutions, molecular recognition between these building blocks, free energy transduction by molecular machines as well as structure formation and transport in cells and tissues. The research activities are focused on four core areas: molecular recognition of carbohydrates, interaction of biomolecules with light, directed intracellular processes as well as directed shape changes of tissues. One general objective is to understand, in a quantitative manner, how the processes on supramolecular and mesoscopic scales between a few nanometers and many micrometers arise from the structure and dynamics of the molecular building blocks. The interdisciplinary research combines bottom-up with top-down approaches, which are pursued by several groups from theoretical and experimental biophysics, from physical and colloid chemistry as well as from biochemistry and molecular biology.

General Framework

The English-speaking doctoral program offers cutting-edge, interdisciplinary research and has been approved for six years, with a possible extension for another six years. Headquarter of the school is the MPI of Colloids and Interfaces. In line with the general rules for all IMPRS, less than half of the admitted students can be from Germany. In the years from 2013 to 2016, we have received about 1400 applications and recruited 36 doctoral students, eleven from Germany and the rest from thirteen different countries. The recruitment of new students is based on a three-step procedure, in which applicants first apply for a project proposed by a group of two or more faculty members. In a second stage, selected applicants are invited for an interview by the faculty members, who evaluate the quality of each applicant. Finally, those candidates who have convinced the IMPRS steering committee and their future supervisors receive an offer.

Research Training Activities

Every doctoral student works on a project under the supervision of a Thesis Committee composed of at least three persons, who meet regularly to discuss progresses and adjustments of the project. The school organizes two workshops per year, where all groups meet and discuss about each of the current projects. Talks by the doctoral students and plenty of time during the poster session allow anybody to personally discuss with the doctoral students and their supervisors. Furthermore, the school organizes a lecture series where faculty members of the school as well as invited speakers deliver pedagogically oriented lectures covering all four core areas of the school. So far, the school has organized 43 such lectures. The school offers a variety of soft skills events, including workshops on scientific writing, presentation skills, German language courses as well as lectures on career possibilities. The school offers also semester courses to cover broad topics in depth. Until the summer semester 2017, the school has offered 42 courses, covering topics from biochemistry to statistical physics, in order to bridge the gap between different disciplines. Group leaders, junior group leaders and professors of the Max Planck Institute of Colloids and Interfaces, the Potsdam University, FU Berlin, HU Berlin, and the Fraunhofer Institute for Cell Therapy and Immunology IZI participate in the program and offer training and mentorship.



For further information see:
imprs.mpikg.mpg.de

Reinhard Lipowsky and
Angelo Valleriani

Presse- und Öffentlichkeitsarbeit

Das Max-Planck-Institut für Kolloid- und Grenzflächenforschung informiert innerhalb seiner Presse- und Öffentlichkeitsarbeit über die wissenschaftlichen Innovationen am Institut und deren Ergebnisse in Lehre, Forschung und Anwendung. Auf diese Weise möchten wir ein eigenständiges, positives Image und Vertrauen schaffen. Gleichzeitig soll dazu beigetragen werden eine Brücke von der Lehr- und Forschungsstätte in die Öffentlichkeit zu schlagen, aktuelle Impulse aufzunehmen, neue Ideen zu finden und umzusetzen. Ein Hauptziel ist es, unsere aktuelle Forschung in das Bewusstsein der allgemeinen Öffentlichkeit, der Politik, der Presse, unserer KooperationspartnerInnen, zukünftiger StudentInnen, ehemaliger Institutsangehöriger sowie der internen Gemeinschaft zu bringen. Aufmerksamkeit und Interesse für die Wissenschaft und damit letztendlich Akzeptanz, Sympathie und Vertrauen zu gewinnen, gehören zu unseren wichtigsten Anliegen.

Fach- und Publikumsjournalisten werden über das aktuelle Geschehen mit Hilfe von fundierten Nachrichten und Hintergrundwissen informiert. Regelmäßig veröffentlichen wir unseren Zweijahresbericht, Presse-Informationen, beantworten Presseanfragen und halten zu den Medienvertretern persönlichen Kontakt. Neben der klassischen Pressearbeit stellt die Konzeption, Organisation und Durchführung von Veranstaltungen den zweiten Tätigkeitsschwerpunkt des Referats dar.

Der Tag der Offenen Türen im Wissenschaftspark Potsdam-Golm ist dabei einer unserer Höhepunkte. Gemeinsam mit den Max-Planck Instituten für Gravitationsphysik und Molekulare Pflanzenphysiologie, den Fraunhofer-Instituten für Angewandte Polymerforschung IAP sowie für Zelltherapie und Immunologie IZI, dem Golm Innovationszentrum GO:IN sowie dem Brandenburgischen Landeshauptarchiv bieten wir im zweijährigen Rhythmus interessierten Besuchern aller Altersklassen einen faszinierenden Einblick in die Forschung. Da am 13. Mai 2017 der Potsdamer Tag der Wissenschaften im Wissenschaftspark Potsdam-Golm durchgeführt wurde, wurde der Tag der Offenen Türen zugunsten dieser Veranstaltung verlegt.

In über 200 Einzelveranstaltungen präsentierten sich 40 Hochschulen und Forschungseinrichtungen aus Brandenburg. Von 13 bis 20 Uhr hatten die rund 15.000 Besucher die Möglichkeit, hinter die Kulissen der interdisziplinären und internationalen Grundlagenforschung und angewandten Wissenschaften zu schauen.

Ein weiterer Höhepunkt konnte am 21. September 2015 mit der Einweihung des Erweiterungsbaus gefeiert werden. Durch die Fertigstellung des neuen Gebäudes mit 2300 qm Nutzfläche gewinnt das Institut nach zwei Jahren Bauzeit zusätzlich Platz für den Betrieb moderner Großgeräte, die Einrichtung von Nachwuchsgruppen wie auch für die Forschung von 100 weiteren Mitarbeitern.

Darüber hinaus werden am Institut Führungen für Interessierte, insbesondere für Schulklassen, sowie Vorträge an den Schulen selbst organisiert. Das Institut beteiligt sich ebenfalls jedes Jahr am „Girls' Day – dem Mädchenzukunftstag".

Ehemalige Mitarbeiter des Max-Planck-Instituts für Kolloid- und Grenzflächenforschung arbeiten auf der ganzen Welt. Sie sind in der Wissenschaft, Wirtschaft und Verwaltung tätig, beeinflussen Entwicklungen und zukünftige Strukturen – Grund genug, alljährlich ein Ehemaligentreffen zu veranstalten, das über die "Trends in Colloids and Interface Science" informiert. Im Rahmen der Veranstaltung werden zwei Preise an Nachwuchswissenschaftler verliehen. Zum Einen der Preis für die beste Promotion und zum Anderen der Preis für die überraschendste Entdeckung.

Der Internetauftritt, aber auch die interne Kommunikation stellen zudem weitere wichtige Bereiche der Öffentlichkeitsarbeit dar. Wir sehen es als Aufgabe an, die Bedeutung der Grundlagenforschung und der zukünftigen Entwicklungen in der Kolloid- und Grenzflächenforschung an die breite Öffentlichkeit zu transportieren. Entdecken Sie auf den folgenden Seiten, dass Wissenschaft faszinierend, kreativ und fesselnd ist! Sollten Sie bei auftretenden Fragen unsere Hilfe benötigen, unterstützen wir Sie jederzeit gern.

Katja Schulze
Presse- und Öffentlichkeitsarbeit
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Foto: Friedrich Bungert

Press and Public Relations

Press and Public Relations at the Max Planck Institute of Colloids and Interfaces serve as the interface between the scientists' work and the public. We inform you about the research results, and want to create an independent, positive image and thus trust in scientific work. Simultaneously we try to bridge the gap between research institution and general public and hence get new impetus and ideas. We promote the perception of our research among the community, the press, government, corporate partners, prospective students, alumni and our own internal community. It is a matter of great importance that not only the scientific community but in fact anyone interested in modern science should have the opportunity to get an idea about the aims of our institute. Attention, interest and finally trust in science must be one of our most important concerns. Therefore we inform journalists with profound news and background knowledge about current research. To pursue this task press releases are edited, brochures – such as this Report – are published and distributed on request and informal support is provided whenever necessary.

Beside classical Press and Public Relations the complete conception, organization and realisation of events is a second core theme. One of our highlights every two years is the Open Day, which is an interesting and fun-packed day, combining demonstrations of high-tech learning facilities with hands on activities for all age groups. The Open Day is held together with the Max Planck Institutes of Gravitational Physics and Molecular Plant Physiology, the Fraunhofer Institutes for Cell Therapy and Immunology IZI and for Biomedical Engineering IBMT, the Golm Innovation Center GO:IN and the Brandenburg Main State Archive. As the "Potsdamer Day of Science" took place on May 13th 2017 in the Potsdam-Golm Science Park we shifted the Oped Day in favour of this event. 40 universities and research institutes from Brandenburg presented themselves with more than 200 individual events. From 1pm to 8 pm about 15.000 visitors took the chance to look behind the scenes of interdisciplinary and international basic science as well as of applied science.

Beside this the MPICI has celebrated the inauguration of its extension building on September 21st 2015. The new building with most modern laboratories and further 2300 square meters gives now space for largescale facilities, for junior research groups as well as for the research of 100 additional employees.

Furthermore the institute takes part in the Germany-wide campaign „Girls'Day – Future Prospects for Girls" every year.

Former members of the Max Planck Institute of Colloids and Interfaces work around the world. They are employed in science, business and administration, influence developments and future structures. Reason enough to organize together with the "Freunde der Kolloid- und Grenzflächenforschung e.V." an annual alumni meeting, which informs about the "Trends in Colloids and Interface Science". Within the event two prices were awarded to early-stage researchers, the "Doctoral Thesis Award" and the "Most Surprising Discovery". Through this forum alumni can stay in touch with other alumni, and the Institute at large. In addition it helps alumni to stay connected with academic departments, bringing both personal and professional benefits.

But also the internet presence and the internal communication are additional important fields within Press and Public Relations. We try to create awareness for the role of basic research in general, especially with regard to future developments in colloid and interface science. We also seek to show that the world of science and technology is fascinating, challenging, varied and rewarding. Within these pages you can find the latest news from the institute as well as a more in depth look at our research. If you have any further questions, please contact us. We are pleased to help you.

Katja Schulze
Press and Public Relations
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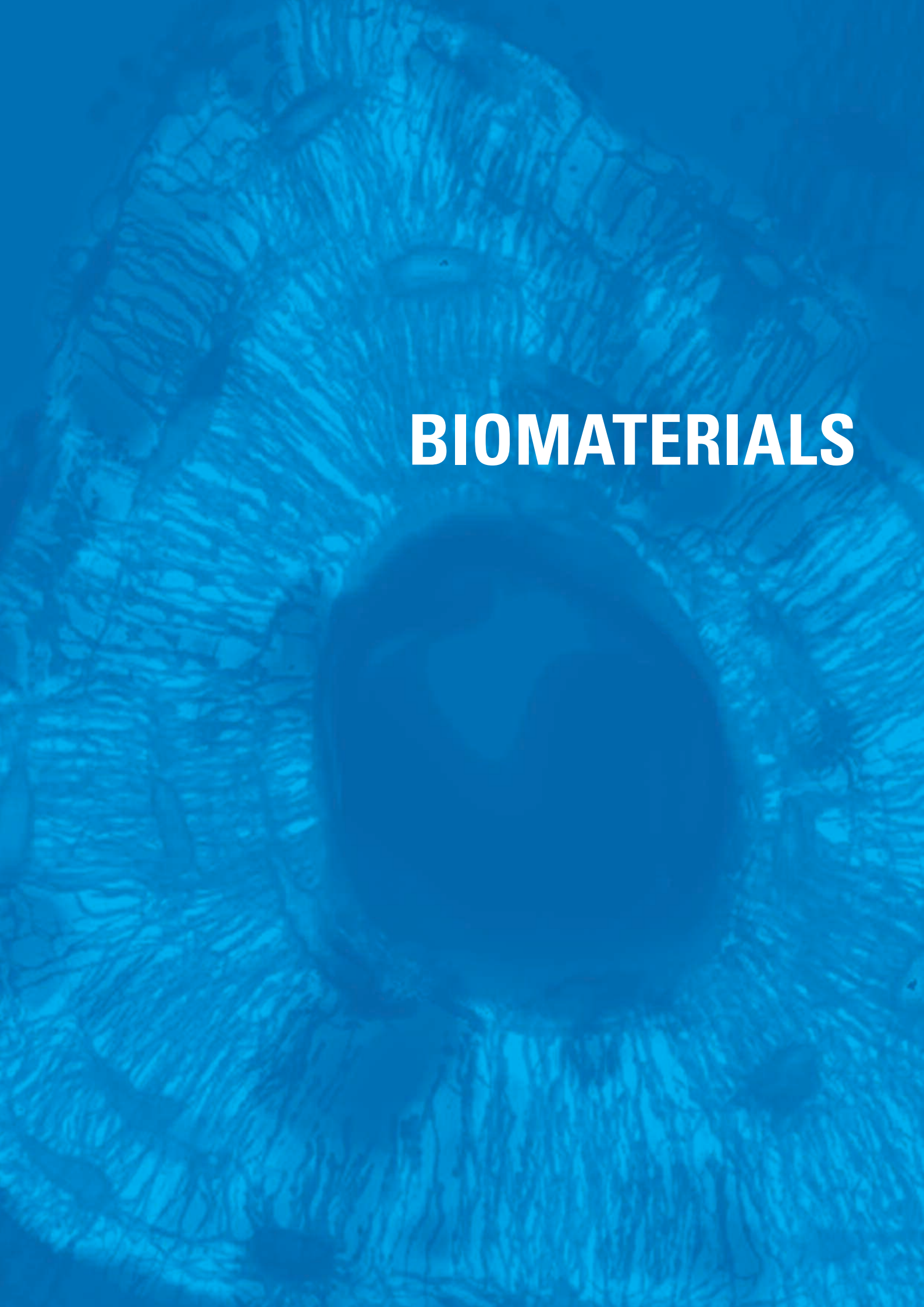

BIOMATERIALS

Department of Biomaterials

Peter Fratzl 13.09.1958
1980: Diploma (Ingénieur Diplômé de l'Ecole Polytechnique, Paris)
1983: PhD, Physics (University of Vienna)
1981-1985: Research Scientist (Austrian Academy of Sciences, Vienna; Laboratoire Leon Brillouin, Saclay, France); Visiting Research Fellow (Hahn Meitner Institute, Berlin; New York University)
1986-1998: Assistant and Associate Professor (Institute for Materials Physics of the University of Vienna, Austria)
1988 and 1989: Visiting Professor (Rutgers University, New Jersey, USA)
1991: Habilitation, Solid State Physics (University of Vienna)
Since 1993: Associated member (Ludwig Boltzmann Institute of Osteology, Vienna).
1993-1994: Visiting Research Fellow (Heriot-Watt University, Edinburgh)
1997: Visiting Professor, (Physics Department of the University of Munich)
1998-2003: Chair of Metal Physics (University Leoben, Austria)
Director (Erich Schmid Institute for Materials Science of the Austrian Academy of Sciences)
Since 2003: Director, Department of Biomaterials (Max Planck Institute of Colloid and Interfaces, Potsdam-Golm)
Since 2004: Honorary Professor of Physics at Humboldt University Berlin
Since 2009: Honorary Professor (Physics of Biomaterials) at the Potsdam University, Fellow of the Materials Research Society, Member of the Austrian Academy of Sciences, the Academy of Science and Literature Mainz, ACATECH as well as the Berlin-Brandenburg Academy of Sciences)
Since 2017: Chair of the Chemistry/Physics/Engineering Section of the Max Planck Society

The overarching research area of the Department is biological materials science, which connects materials science and biology in a reciprocal way: First, biomedical questions are addressed by methods and approaches borrowed from physics, chemistry or materials science. One such example is the extracellular tissue in the case of skeletal diseases and during regeneration. Second, we tap into the diversity of natural organisms to study naturally evolved solutions of engineering problems encountered by these organisms. Examples are materials combining stiffness and fracture resistance or providing capabilities for sensing, self-healing or shape-change. Many types of natural materials, often based on common classes of natural polymers, such as cellulose, chitin or protein (collagen and others) are addressed in these ways.

This research is carried out by scientifically independent research groups with diverse backgrounds, including mathematics, physics, chemistry, materials science, physical chemistry, biochemistry, wood science, botany, zoology and molecular biology. The group leaders were assembled not only based on their scientific excellence but also on their capability of collaborating – where needed – with each other groups as well as with the director who mainly contributes expertise in x-ray scattering, mechanical modeling as well as general materials science.

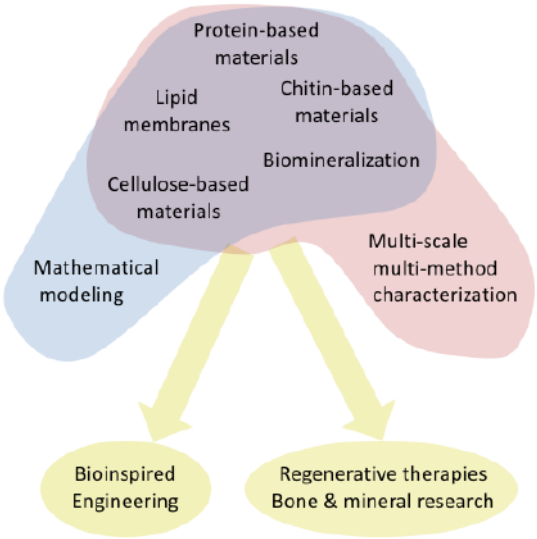

Fig. 1: Schematic of research topics in the biomaterials department. Most biological materials of interest are based on protein, cellulose, lipids and minerals (top). They are analyzed by multi-scale, multi-method approaches (pink) and by mathematical modeling (blue) and they lead to multiple collaborations in the contexts of bio-inspired engineering and of regenerative therapies (yellow).

Natural Materials Based on Proteins, Lipids, Polysaccharides

Matt Harrington's group addresses primarily extracellular protein-based materials and is interested in their assembly and in their often exceptional properties.

Yael Politi studies the chitin-spaced cuticle of arthropods, such as spiders. This cuticle supports a variety of tools and sensory devices that are essential for the survival of the animal. The fiber architecture of the cuticle as well as its composite character comprising chitin, protein and water are key for its functionality.

Michaela Eder works with her research group primarily on cellulose-based biological materials, such as wood and certain seed capsules that open with changing air humidity or temperature. These capsules are particularly interesting because they represent models for shape-changing polymeric materials.

Emanuel Schneck runs an Emmy-Noether group (supported by DFG) on the physics of biomolecular interfaces. The research addresses interaction between membranes and with biomolecules. He makes use of x-ray and neutron reflectivity studies as well as numerical modeling.

Mason Dean studies cartilaginous skeletal elements and, in particular, the formation, structure and mechanical performance of tesserae, mineralized tiles covering all skeletal elements.

Reinhard Miller's research focusses on solution-air interfaces and their dynamics. He retired by the end of 2016.

Biomineralization

Biomineralization is a widely represented topic in the department **[1]** involving the work of several groups. *Damien Faivre* heads a group focusing on magnetotactic bacteria and the synthesis and application of magnetic nanoparticles. *Wouter Habraken* reports on his work studying nucleation and growth of calcium phosphate minerals in-vitro to help our understanding of biomineralization. Very surprisingly, a calcium carbonate phase was discovered in the process that had not previously been described. Wouter Habraken was supported by a 5-year collaborative project with the Weizmann Institute (Lia Addadi and Stephen Weiner, among others), also involving *Yael Politi* and *Luca Bertinetti*. Results included the discovery and characterization of mineral precursors, probably transported within vesicles and deposited at the growth front of bone in zebrafish **[2,3]** and in chicken embryo **[4].** Other results of this collaboration are mentioned in *Wouter Habraken's* report.

Methodological Approaches

The experimental approach is based on multi-method 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 developing and using multi-method characterization approaches combining x-ray tomography; scanning electron microscopy and scanning x-ray diffraction as well as spectroscopic imaging to

characterize micro- and nanostructure and many levels of structural hierarchy **[5]** (see also report by *W. Wagermaier*). We use nano-indentation as well as acoustic microscopy to estimate local mechanical properties. *Igor Zlotnikov* has established modulus mapping techniques which push the lateral resolution of mechanical characterization into the nanometer range (see his report). The strength of this multi-method approach is that the different parameters measured on the same specimen can be correlated at the local level with micron (or even smaller)-scale spatial resolution. This facilitates the extraction of structure-property relationships even in extremely heterogeneous materials **[6].**

In a related type of approach, we study *in situ* changes in various materials (e.g. due to mechanical stress or to chemical or thermal processing) by time-resolved scattering or spectroscopy during mechanical deformation or thermal or hygroscopic treatment. This gives insight into the molecular and supramolecular mechanisms which are responsible for the noteworthy properties of these materials. In some cases, such measurements can be performed in the laboratory (e.g. with Raman or infrared spectroscopy or in the environmental scanning electron microscope), but in many cases synchrotron radiation is needed (e. g. for x-ray diffraction or small-angle scattering). A dedicated beamline end station for scanning small- and wide-angle scattering and fluorescence spectroscopy is operated at the synchrotron BESSY at the Helmholtz Zentrum Berlin. A particular challenge is related to the big amount of data generated in such experiments, which led us to head an effort in developing software for the online analysis of large x-ray scattering datasets. This approach is now complemented by recent large investments in the Institute that provide new capabilities with high-resolution transmission electron microscopy as well as (cryo)-focused ion beam 3D electron imaging (via slice and view scanning electron imaging).

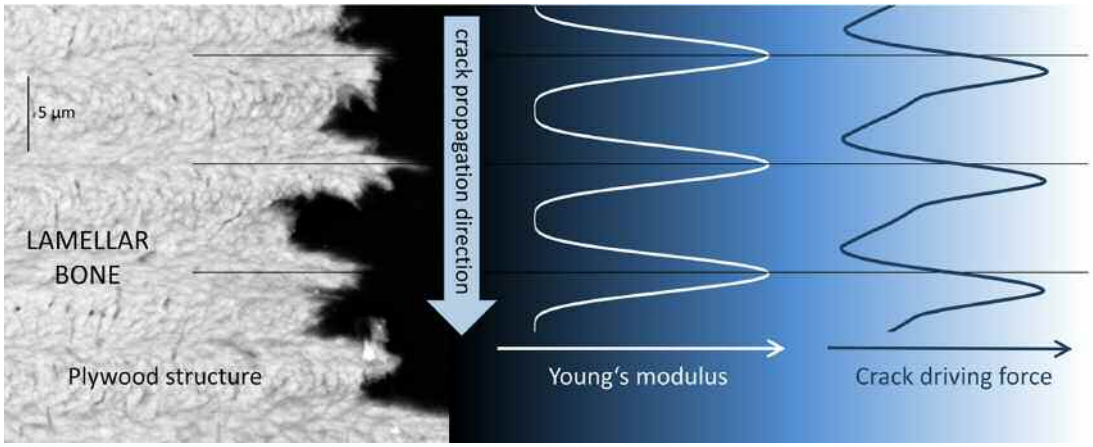

Fig. 2: Variation of stiffness (Young's modulus) and of the resulting crack driving force in lamellar bone. The plywood-like structure leads to a periodic modulation which implies larger energy dissipation when a crack propagates. In this way the toughness of bone tissue is increased by a large factor ***[15].***

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 (see for example the reports by *John W.C. Dunlop* and *Richard Weinkamer*). The Humboldt Award Winner F. Dieter Fischer from Montanuniversität Leoben (Austria) is a long-standing collaboration partner in this context.

Active Materials

The classical concept that materials are a passive support for the activity of devices is currently challenged by research on active materials which are responsive or adaptive, which regenerate or allow shape changes. The Department takes part in these research activities by focusing on shape-changing materials of natural origin and artificial systems inspired from these **[7].** Plant-based systems, such as seed capsules, are systems where shape change is induced by the absorption of water from air. Both the underlying mechanisms as well as the physical chemistry of water absorption and osmotic stress are investigated (see report by *Luca Bertinetti*). Osmotic stress is also generating a contraction of the collagen molecule which was studied in detail by in-situ x-ray diffraction **[8].** One consequence is the generation of compressive pre-strains on the mineral phase of bone [9] and of dentin **[10,11],** which is likely to greatly improve the fracture resistance of these materials. Finally, research on active materials is also one of the focus areas of the Cluster of Excellence "Image-Knowledge-Gestaltung" supported by the German Science Foundation (DFG) and located at Humboldt University Berlin. This Center is an interdisciplinary research laboratory including sciences, humanities and the design disciplines (with the spokespersons: W. Schäffner - Cultural History and Theory, H. Bredekamp – Art History, and P. Fratzl – Science).

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[3] A. Akiva et al.: On the Pathway of Mineral Deposition in Larval Zebrafish Caudal Fin Bone. Bone 75, 192-200 (2015).

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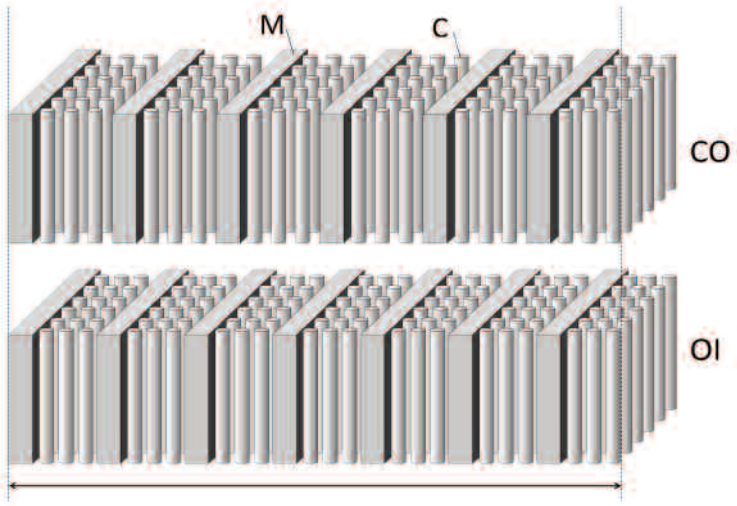

*Fig. 3: Schematic representation of the packing of plate-like mineral particles (M) associated with collagen molecules (C) in bone matrix of osteogeneis imperfecta (OI) and controls (CO). Electron backscattering imaging and Raman spectroscopy indicate the larger density of mineral in OI but similar protein/mineral ratio. Small angle x-ray scattering also shows similarly sizes particles. Hence, the higher density must be linked to a reduced water content (or nanoporosity) of the matrix confirmed by Raman spectroscopy (from **[14]**).*

Among many other activities, the Cluster organized a public exhibition on the interaction between science, humanities and design in a Berlin Museum ("+ultra – gestaltung schafft wissen" at Gropiusbau, Berlin, November 2016) **[12].**

Research on Bone and on Tissue Regeneration

In collaboration with partners from the Montanuniversität Leoben and the Austrian Academy of Sciences (F. Dieter Fischer and Otmar Kolednik) we study by theoretical methods the fracture behavior of multilay-ered materials and, in particular, of lamellar bone. Recent work shows that the lamellar architecture increases the fracture toughness of bone by more than an order of magnitude **[15, 16]** (see **Fig. 2**).

John Dunlop studies micro-tissues in vitro and investigates how they grow as a function of three-dimensional geometry. The approach is primarily biophysical but – since micro-tissues may be composed of bone cells or fibroblasts – also teach fundamental lessons about bone regeneration and wound healing.

Katja Skorb with her group develops methods for nanostructuring metallic surfaces using ultrasound treatment. These surfaces, studied in the context of cell adhesion, proliferation and differentiation; may play an important role for the development of new surface treatments for implant materials.

In a long-standing collaboration with the Ludwig Boltzmann Institute of Osteology in Vienna, Austria, we study bone structure and properties in genetic or metabolic bone diseases, such osteogenesis imperfecta (brittle bone disease) and osteoporosis, see **[13,14]** and reports by *Richard Weinkamer* and *Wolfgang Wagermaier*. As one example, we could show by a combination of electron microscopic, x-ray scattering and spectroscopic techniques, that one common feature of many forms of OI is a larger number of similarly sized mineral particles in the bone tissue, which implies increased fragility (see **Fig. 3**). Moreover, we are particularly interested in the dense osteocyte cell network that perfuses all bone tissue and acts both as an endocrine organ and a mechanosensory system. We study its network structure in relation to the architecture of the extracellular matrix. In the context of bone regeneration, the Department is also involved in a consortium on bone regeneration with the Berlin Brandenburg School of Regenerative Therapies (supported by the DFG Excellence initiative).

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.

Peter Fratzl
Director of the Department of Biomaterials

Evolutionary Perspectives on Vertebrate Hard Tissues

The study of skeletal biology is dominated by work on a few model mammalian species, although mammals represent <10% of living vertebrate species. In contrast, the number of living fish species is staggering, being half of all vertebrates and having an astounding range of morphological, functional and ecological diversity. Fishes are the oldest non-extinct lineages of vertebrates, with the primary taxonomic groups – the cartilaginous fishes and bony fishes – offering two very different primary skeletal materials. Our group exploits the rich diversity and evolutionary history of fishes, using investigations of development, ultrastructure and function to understand skeletal tissue evolution, adaptation, and mechanics.

How do Mineralized Skeletal Tissues Develop? How is "Structure" Regulated?

Vertebrate skeletons vary considerably in microstructure, but a common necessity in their growth is the regulation of the location and timing of mineralization. Shark skeletons are an unappreciated but ideal system for investigating the control and development of mineralization, in that they possess a vast and accessible array of mineralization fronts, arranged in visually striking patterns (**Fig. 1**). We show, using histological, imaging and material characterization techniques, that mineralized shark cartilage is a curious mosaic of skeletal characteristics, marked by different collagens, cellular processes and mineral density patterns than the bone or cartilage of other fishes or mammals, but exhibiting networks of communicating cells and enzymatic mineralization regulation that mirror those of bone **[1–3].** By rooting these investigations in comparisons with other mineralized shark and ray tissues, the skeletal tissues of bony fishes, and well-known mammalian systems **[3–5],** we begin to characterize the conservation of mineralization and growth mechanisms among vertebrates.

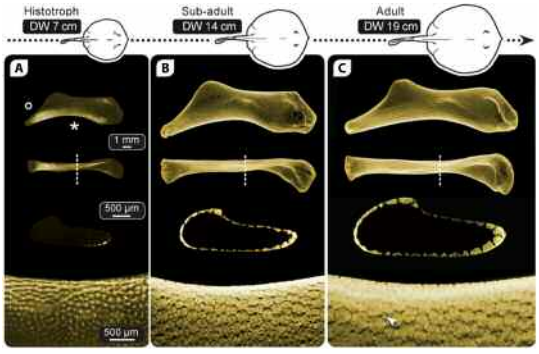

Fig. 1: MicroCT images of the development of skeletal mineralization in a stingray; note the tiling on the outside of the skeleton and the local variation in cortical thickness and calcification.

How do the Levels of Structural Hierarchy Mediate Skeletal Mechanical Properties?

All vertebrate mineralized tissues are mixtures of mineral, organic materials like collagen, and water, but few offer morphologies as geometric and amenable to modeling as shark cartilage. By combining techniques for quantifying and imaging the structure of the component parts of shark skeletons and for testing and modeling tissue mechanical properties, we provide the first insights into the high level of performance of shark cartilage **[1, 6–8].** Through a Human Frontier Science Program-funded collaboration with computer scientists and engineers in two countries, we define principles of tissue mechanics by incorporating high-resolution structural data (e.g. from synchrotron radiation tomography of biological tissue) into analytical and finite element models and multi-material 3D printed objects for mechanical testing (**Fig. 2**). This workflow allows us to query relationships between tissue form and function, even for very small structural features (e.g. the ~1µm wide joints between the mineralized tiles covering the skeleton), and to begin to abstract design rules of the system for translational science applications (e.g. building of biomimicked low-density, high-stiffness composites).

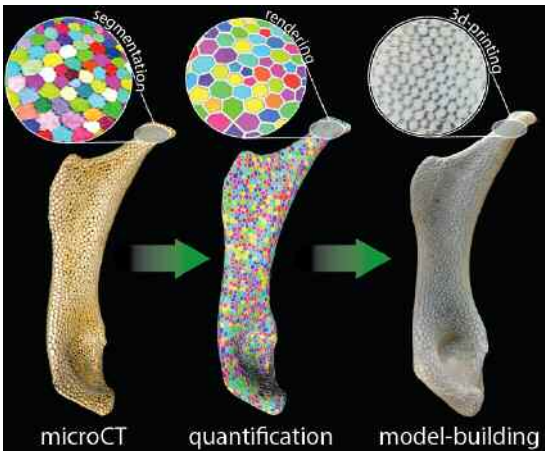

Fig. 2: Morphology-to-modeling workflow. MicroCT scanned skeletal elements are semi-automatically segmented and 3d physical models printed with different optical and material properties to quantify mechanics-shape relationships.

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Plant Material Adaptation

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The functionality of plant materials in given environments is the main interest of our research group. We define plant material as any material forming the plant body: cellular components form cells which agglomerate to tissues, which in turn are the building blocks of organs of whole plants. The plant cell wall, its chemical composition and structure as well as its proportion in a given volume plays a major role for the material performance at larger length scales such as at the organ level. A deeper understanding of plant materials implies therefore investigation at multiple length scales. The groups' activities can be assigned to both living and dead tissues. As long as cells are growing they are surrounded by the primary cell wall, rigid enough to withstand internal and external forces but at the same time pliable to allow for growth. This is achieved by the spatial orientation and interplay between the primary cell wall components cellulose, hemicelluloses and pectins. Dependent on the orientation of stiff and softer cell wall components different cell geometries emerge. After cells have reached their final form, thick, lignified secondary cell walls are synthesized in many cells. If one compares tissues with mainly primary cell walls to tissues with secondary cell walls the material properties are highly different. Eg. both hypocotyls and wood consist of elongated, cylindrical cells, however the stiffness of hypcotyls in the longitudinal direction is ~ 25 MPa **[1]** whereas in plant based fibrous materials with secondary cell walls 200 – 1000 fold higher tensile stiffness can be reached (eg **[2,3,4]**). Both primary and secondary cell wall systems, with and without active metabolism (living and dead) are interesting systems to study adaptations/adjustments of plant materials to given environments. We think this is equally interesting for a basic understanding of biological systems, for a deep understanding of the renewable resource plant material which is a prerequisite for targeted use and for the development of new (bioinspired) materials **[5].**

In the following some examples of recent research activities are given.

Primary Plant Cell Walls: The Effect of Age on Dark Grown Arabidopsis Hypocotyls

Dark grown Arabidopsis hypocotyls are a primary cell wall model system for a large scientific community. Numerous studies on the 200–400 µm thick and up to several mm long hypocotyls are performed to better understand the influence of molecular processes and genetic modifications on cell wall structure and growth. However, only few studies include experimental micromechanical data that give insights how such processes and modifications relate to Arabidopsis primary cell wall mechanics. Furthermore it is still unclear how hypocotyl age influences mechanical properties. We studied effects of age on hypocotyls of different seed batches with two tensile-testing-setups designed in our lab **[1, 6].** They offer complementary possibilities of studying mechanical properties of *Arabidopsis* hypocotyls. Data were evaluated and discussed by considering age, geometrical parameters, hypocotyl density and cellulose content. Tensile stiffness and breaking stress of 4 day old hypocotyls were significantly lower than of 5–7 day old hypocotyls where no clear differences could be found (**Fig. 1**). Naturally the hypocotyls got longer with age. Furthermore the dataset allows estimations concerning biological variability of this model system. With this study we were able to establish both experimental protocols and reference values for the mechanical parameters tensile stiffness and fracture stress, useful for future studies on both wild-type and modified hypocotyls grown under various conditions.

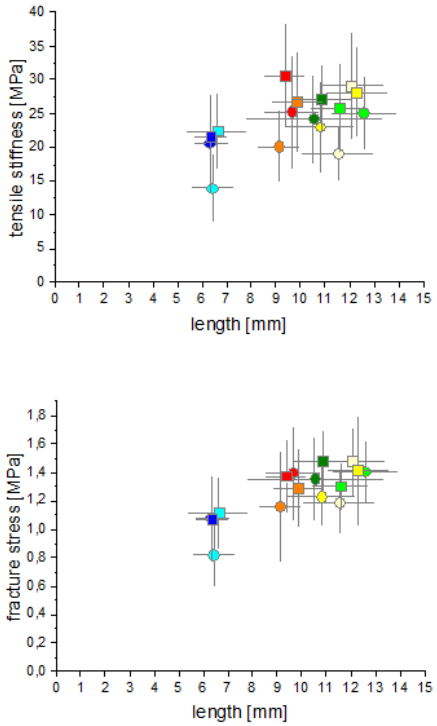

*Fig. 1: Arabidopsis hypocotyl mechanics **[2]:** circles show experiments of the first seed batch, squares experiments of the second seed batch. Dark colors are related to the first experiment, light colors to the second experiment of one seed batch. Colors relate to the hypocotyl age: blue – 4days, red – 5days, green – 6days and yellow – 7days.*

Secondary Plant Cell Walls: Important Components in Many Seed Pods

Fruits and seed pods are plant structures essential for long-term species survival. Hence, it is not surprising that functionalities are incorporated in the material. Frequently, seed pods are composed of dead tissue which still provides possibilities for mobility and movements to allow for seed dispersal and distribution. E.g. the devils claws (Martyniaceae fruits) interlock with hooves and ankles of large animals to disperse seeds **[7].** This is possible since the flexibility of the structures allow for attachment during dynamic locomotion and the high strength and stability prevent premature failure due to heavy loads which has been described in detail in the article "A materials perspective of Martyniaceae fruits" **[7].** In contrast to seed dispersal based on attaching to animals and

the forces created by the animals, seed dispersal often relies on the movement of the seed pod itself. This is particularly interesting when initiated by an environmental trigger:

Serotiny – Elevated Temperatures Trigger Seed Release

A so-called serotinous plant does not release seeds upon maturity (such as wheat or pine cones in temperate regions) but it rather needs an environmental trigger for release and dispersal. Often the triggers are rain or drastic changes in temperature. In the last years we got interested in the seed pods of Banksia species which require heat – typically caused by bush fires – for seed release. The plant genus Banksia is native to Australia and received its name from the British botanist Joseph Banks who collected the first Banksia samples in 1770. Banksias are also considered being iconic Australian plants, they are frequent motives in indigenous and other arts, probably because of their impressive flower spikes (inflorescence) which can contain up to 6000 single flowers (**Fig. 2A**).

Fig. 2: (A) Flower spike of B. attenuata, (B) follicles developed out of pollinated flowers (C) initial follicle opening caused by fire and (D) completely open follicles, seeds and separator have fallen out

Some of the flowers get pollinated, often by mammals, such as nectar-sucking opossums and develop into follicles, the seed containing structures (**Fig2B**). Many species accumulate cones (without active metabolism) in the canopy for up to 17 years until a bush fire. The fire initiates follicle opening (**Fig 2C**). The gap between the follicle halves is large enough to expose the inner surface to the environment but too small for immediate seed release. Wetting and drying cycles are necessary for further follicle opening (**Fig. 2D**).

From a materials science perspective an understanding of the long-term dimensional stability and functionality of the woody and polymeric Banksia follicles during fire is interesting and might contribute to a better use of renewable resources and polymers since many plant based materials such as wood are not suitable for various applications due to swelling and shrinkage upon humidity changes. On the other hand many polymers lack stability at elevated temperatures causes problems for applications.

Together with the Botanical Garden in Perth we collected cones of Banksia attenuata at 5 sampling sites from Perth to Wannaroo, following a climatic gradient. By exposing the collected samples to stepwise heating we found that the opening temperatures gradually changed along the climatic gradient **[8]:** the southernmost follicles opened at 54 °C, the northernmost at 72 °C. These temperatures were much lower than the ones found in literature. When the follicles open they separate along the junction zone which is characterized by interdigitating cells and a substance gluing the follicles halves together (**Fig. 3**).

Fig. 3: (A) Follicle starting to separate along the junction zone, (B) completely open follicle, (C) longitudinal cut of a follicle, seed and separator between the follicle valves (D) globular structure of exocarp, segmented µCT (bar 1mm), (E) junction zone showing interdigitating cells (bar 50 µm)

Investigations on the melting behavior of the substance between the two follicle halves, a wax, revealed no differences in melting temperatures between the sampling sites (~45–50 °C) and were below the opening temperatures. This indicates that the wax might act as a sealing agent for microcracks since 45–50 °C can be reached in the field. Keeping the follicle tight is essential for avoiding any microbial attack, such as degradation caused by bacteria or fungi. Furthermore in the outer layer – the exocarp – sclerenchymatic fibres without preferential orientation form globules which are in contact to each other similar to puzzle pieces. Probably small movements in the plane of the follicle surface are possible; at the same time outward bending of the follicles valves seems to be prevented by the geometry and arrangement of the globules **[9].** Banksia follicles are an excellent example for long-term stability of a purely polymeric material, properties highly desirable for plant-based materials for buildings and/or constructions

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Biochemical Strategies in Load-Bearing Natural Materials

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Organisms such as mussels, spiders and hagfish, are able to rapidly fabricate remarkable biopolymeric fibers from bottom-up assembly of protein building blocks possessing properties that rival those of the best man-made polymers. As our fundamental knowledge of these materials improves, they are emerging important archetypes for inspiring the development of high performance synthetic polymers **[1].** However, this requires a deep, holistic understanding of the underlying biogenic design principles. Along these lines, the overarching goals of our research group are to:

1) Elucidate structure-function relationships and bio-fabrication processes from biogenic materials.
2) Adapt natural design principles for development of advanced bio-inspired materials.

Structure-Function Relationships of the Byssus

Learning from nature requires the in-depth characterization of structure-function relationships of biological materials. X-ray diffraction studies coupled with *in situ* mechanical testing led by Antje Reinecke have identified the critical role of cross β-sheet protein conformation in the characteristic large extensibility and elastic recoil of mussel byssal threads **[2].** A complementary project led by Clemens Schmitt in collaboration with Yael Politi (Dept. of Biomaterials) employed X-ray absorption spectroscopy (XAS) coupled to mechanical testing in order to probe the hypothesis that protein-metal coordination is essential for thread mechanical properties. These results reveal the presence of a strong, yet reversible sacrificial network of histidine-Zn^{2+} cross-links that contribute to the high stiffness, toughness and self-healing behavior of the threads **[3].** Taken together, these studies

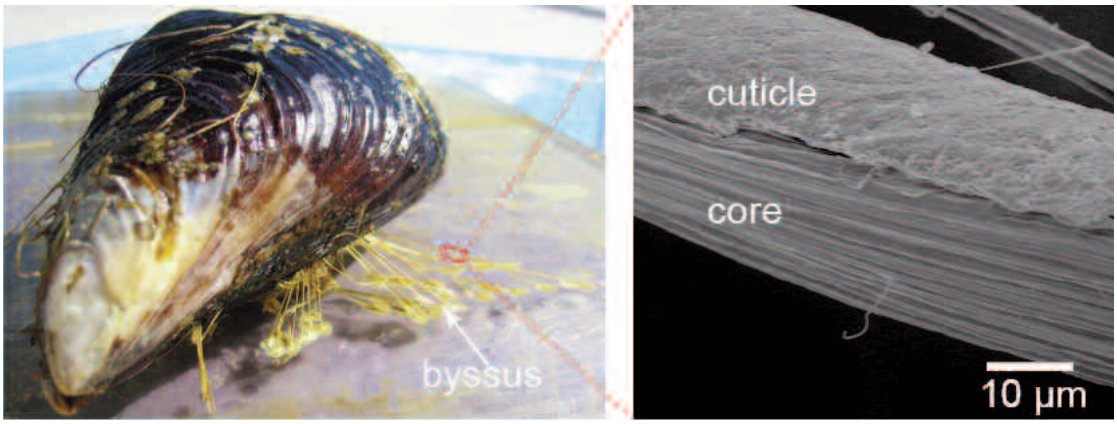

Fig. 1. Mussel byssus holdfast. A mussel byssus consists of 50–100 protein-based byssal attachment threads. Each thread possesses of a tough and self-healing fibrous core sheathed by a hard and extensible protective cuticle.

Our primary model system is the byssus, a collection of tough proteinaceous fibers, which are externally extruded by marine mussels to anchor on surf-beaten substrata at the rocky seashore (**Fig. 1**). These fibers exhibit remarkable properties, such as wet adhesion, high toughness and self-healing capacity. Using a cross-disciplinary research approach and employing a broad range of analytical techniques, we focus on answering questions related to the biochemical and biophysical mechanisms defining these material properties. Below are some major breakthroughs that we have made during the last two years.

greatly improve our picture of the underlying mechanism of thread performance, which can adapted for developing new polymers as described below **[1].**

In addition to work on the thread core, another project led by Clemens Schmitt established a clear connection between the mechanical behavior of the hard, yet extensible outer cuticle of byssal threads (**Fig. 1**) and the presence of metal coordination bonds mediated by 3,4-dihydroxyphenylalanine (DOPA) – a post-translational modification of the amino acid tyrosine. Particularly surprising was the observation that the DOPA-metal complexes provided over 80% of the stiffness and hardness of the protective outer coating, but that the metal center could be replaced by iron, vanadium or aluminum without a major influence on mechanical properties **[4].** This strongly suggests that the mussel byssus has evolved to be opportunistic to changing metal conditions in the seawater.

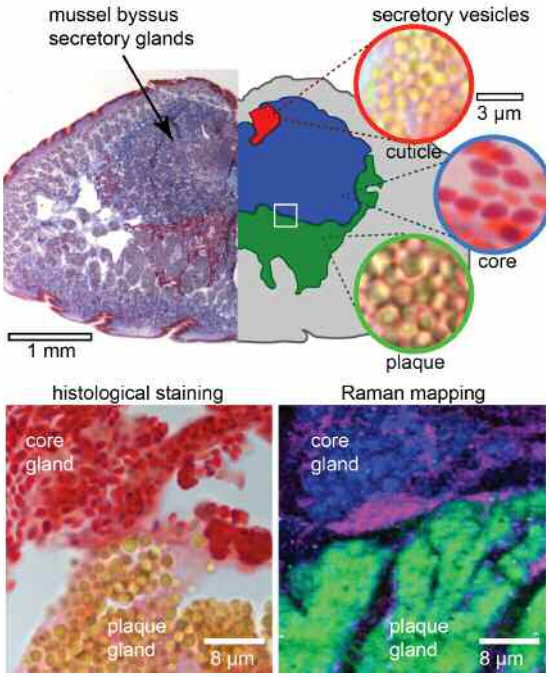

Fig. 2. Mussel byssus biofabrication. Byssal threads are produced as a secretion of protein building blocks stored in secretory vesicles in the byssus secretory glands. Using a combination of histological staining and confocal Raman spectroscopic imaging, the dynamic byssus assembly process was investigated.

Processing and Assembly of Mussel Byssus

In a remarkable feat of material processing, each byssal thread is produced in just three minutes as a external secretion of over ten different protein building blocks under ambient conditions, which self-organize into the complex nano- and micro-architectured structure observed in the native thread. A recently published study led by Elena Degtyar and Tobias Priemel have used a unique combination of traditional histology and cutting edge confocal Raman spectroscopic imaging to follow the processing steps of the byssal proteins in mussel tissue as a thread is formed **[5].** Among other things, this study revealed that a large part of the impressive structure of the byssus is acquired via spontaneous self-assembly of proteins, rather than through biologically regulated steps. Additionally, a separate project led by Antje Reinecke in collaboration with Gerald Brezesinski (Dept. of Biomolecular Systems) examined how histidine-rich protein sequences in the byssal proteins responsible for the self-healing behavior also function as pH-sensitive triggers during thread assembly **[6].** These projects provide a foundation for a number of future characterization studies and have clear implications for the development of sustainable materials fabrication.

Mussel-Inspired Materials

Our group maintains an ongoing DFG-funded collaboration with the group of Prof. Ulrich Schubert (Friedrich Schiller University) through priority program SPP-1568 with the goal of developing and characterizing mussel-inspired self-healing polymers based on metal coordination. This has culminated in two joint publications describing metallopolymeric coatings containing His-Zn^{2+} complexes, which are able to heal scratches following mild heating **[7,8].** Furthermore, two projects led by Franziska Jehle and Ana Trapaidze, respectively, are attempting to harness histidine-rich peptides based on byssal thread protein sequences to fabricate new materials exhibiting higher order organizational structure and tunable viscoelastic or self-healing properties.

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Biological Chitin-Based Tools and Sensors

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The cuticle of arthropods, a fascinating multi-purpose functional material, is made up primarily of chitin and proteins. The cuticle is the arthropod exo-skeleton so that it also serves as skin and holds sense organs and functional tools **[1].** These structures are all built of similar material however their underlying architectures and compositions are locally modified yielding fine-tuned materials properties. The study of chitin and chitin-based materials therefore holds a promise for clever bio-inspired materials design.

Despite many years of studies, there is still much to discover regarding the manner in which the cuticle components are assembled and how they interact within the final material. One of the goals of our group is to obtain basic understanding of the cuticular material, to gain insight into the structure-properties-function relations in specific structures such as cuticular tools (e.g. fangs, claws) and sensors and to investigate the manner in which they are formed. We work in close collaboration with Prof. Friedrich Barth, from the University of Vienna (Vienna, Austria) Prof. Bernard Moussian from the Technical University in Dresden (Germany), Prof Jan-Henning Dirks from Hochschule Bremen (Germany), Prof. Emil Zolotoyabco from the Technion Institute of technology (Haifa, Israel), Prof. Benny Bar-On from Ben-Gurion University (Beer Sheba, Israel), James Weaver from the WYSS institute, (Cambridge, USA) and others.

Chitin-protein-water Interactions

The cuticle can be described as a fiber reinforced composite material, where α-chitin crystallites are tightly coated by a protein shell. We studied the tarsal tendon of the spider *Cupiennius salei,* in which the chitin-protein fibers are highly aligned, using synchrotron-based X-ray diffraction and Raman spectroscopy in its intact, deproteinized, hydrated and dried states in order to shed light on the chitin-protein-water interactions in this system.

We observed high degree of order within the protein matrix and we identified protein β-sheet signature with highly defined orientation: the direction orthogonal to the β-strand long axis is slightly inclined with respect to the chitin c-axis.

In addition we observed variations in the position of the (020) diffraction peaks in pristine and treated chitin samples (**Fig. 1C**). Such that the lattice parameter b, extracted directly from the (020)-reflection, showed a large apparent increase relative to the bleached dry state – up to about 9% wet and 6.5% for dry samples. Although to a smaller extent (1.5%), such an increase was also found in 'wet' deproteinized and bleached samples. These findings were best explained by modeling the protein- and water-induced shifts in the diffraction profiles resulting from the tight interactions between them and the chitin crystallites. In this model X-ray interference effect is caused by the electron density modulation at the interface of chitin and surrounding protein coat and water due to their coherent ordering with the chitin crystalline organization. Based on this analysis, we predict protein ordering up to 2 nm and water ordering up to about 0.5 nm with protein sub-layers, spaced by 1.13 nm, and water molecules spaced by 0.25 nm. Such protein spacing is typical to β-sheets inter-sheet stacking in amyloids (see also report by Matt Harrington), whereas the distance found for water spacing is only slightly smaller than the mean distance between molecules in liquid water (0.29 nm). Moreover, we observed that the hydration caused swelling of the protein-coat and brought about larger order both in terms of the smallest dispersion in protein spacing and in chitin mis-orientation.

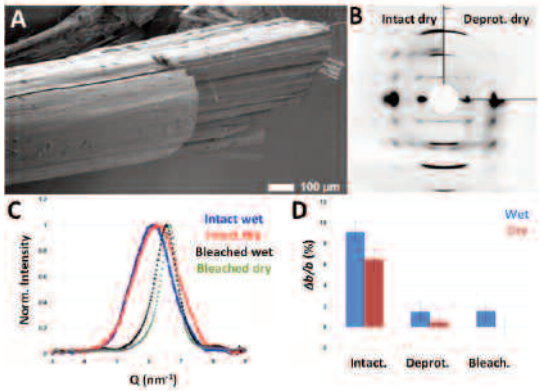

Fig. 1: (a) Scanning electron microscopy image of cryo-fractured spider tarsal tendon revealing nearly parallel fiber arrangement. (b) Diffraction pattern of an intact tendon compared with a tendon deproteinized by chemical treatment (upper right corner insert) (c) Normalized (and background subtracted) (020) diffraction profiles, measured from intact and bleached tendon samples (wet and dried). (d) Apparent relative change of lattice parameter, b (%), in treated samples with respect to that in the bleached and dried chitin.

Our results highlight the importance of hydration to the structural integrity of chitin based materials and may bare significance to the understating of fiber ordering during cuticle formation with implications for materials synthesis and design.

Nano-channels at the Tip of Spider Fangs and Cuticle Fortification

Metal ion cross-linking is used by many invertebrates for fortifying their hard parts **[3],** however, not much is known about the chemical nature and the mechanisms of this incorporation. We studied the spider fang, which is a natural injection needle comprising multi-scale architectural gradients, including high levels of Zn incorporation at its tip **[3,4]** to gain insight into these questions. We used high-resolution transmission electron microscopy (HR-TEM), spectroscopic methods and amino-acid analysis of fangs from adult spider as well as from spiders shortly after ecdysis - the shedding of the old cuticle during molting.

We found an array of multiple vascular nano-channels, which seem to attend the transport of zinc to the tip of the fang. The channels are filled with Zn precipitate in adult spiders, but not during and right after ecdysis. On the other

hand, amino-acid analysis of the same samples shows that the protein matrix composition is similar during ecdysis and in adult spider fangs, including a high content of histidine residues at the tip of the fangs. Thus His-rich proteins, which are the expected to bind Zn, are deposited before Zn is incorporated into the cuticle.

Using Electron Energy Loss Spectroscopy (EELS) at the N K-edge we demonstrated that His-Zn cross-links indeed occur within the protein matrix of adult spider fangs, but not in fangs of spiders during ecdysis.

We believe that our observations of the nano-channel array serving the Zn-transport within the pre-deposited His-rich protein matrix may also contribute to recent bio-inspired efforts to design artificial vascular materials for self-healing and in-situ curing.

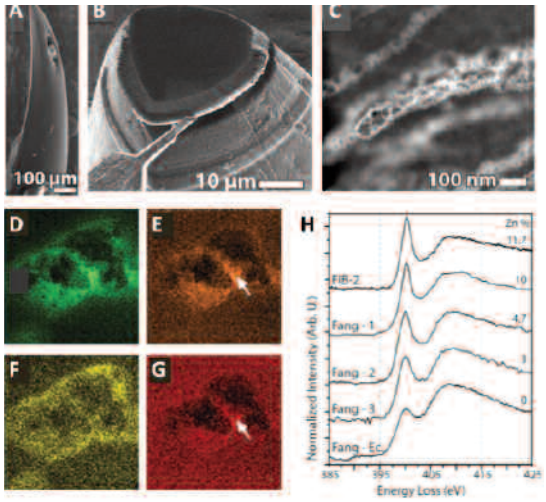

Fig. 2: Electron micrographs of the spider's fang. (A) SEM image showing the distal part of the spider fang. (B) Focused Ion Beam (FIB) lamella preparation for HR-TEM analysis (C) HAADF image of one nano-channels showing multiple Zn-rich precipitate (D-G) EDS Mapping of one of the nano-channels, FOV=400nm (D) Zn distribution, (E) oxygen, (F) chlorine and (G) nitrogen. (H) N K-edge EELS spectra performed at various parts of adult fangs containing different Zn levels (Fang 1-3, FIB-2), and of the tip of the fang of a spider undergoing ecdysis (Fang Ec). The relative atomic percent of Zn present in the sample is indicated for each spectrum.

Biomineralization

Many biominerals are formed by the crystallization of a disordered precursor phase resulting in crystals with intricate shapes and properties **[7].** Although the transformation mechanisms are still poorly understood, it is expected that they have a bearing on the nanoscale texture and on the physical properties of the crystalline product **[8].** The amorphous phases can incorporate more impurities than a crystal. This often leads to impurities being pushed out by the crystallization front and accumulate in grain boundaries.

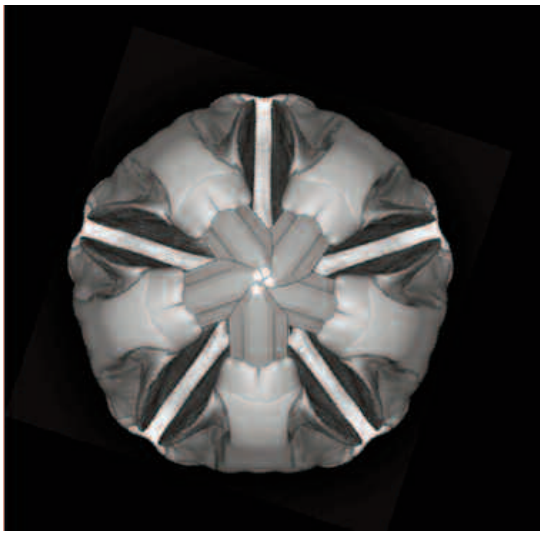

Figure 3: Three-dimensional reconstruction from microCT data of sea urchin "Aristotle lantern" comprising five jaws and five continuously growing teeth.

Amorphous calcium carbonate, the precursor phase in sea urchins, is hydrated, whereas the crystalline form into which it transform, calcite is anhydrous. Most of the dehydration is thought to take place before the crystallization **[9].** However the details of this mechanism and the manner in which access water and the organic molecules are incorporated in the final biomineral are still unknown. We are currently investigating the structure and properties of sea urchin spine using high-resolution x-ray powder diffraction (HR-XRPD) and in-situ heating small angle scattering (SAXS) in order to gain understating of this process, which appear to be fundamental for various biomineralizing systems.

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From Magnetite to Calcite

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Biomineralization is the process by which organisms form materials. These materials are as different as the function they fulfill. Examples encompass calcium phosphate in bones for mechanical support, calcium carbonate in sea shells for protection against predators and magnetic minerals for orientation. Over the years, it has become evident that the biological materials not only have outstanding properties when compared to man-made materials of similar composition but also that they are also formed under physiological conditions. Accordingly, materials scientists can learn from the design principle to produce engineered materials with reduced ecological footprints when compare to current state of the art techniques. In my group, we thus study the formation of these biological materials and their unmatched properties as well as we test extracted principles to form similar materials synthetically.

Biological Materials

Biomineralization is typically of primary importance for the biomineralizing organisms as stated above. It may even be vital and as such, it may be impossible for example to completely turn off bone formation to study the associated mineralization pathway. In contrast, biomineralization in unicellular organisms can be turn on and off. This is in particular the case in coccolithophorid algae or magnetotactic bacteria when they are deprived from the main constituent building the mineral (Calcium for the former and Iron for the later). In addition, these organisms play strategic geological roles for CO_2 fixation or in the Fe-cycle. In the last years, we have studied the mineral formation in these organisms by a variety of analytical approaches as described below.

Calcite Biomineralization in Coccolithophores

Coccoliths (**Fig. 1**) are calcite crystals produced by coccolithophores, which are a group of unicellular algae representing a major part of the marine phytoplankton with potential effect on the geological sequestration of carbon dioxide. Each cell is surrounded by several coccoliths **[1].** The biological function of coccoliths is currently unclear.

The mechanism leading to the formation of the coccoliths has remained unclear; in particular the exact pathway followed by Calcium has remained elusive. We have thus developed an approach minimizing potential artefacts to follow the dynamics of the process. We studied cryo-preserved cells by X-ray absorption spectroscopy, X-ray imaging, focused ion beam sectioning coupled with scanning electron microscopy imaging, analytical transmission electron microscopy and optical microscopy. Thereby, we identified a compartment that is distinct from the coccolith-producing compartment, and which is filled with high concentrations of a disordered form of calcium **[2].** Surprisingly, we did not observe carbonate co-localized Calcium but rather phosphorus. We will continue to analyze the role of this intermediate in the future.

In parallel, we studied the role of the so-called baseplate, which is an organic template onto which calcite nucleate *in vivo*. This template was expected to spatially direct the mineralization of calcite to its outermost region (**Fig. 1**). We showed that a specific interaction between soluble biological determinants and this baseplate indeed directed Calcium-based compounds to this region, but that these compounds were at least initially non-crystalline **[3].** The macromolecules therefore here do not control mineralization, but already play a critical role prior to it.

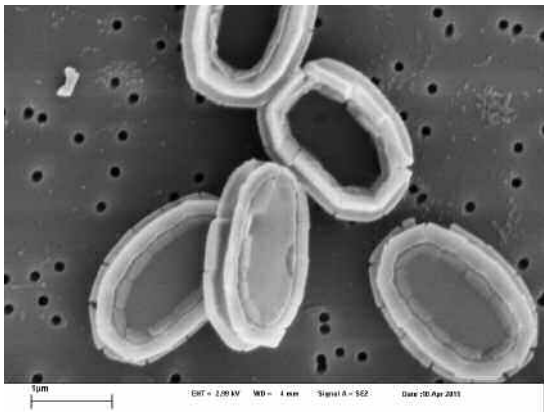

Fig. 1: SEM image of a typical coccolith. These scales are isolated from the cell. The additional layer seen on the bottom particle is the baseplate.

Magnetite Biomineralization in Magnetotactic Bacteria

Magnetotactic bacteria (**Fig. 2**) are a group of microorganisms that synthesize and organize magnetic nanoparticles called magnetosomes **[4].** The magnetosomes are membrane-enveloped magnetite (Fe_3O_4) or greigite (Fe_3S_4) nanoparticles that are supposed to help the cells navigating along the magnetic field lines of the Earth's magnetic field to reach their preferred conditions at the bottom of lakes / seas **[5].**

One of our long-standing works has been to elucidate the chemical route by which magnetite is intracellularly formed. In our most recent study, we investigated the early stages of magnetosome formation by utilizing advanced analytical electron microscopy techniques. We correlated the size and emergent crystallinity of magnetosome nanoparticles with the changes in chemical environment of iron and oxygen. We in particular discovered that magnetosomes in the early stages of biomineralization with the sizes of 5–10 nm were amorphous, with a majority of iron present as Fe^{3+}, indicative of ferric hydroxide **[6].** In turn, the magnetosomes with intermediate sizes showed partially crystalline structure with a majority of iron present as Fe^{3+} and trace amounts of Fe^{2+}. These findings corroborate the results obtained on other species.

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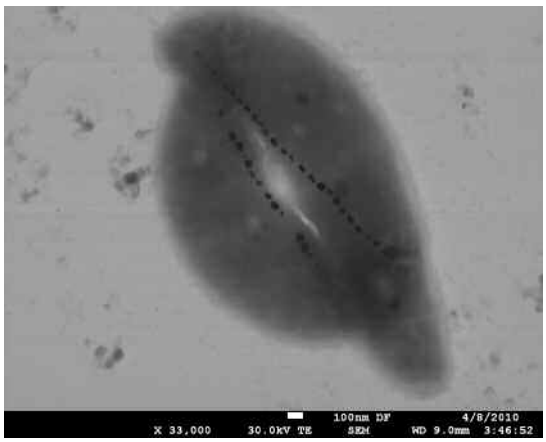

Fig. 2: TEM image of typical magnetotactic bacteria and their characteristic magnetosome chains.

Magnetotactic bacteria do not simply form magnetosomes, they also arrange them in chain **[7][8].** This feature, however, drastically complicates their division when they have only one flagellum or one bundle of flagella. In this case, the bacteria indeed have to pass on to their daughter cells two types of cellular polarities simultaneously, their magnetic polarity and the polarity of their motility apparatus. The specific magnetotactic bacteria magnetotactic bacteria solve this problem by synthesizing the new flagellum at the division site, a division scheme never observed so far in bacteria **[9].** Even though the molecular mechanisms behind this scheme cannot be resolved at the moment due to the lack of genetic tools, this discovery provides a new window into the organizational complexity of simple organisms.

Biomimetic Systems

Random Synthetic Magnetic Swimmers

In the previous years, we have studied the formation of magnetite nanoparticles in a synthetic process but with a particular focus towards low-temperature process **[10].** We also tried out several strategies to form 1D magnetic materials **[11][12].** We now profit from our expertise to assemble nanoparticles and use these aggregate as steerable micro- to nanoswimmers.

In contrast to previously designed magnetically actuated devices that all are of helicoidally- shaped, ours are of random morphology (**Fig. 3**). This enable the same materials not only to be used with different actuation strategies such as rollers, swimmers or propellers **[13],** but also to profit from their different properties to be able to actuate them concomitantly along independent trajectories **[14].** We finally showed that out of a pool of such propellers, we could select particularly fast devices outperforming any state-of-the-art materials **[15].**

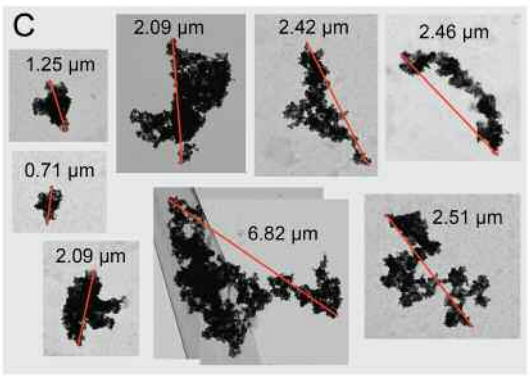

Fig. 3: TEM images of selected microswimmers (image from Vach et al., Nano Letters, 2013).

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Biomimetic Actuation and Tissue Growth

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The ability of biological tissues to change both their external shape and internal structure, allows organisms to grow, to adapt to their environment, and even to heal damage. Shape changes may even perform a function in tissues without an active metabolism, such as found in seed dispersal units in the plant world (see the group Plant Material Adaptation of M. Eder). These processes of morphogenesis are mediated by biochemical and genetic signals operating within the physical constraints of their surroundings. The importance of these physical constraints has become clearer in recent years with the observation that cells and growing tissues indeed respond to mechanical signals. An important feature of mechanical signalling is that it can act at long range, meaning the shape of external constraints can be "felt" deep inside the tissue itself. Such mechanical signals may arise due to loads acting on the external boundary or even be created by active stress-generating processes occurring inside the tissue itself (see the Mechanobiology group of R. Weinkamer).

In our research group we explore how mechanical boundary constraints influence growing and swelling tissues. The research uses a combination of theoretical and experimental techniques and is performed in collaboration with several groups both within and without the department.

Tissue Growth

In previous work we have shown that cells respond to the curvature of the substrate to which they are adhered to (See refs **[1-4]** and earlier references contained therein). We use 3D printing techniques to produce scaffolds of controlled geometry and have shown using cell culture experiments on these surfaces, together with theoretical modelling, that surface curvature influences the microstructure of tissue as well as its local growth rate. Due to experimental restrictions, in our early work we explored the response of growing tissues to rather simple geometries consisting of prismatic pores. As these pore have straight sides, one of their (starting) surface curvatures is zero, which allowed us to model the role of curvature in 2D. To explore more thoroughly the role of curvature in 3D, we have extended our modelling approach to 3D **[1].** In a collaboration with D. Fischer (Montan University Leoben) we have used these 3D models to highlight that when growing tissues are considered as viscous fluids then a simple pressure based model for growth can explain many features observed in the process of bone healing (**Fig 1**).

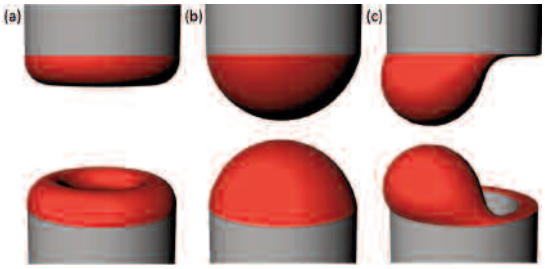

*Fig. 1: Three example configurations of simulated "bone-healing" after osteotomy **[1].** Tissue is shown in red and bone is shown in grey.*

From an experimental perspective we have also explored how stem cells respond to curvature **[2].** Our results indicated that the controlled response we observed previously in osteoblasts can be generalised to other similar cell types (collaboration C. Werner, Dresden). The role of surface geometry on extra-cellular matrix (ECM) organisation was further explored in a collaboration with two former group members (C. BIdan, UJF Grenoble, and P. Kollmannsberger, P, ETH Zurich). In this study we used a novel ECM labelling method to explore the temporal sequence of ECM deposition in pores of controlled geometries **[3]** and showed that not only cells but also ECM components are influenced by shape.

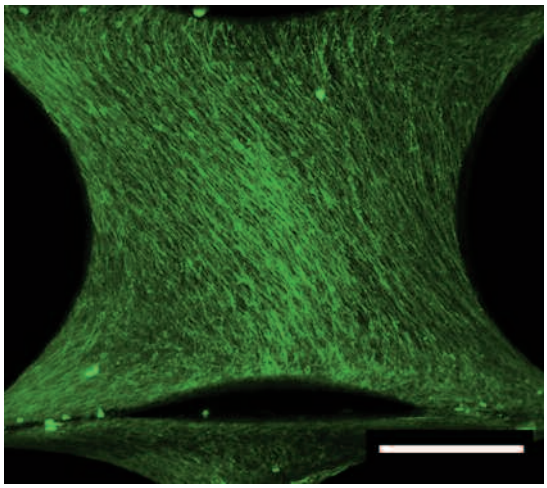

Fig. 2: A maximum projection of tissue grown on a constant mean curvature surface (MC3T3 pre-osteoblasts). Tissue is stained for actin and imaged using a light-sheet fluorescence microscope. Scale bar 400µm.

Fundamental work on the mechanisms of curvature sensing in cells has been done in collaboration with A. Petersen (Charité Berlin), which illustrated that convexly curved surfaces increased cytoskeletal tension. This in turn resulted in more nuclear deformation of the cells, expression of Lamin-A and thus promoting osteogenic differentiation **[4].** More applied research on titanium substrates has been done with K. Skorb where we have started exploring how nanostructured titanium surfaces influence cell behaviour in 2D and tissue growth in 3D **[5-6].** Recent progress in scaffold manufacturing techniques has enabled us to produce non-zero Gaussian curvature surfaces on which we can perform cell-

culture experiments. Interestingly tissues growing on these surfaces spontaneously form chiral patterns of cell alignment (**Fig. 2**). This seems to be a collective response of cells to geometric constraints, and highlights how cells in 3D can self-organise in ways much akin to liquid crystals. These ideas are supported by work we have done in developing active particle models confined to surfaces in 3D **[7],** where we see a strong coupling between surface curvature and particle ordering on curved surfaces (**Fig. 3**). It is hoped that these observations and models of pattern formation in 3D will help in the understanding of complex 3D architectures observed in many tissues e.g. **[8].**

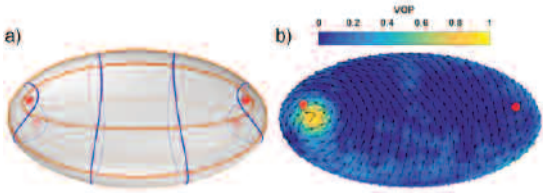

*Fig 3. Active particle simulations on ellipsoidal surfaces reveal an intrinsic coupling between particular geometric features (a) umbilic points (in red) and the dynamics of vortices highlighted in yellow in (b) that appear due to the collective movements of interacting particles **[7].***

Actuation

Macroscopic shape changes also occur in tissues due to differential swelling of spatially separated regions inside a tissue or organ. This actuation behaviour is well illustrated by the example of the ice-plant **[9],** whose seed-dispersal unit is powered by the swelling induced by liquid water. The unique diamond lattice cell structure of this tissue converts isotropic expansion into anisotropic tissue motion thus opening the capsule. We used advanced multi-material 3D printing of swellable and non-swellable polymers, combined with finite element simulations to investigate the role of cell shape on the actuation behaviour **[9,10]** (see. **Fig. 4** for an example).

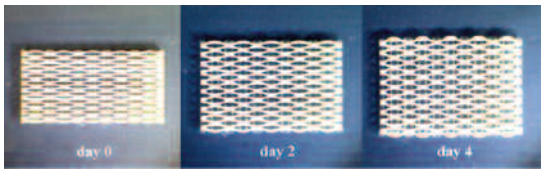

*Fig 4. Swelling of a 3D printed honeycomb structure containing of transparent swellable and white non-swellable materials **[9].***

We are also working with the plant biomechanics group of M. Eder, to model the actuation behaviour of other plant tissues. For this we mainly focus on developing theoretical tools to simulate plant organ actuation based on segmented micro CT mages. In addition to investigating natural actuators, together with polymer chemists, we have explored how shape and structure can influence actuation of artificial polymeric materials. In two separate collaborations with the groups of J. Yuan (Colloid Department) and L. Ionov (Georgia University, USA) we have investigated the role of internal structure and external geometry on the actuation of planar polymeric films **[11-14].** The group of J. Yuan have developed porous poly-ionic liquid (PIL) actuators that respond to multiple solvents extremely rapidly **[11].** Actuation is achieved via a chemical gradient across the membrane thickness. By modifying the internal microstructure of these membrane actuators using carbon nanotubes **[12],** or cloth **[13],** it is possible to control and direct actuation in particular directions with respect to the principle fibre orientation. An alternative way to control actuation is to control when actuation occurs in a particular location. These concepts were explored together with L. Ionov who produced actuating polymeric bi-layers with a variety of different geometries **[14].** As these bi-layers start swelling from the edges, different geometries (i.e. the presence of holes) gives rise to different rates of swelling which in turn force the membranes to roll or fold into non-equilibrium configurations. This opens up the possibility of using geometry to program multiple 3D states of an actuator, which could be interesting for a variety of applications such as soft robotics and cell manipulation.

Our group, together with the group of M. Eder, have also been involved in research and teaching within the context of the DFG excellence cluster Bild Wissen Gestaltung in the area of Active Matter. With the biologist T. Stach and cultural historian C. Vagt (Humboldt University) we have been investigating the structure of self-moving materials from a variety of different perspectives. We focus on understanding two biological examples, the house of the tunicate and the opening of seed protecting structures in plants, and equivalent structures in architecture. On one hand the interaction with scientists from very different disciplines can give new insights into our understanding of our biogical materials, but also we hope can also inspire new concepts in design and architecture.

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Mechanobiology

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The ability of biological materials for structural adaptation and self-healing depends often on an adequate response to mechanical stimulation. Mechanobiology studies this link between a mechanical stimulus and the resulting structural change in biological systems. Bone is a relevant mechano-responsive material not only from a material science perspective, but also due to important medical implications. Age-related bone loss is a serious problem in our aging Western societies. Although structural adaptation of bone was already described more than 100 years ago by Julius Wolff, only now serious attempts are undertaken to obtain a more quantitative description between the local mechanical stimulation and the probability to resorb or deposit bone at this location. Wolff's law states a higher probability for bone formation at sites of high mechanical loading, and preferred resorption at locations of low load. Aiming at a quantitative formulation of Wolff's law most fundamental questions that are arising concern the universality of such a formulation: Does Wolff's law depend on the species and/or the skeletal site, does it change with age?

The structural adaptation of bone is enabled by specialized cells. Beside the bone resorbing and bone forming cells (osteoclasts and osteoblasts, respectively), osteocytes recently receive particular attention of researchers. These most abundant bone cells are embedded in the mineralized bone matrix. They use a network of thin channels – the canaliculi – to connect with each other via their long cell processes. Multiple functions have been attributed to this osteocyte network: (i) mechano-sensation via the detection of the fluid flow through the canaliculi; (ii) contribution to mineral homoeostasis by using the large surface area of the network; (iii) transport of nutrients and signaling molecules.

The aim of the research group is to obtain a more quantitative description of how mechanical stimuli influence processes in bone. Using a combination of experimental and computational methods, the research focuses on the processes of bone remodeling and healing.

Mechano-regulation of Bone Remodeling

With the aim of an experimental assessment of Wolff's law, experiments on living mice were performed at the Julius Wolff Institute, Charité, (Bettina Willie, Sara Checa). Multiple micro-computed tomography images with a time lapse of about 5 days allowed the determination of the exact location where bone was remodeled **[1].** An non-invasive in vivo loading device combined with Finite Element calculations provided the information about the local mechanical stimulation in the same mouse bone **[2].** The combination of the information where bone was remodeled and how large the mechanical stimulation was at this site allows a quantitative assessment of the mechano-regulation (**Fig. 1**). The experiments were performed in mice of three different age groups (young, adult and elderly). The comparison of the mechano-regulation in adult and elderly animals demonstrate that in both age groups remodeling is mechanically regulated with the highest probability for bone formation at large mechanical stimulation (strain), while low mechanical stimulation results preferentially in bone resorption. However, the mechanical control of remodeling becomes more dysregulated with age. This is most obvious by the broader range of strains where both formation and resorption occurred in the elderly animals **[3]** (**Fig. 1**). Evaluation of remodeling events on the same long tube-like bone, but distinguishing events at the inner (endosteal) surface of the hollow tube compared to the outer (periosteal) surface) showed a reduced mechano-responsiveness of the periosteal bone surface **[4].**

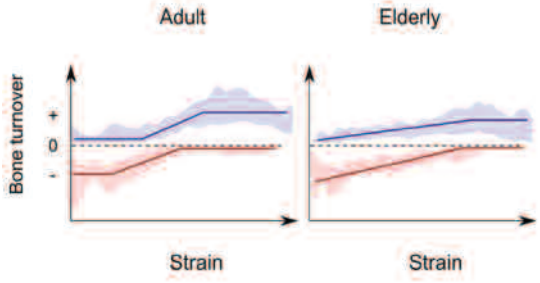

*Fig. 1: Mechano-regulation of remodeling of a long bone (tibia) in adult (26 weeks) and elderly (78 weeks) mice. Plotted are the probabilities for bone formation (blue) and bone resorption (red; plotted negatively for better visibility) as a function of the maximum principal strain (obtained by Finite Element calculations) at the same location on the bone surface. The results from several animals (n=9) (colored area corresponds to standard deviation) is summarized by a piecewise straight function to guide the eye **[3].***

Structural Analysis of the Osteocyte Network

To make progress towards an understanding of the cellular implementation of the mechano-regulation in bone, we analyzed the structure of the osteocyte lacuno-canalicular network (OLCN). It is thought that fluid flow through this network caused by the loading of the bone is sensed by the cell processes of the osteocytes. The investigations focused on human osteons, the cylindrical building blocks of cortical bone formed during remodeling (**Fig. 2**). The network structure is imaged using rhodamine staining followed by confocal laser scanning microscopy. An image analysis provides information about the density and connectivity of the network, and its orientation with respect to the overall osteonal structure **[5].** The network was found to be impressively dense with one cubic center of healthy human bone comprising a network of 74 km in length. However, osteons show a substantial variability of the canalicular density with roughly 10% of the volume having a canalicular density twice the average value and large regions lacking an accessible network. Hints about the formation of the network are provided by our observation that the network density increases in direction of bone formation from the outer cement line towards the Haversian canal **[6].** Future investigations have to show the diagnostic potential of our method, in particular with respect to a structural deterioration of the OLCN with age.

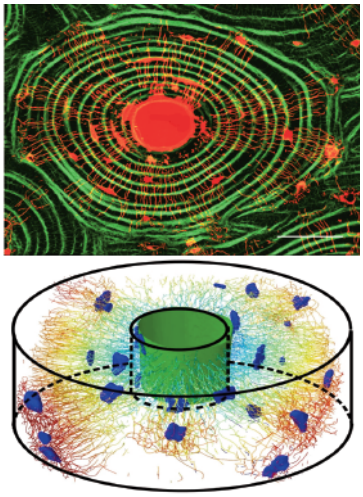

Fig. 2: Top, circular structure of a human osteon with the central Haversian canal (red circle) housing a blood vessel. The red fluorescence signal shows further the lacunae, in which the cell bodies of the osteocytes find their place, and the fine canals (canaliculi) for the cell processes. The green second harmonic generated signal of collagen highlights the lamellar arrangement of the bone matrix; scale bar 30 µm. Below, three-dimensional rendering of the canalicular network within an osteon as the result of the image analysis. Lacunae are shown in blue, canaliculi are colored from blue to red depending on their distance from the Haversian canal (green).

Bone Structural Adaptation and Healing

Implementing a simple version of Wolff's law into a computer model we studied the influence of mechano-regulated bone remodeling on the structural stability of foam-like trabecular bone. Our simulations demonstrated that the rather complex loading pattern in the dynamic foam-like structure does not support the commonly believed hypothesis that thinner trabeculae are mechanically protected from resorption. Remodeling rather led with age to structural deterioration by preferred loss of trabeculae in confined regions **[7].**

The jaw bone offers a particular interesting example of bone structural adaptation. Alveolar bone comprises the thickened ridge of the mandibular and maxillary bones that serves as primary support structure for teeth. The maintenance of the alveolar bone relies completely on a continuous mechanical stimulation due to mastication with mechanical disuse resulting in alveolar bone loss. The high mechanobiological sensitivity of this bone and high remodeling activity enables fast tooth movement, but has also detrimental effects on the progression of periodontal diseases. Together with the Japanese company LION corporation we studied the structure of alveolar bone and tooth in mice influenced by diabetes and age. Due to the hierarchical structure of these mineralized tissues **[8]** an experimental characterization on multiple length scales was performed. Synchrotron small- and wide-angle X-ray scattering (SAXS/WAXS) provides a microscopic spatial resolution with each scattering pattern yielding nanostructural information about mineral particle size and arrangement. The measurements (performed with Wolfgang Wagermaier) demonstrated structural differences not only between the tooth and the alveolar bone, but also between the buccal and the lingual side of the alveolar bone – most likely an adaptation to an asymmetric loading. Within the alveolar bone structural gradients were found with the thinnest mineral particles at locations close to the tooth. In diabetic mice particle thicknesses were smaller compared to control animals **[9].**

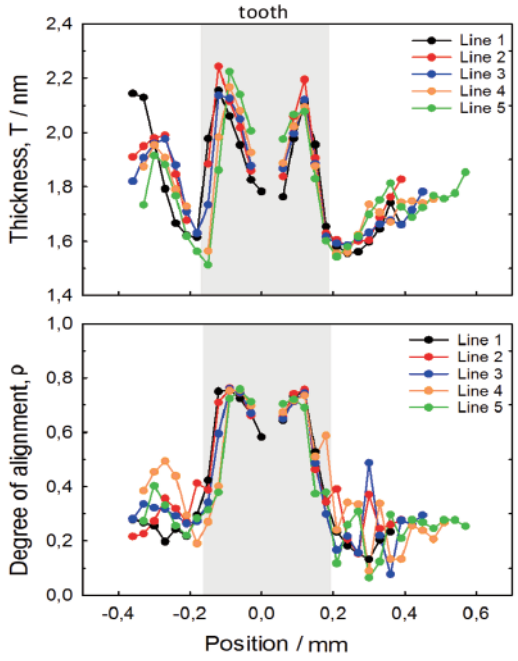

Fig. 3: The mineral nanostructure of alveolar bone and tooth of a diabetic KK+ mouse obtained by scanning SAXS/WAXS experiments. The 5 lines correspond to 5 horizontal scans from the buccal side (left) to the lingual side (right). The position of the tooth in the middle of the plots is highlighted by the gray shading. The black line corresponds to the uppermost scanning line closest to the tooth crown. Obtained parameters included the mineral particle thickness T (top) and the degree of mutual alignment ρ of the particles (bottom).

Beside adaptation, biological materials exhibit fascinating healing abilities **[10].** During bone healing the differentiation of stem cells migrating to the fracture site is another process which is mechanically influenced. With computer simulations we tested hypotheses how mechanical stimulation is regulating bone formation, which can occur either directly by the action of osteoblasts or indirectly via a transient formation of cartilage. Comparing the simulation results with experiments on sheep bone showed that the healing process is so robust that active mechano-regulation only during crucial healing phases is sufficient for a successful healing outcome **[11].**

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Hierarchical Structure of Biological and Biomimetic Materials

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Understanding structure-function relations within biological materials highlights biological, physical and chemical principles, which can be beneficial for bio-inspired materials research. In our group, we use combinations of materials science approaches (i) to answer biologically driven questions in natural materials and (ii) to understand structure-function relations in biological and synthetic materials. By this approach we aim to elucidate biological processes and to transfer knowledge from natural materials to the design of man-made materials, such as polymer-based hybridmaterials and nanostructured mineral-based materials.

In our research, bone serves as a prototypical system for a hierarchically structured material with extraordinary mechanical properties. Bone as a living organ has the capability to adapt to environmental conditions and to regenerate after injury. These processes are closely related with changes in the material structure at all size levels and can therefore be assessed indirectly by materials science methods. The research on bone is performed in cooperation with partners from the Julius Wolff Institute at the Charité in Berlin as well as the Ludwig Boltzmann Institute of Osteology in Vienna, Austria.

Our central experimental methods are X-ray scattering (SAXS, WAXS), X-ray fluorescence (XRF), polarized light microscopy (PLM), confocal laser scanning microscopy (CLSM), electron microscopy (EM), micro-computed tomography (µCT) and nanoindentation (NI). For X-ray scattering experiments we use our lab sources as well as synchrotrons, in particular the MPI µSpot beamline at BESSY II (Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin Adlershof).

Fragility and Toughness of Bone

Bone material exhibits a complex multiscale arrangement of mineralized collagen fibrils. In the prevention of fractures, the most important mechanical property is toughness, which is the ability to absorb impact energy before complete failure. Toughness depends in a complex way on the internal architecture of the material on all scales from nanometers to millimeters. The related mechanisms include plastic deformation of glue-like organic layers between mineral platelets and fibrils, micro cracking, crack deflection and crack bridging. Therefore, bone fragility has several different mechanical causes. We described these mechanisms for bone material and put them in a clinical context **[1].**

Bone Healing

A fracture in bone results in a strong change of mechanical loading conditions at the site of injury, where a bony callus is formed. We investigated bone during healing by means of µCT and different two-dimensional methods **[2].** Backscattered electron images (BSE) were used to assess the tissue's calcium content and served as a position map for other experimental data (NI and SAXS). Together with visualization experts from Zuse Institute Berlin we developed a software package enabling a combined visualization of information from these two-dimensional methods and three-dimensional µCT-data. Fig. 1 shows the combination of (a) µCT, (b) BSE-images and (c) the combination of (a), (b) and corresponding X-ray scattering data.

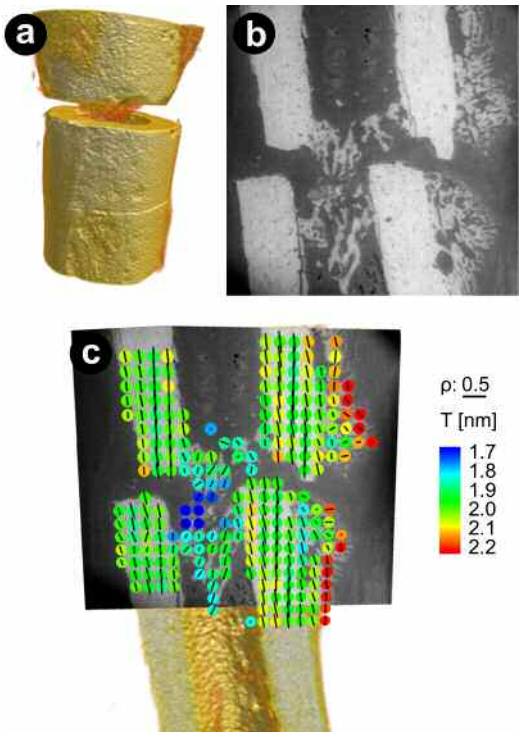

Fig. 1: Bone healing visualized by a combination of 3D and 2D methods [2]: (a) µCT image of a osteotomized rat femur, (b) backscattered electron microscopy image of a longitudinal section from the same femur as shown in (a), (c) combination of images (a) and (b) together with results from SAXS measurements: Color-coded measurement points represent the mean mineral particle thickness (T). The degree of orientation (ρ) and the predominant particle orientation are denoted by the length and orientation of the bar.

Mineralization in Healthy and Diseased Bone

The course of bone mineralization is a crucial determinant that affects the properties of healthy and diseased bone. The detailed mechanism by which calcium is deposited during mineralization and removed during absorption is largely unknown. We investigated samples from patients with osteogenesis imperfecta (OI), also known as brittle bone disease. This disease relates to a group of connective tissue disorders characterized by mutation in genes involved in collagen synthesis. Beside increased bone fragility, OI leads to low bone mass, impaired bone material properties and abnormally high bone matrix mineralization. We investigated mineral particle properties in human bone of children with OI type VI and compared it with a control group **[3].** Main characteristics of OI type VI were (i) the coexistence of a highly mineralized bone matrix with seams showing abnormally low mineral content and (ii) a heterogeneous population of mineral particles with unusual size, shape and arrangement, especially in the region with lower mineral content.

Hybridmaterials with Specifically Designed Interfaces to Improve Mechanical Properties

Hybridmaterials consist -like bone- at the nanoscale of an inorganic phase embedded in an organic matrix. In order to imitate such interfaces in synthetic materials similar to those of nature and to achieve enhanced mechanical properties, we produced hybrid materials with partners from HU Berlin (Prof. Hans Börner). This model system is based on magnesium fluoride nanoparticles (MgF_2) embedded in a PEO matrix **[4].** The interface between these two phases consists of conjugates with a peptide side adhering specifically to the inorganic surfaces of the nanoparticles, and the PEO side bonding well with the matrix. In tensile tests we could show that stiffness and toughness of the composites increased with the amount of conjugate. Pure PEO showed a modulus of elasticity of about 700 MPa, an addition of 15% MgF_2 particles increased the elastic modulus to about 820 MPa (**Fig. 2**). These values rose to a maximum of approx. 1400 MPa due to the functionalization of the particle surface with 3 mol% conjugate. The addition of MgF_2 particles reduced the toughness compared to pure PEO as expected. However, the toughness of the hybrid material increased through the peptide-polymer conjugates, but there the maximum is reached at about 1 mol% conjugate **[5].**

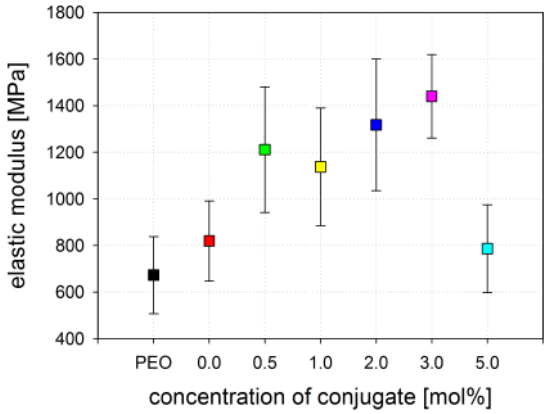

Fig. 2: Elastic modulus of a hybrid material, made from a PEO matrix, MgF_2 nanoparticles (15 wt%) and interface conjugates. The elastic modulus increases with the amount of conjugate from about 700 MPa (pure PEO) to 1450 MPa (3 mol% conjugate).

Nanocrystalline Calcium Carbonate Microlens Arrays

Exploring fundamental formation and crystallization processes in tailored mineral-based materials can contribute to a deeper understanding of complicated biomineralization processes. We produced thermodynamically stable, transparent calcium carbonate-based microlens arrays (MLA) by transforming an amorphous $CaCO_3$ phase into nano-crystalline calcite **[6].** The nano-crystallinity of the formed calcite minimized structural anisotropy and resulted in greatly reduced birefringent effects (Figure 3a). We examined the corresponding structural changes by mapping local lattice parameters and size of the calcite crystallites within the individual microlenses **[7].** The driving force for producing a crystal size of around 10 nanometers in calcite is the minimization of residual stresses and the associated elastic energy by plastic deformation involving grain boundary formation and twinning. Local strains originate from the transformation-induced macroscopic volume changes (**Fig. 3b**), which arise due to differences in the specific volume in ACC and calcite, mostly due to water loss and short-term atomic rearrangements. These MLA represent a striking example of a stress-engineered nanocrystalline material produced by almost no energy costs by phase transformation.

Interestingly, also nature utilizes $CaCO_3$-based materials to produce optical functional materials. In a review, we illustrate basic strategies to produce such optical functional materials by manipulating the material structure **[8]**. These strategies are driven by the aim to eliminate or reduce the birefringent properties of calcite.

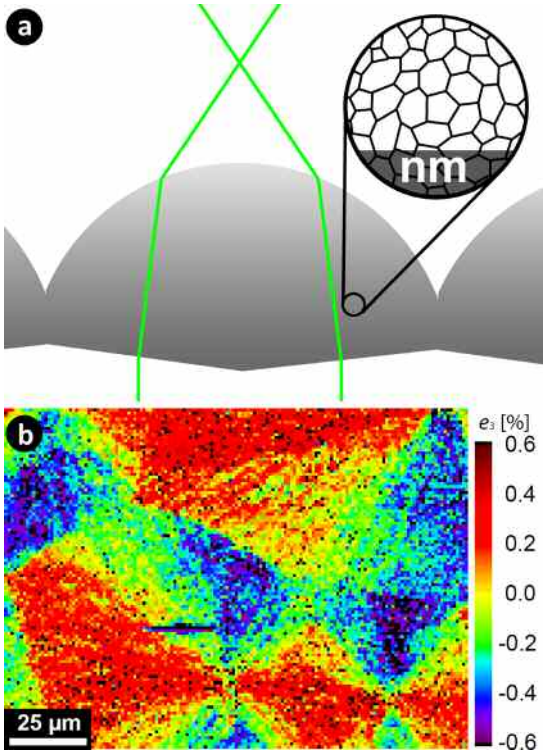

Fig. 3: Nanocrystalline $CaCO_3$ microlens arrays. (a) scheme of the light path through one nanocrystalline microlens. (b) map of relative lattice distortions (in percent), $e_3 = \Delta c/c$ showing relative differences in lattice parameters [6]

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Nanostructuring of Inorganic / Polymeric / Biological Interfaces

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Today increased interest of scientists is focused on dynamic, non-equilibrium processes and materials. It involves needs for effective energy conversion with the focus on oscillation of inorganics' properties, chemical networking, autoamplification reactions, mimicking living systems, using cell metabolic life inspiration and ions, protons, concentration gradients. These themes are investigated in the group through three different topics: 1) non-equilibrium methods for solid mesoprocessing, 2) coupling of light and pH to regulate soft matter dynamics; and 3) dynamic, self-adaptive and stimuli-responsive systems for nanoscale biomachineries. We collaborate with scientists in the MPIKG, other German Institutions and abroad. Our main collaboration partners are Prof. H. Möhwald, Emeritus Group (Interfaces) MPIKG; Dr. D. Andreeva, Institute of Basic Science in Ulsan; Prof. D. Sviridov, Belarusian State University, and Prof. G.M. Whitesides, Harvard University.

Methods for Solid Mesoprocessing

We have a specific interest in nonlinearity solids' engineering and propose to exploit complex nonlinear dynamics (example shown in **Fig. 1**) to achieve superior technological functionalities, metastable materials, which may be difficult or even impossible to achieve with linear systems. High intensity ultrasonic (HIUS) treatment of solids is an ideal target platform for mesoprocessing with possibility to control process dynamics by parameters of HIUS treatment: solvent and additives, intensity and duration **[1-3].**

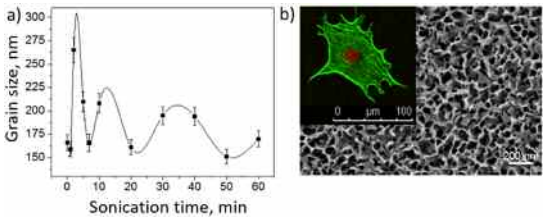

Fig. 1: a) Oscillation of grain size of Ti microparticles vs. sonication time in ethylene glycol. The grain size was determined for (110) Ti using X-ray diffraction data and the Scherrer method. b) Scanning electron microscopy (SEM) image of HIUS nanostructured mesoporous titania surface to guide cell behaviour. Adapted from Ref. ***[1-3].***

Other non-equilibrium methods can be envisaged: hot pulsed plasma discharge, laser focused exposure together with electrochemical processing.

We use metal surface nanostructuring to guide cell behaviour **[1]** (with J. Dunlop (Biomaterials, MPIKG)) that is an attractive strategy to improve parts of medical implants, lab-on-a-chip, soft robotics, self-assembled microdevices, and bionic devices.

Coupling of Light and pH to Regulate Soft Matter

We suggest to investigate photocatalytically triggered local pH changes in semiconductor / polyelectrolyte (PE) Layer-by-Layer (LbL) assembled interfaces, mimicking natural processes in a novel design strategy for inorganic / polymer interfaces. We have shown recently **[4-6]** that under irradiation of TiO_2 a series of photocatalytic reactions leads to a local change in pH, which modulates the pH sensitive LbL assembly. Prime questions are: (i) how many photons are needed to locally change the pH on titania? (ii) what is the optimum LbL architecture to understand the basis of proton trapping and storage, the pH gradient under local irradiation? And (iii) how to achieve reversible actuation of different assemblies for advanced applications? **[4]**

The efficiency of the multilayers' response (**Fig. 2**) was investigated with atomic force microscopy (AFM), *in situ* quartz crystal microbalance (QCM) and ion selective microelectrode technique (SIET) for mapping the activity of protons over the surface under local irradiation.

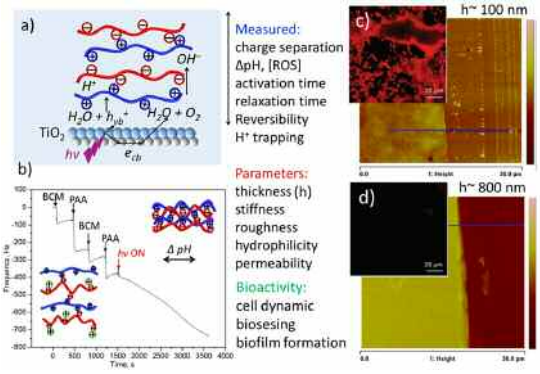

Fig. 2: Surface decoration and photoinitiated light-pH coupled reactions. a) Reactions on TiO_2 resulting in a local change of pH. b) in situ QCM of LbL PEs assembly and their activation under irradiation resulting in water attraction into the LbL and (c, b) LbL thickness change (c) before and (d) after irradiation that possibly affects (insets (c, d)) bacteria detachment from the surface. Abbreviation: BCM, block copolymer micelles; PAA, poly(acrylic acid) (PAA). Adapted from Ref. ***[4].***

We focus for the first time on the possibility of efficient transformation of energy of electromagnetic irradiation into local pH shift to actuate soft matter. This was demonstrated to be efficient to suggest Nanoscale biomachineries to control, for example, cell surface interactions, biosensing development, biocide coatings, and self-healing.

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Structural and Nanomechanical Characterization

Living organisms form complex mineralized biocomposites that perform a variety of essential functions. These biomaterials are often multifunctional, being responsible for not only mechanical strength, but also provide optical, magnetic or sensing capabilities. Many studies have emphasized the complexity of biochemical mechanisms in charge of the delicate equilibrium and interaction chemistry between inorganic precursors and macromolecular components leading to nucleation, assembly and growth of different biominerals. In contrast, mechanical and thermodynamic constraints, governing the microstructure formation, growth kinetics, morphology and mechanical properties of the mineralized tissue are much less understood. Therefore, we aim to address the fundamental question of how nature takes advantage of mechanical and thermodynamic principles to generate complex functional structures.

Eshelby Twist in the Axial Filament of the Sponge *Monorhaphis Chuni*:
We studied the highly-ordered crystalline protein/silica axial filament in the anchor spicule of the marine sponge *M. chuni*, **Fig. 1.** Using microbeam synchrotron X-ray diffraction analysis, we discovered a specific lattice rotation (so-called Eshelby twist) propagating throughout the entire proteinaceous structure. This finding, together with the dislocation-induced deformation field visualized by transmission electron microscopy (TEM), indicated the presence of a screw dislocation situated along the axial filament **[1].** The dislocation-mediated spiral crystal growth is thermodynamically favourable at low supersaturation levels due to the permanent presence of the dislocation-related kink on the growing surface of the crystal. Apparently, only this mode of growth can provide reasonable growth rates (at low temperatures of deep water) needed to form a very long (up to 3 meters) crystalline structure of the axial filament, consisting of perfectly arranged protein units and amorphous silica building blocks. It is fascinating that processes occurring in nature (the protein/silica hybrid crystal growth) and in the field of inorganic man-made materials (growth of nanowires and perfect bulk crystals, such as silicon) independently converged to the dislocation-mediated spiral growth mode, which is favourable from the viewpoint of free energy minimization.

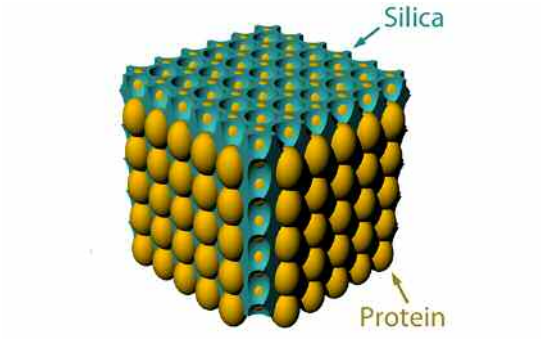

Fig. 1: 3D model of the protein/silica axial filament in the anchor spicule of the sponge M. chuni.

Static and Dynamic Mechanical Characterization of a Single Interface in the Prismatic Structure in the Shell of *Pinna Nobilis*:
Quantification of the local physical properties of internal interfaces in biological structures is complex. Except for nanoindentation-based surface techniques, there was no viable in-situ methodology to directly measure static and dynamic mechanical response of an individual sub-micrometer-thick interface. We developed an indirect experimental-analytical framework designed for (but not limited to) quantifying the elastic and viscoelastic properties of a single organic interface in biocomposite materials and demonstrated it on the calcite-organic composite prismatic structure in the bivalve shell *P. nobilis* **[2-3].** The methodology is based on force-modulation of a micro-cantilever that contains an individual organic interface and is cut-out from the biocomposite using the focused ion beam (FIB) milling technique, **Fig. 2**. During measurement, a modulating force is applied by a standard nanoindentation instrumentation at different locations along the micro-cantilever. By applying a theoretical treatment, the resulting time-dependent flexural deflection is then used to extract the elastic modulus and the damping coefficient of the interface alone.

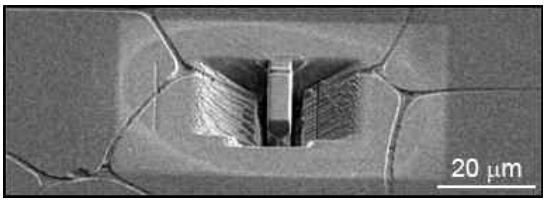

Fig. 2: A micro-cantilever milled from the prismatic structure in P. nobilis containing a single interface.

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Interactions of Water with Biological Materials

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Biological materials are constituted by molecular/supramolecular building blocks which are assembled at several hierarchical levels. They are often complex materials, which evolved to exploit intereactions with water and ions in a desired way. In my group, we address, from the molecular level upward, the effect of water and electrolytes on the molecular components of natural materials and on material's mechanical properties. The aim is to describe the thermodynamic of the interactions and understand what molecular mechanisms are responsible for the observed responses, with particular focus on passive actuation of tissues. Because of the various hierarchical levels of organization, we developed (in collaboration with many groups of the department) *in-situ*, multi-technique approaches, from which we can obtain information from the molecular to the macroscopic level.

Wood and Actuation in Plant Tissues

Although water interactions with plant tissues is of extreme importance for technological and physiological reasons, to date, they have been described only phenomenologically, without taking into account tissues' composition and structure. In the last two years, in collaboration with prof. Thomas Zemb (ICSM – Marcoule - France) we developed a new model, using a force balance approach which, starting from compositional and structural data, describes how, for fibre reinforced polymeric composites, the chemical energy associated to water interactions is used to overcome the work of swelling and can be converted into mechanical work. This approach allows to establish the full thermodynamics of the actuation for non-living plant tissues **[1].** Also, we recently established a way to account for electrostatic effects (impregnation from electrolytic solutions) which allows to describe the ions specifics effects in such tissues **[2].** This knowledge has fundamental consequences in wood technology: it enables the possibility to design new treatments able to turn these processes on or off so that water uptake can be either promoted or avoided at specific humidity ranges. This force balance approach could be used also be used to describe the actuation of synthetic biomimetic systems **[3].**

Collagen Based Tissues

Another molecule strongly interacting with water is collagen, which is the most abundant protein in mammals' tissues. In collaboration with A. Masic (MIT - Boston), we could describe how, by changing the collagen hydration state the molecule undergoes structural changes that result in the generation of tensile stresses up to 80 MPa. In mineralized tissues, this contraction of collagen puts mineral particles under compression leading to strains of around 1%, which implies localized compressive loads in mineral up to 800 MPa. Interestingly, as collagen partially dehydrates when mineralized, this mechanism could be in place to protect the mineral phase from tensile loads in collagen based mineralised tissues **[4].** In the last year, we have started to investigate the effect of the temperature on the structure and stability of collagen in hydrated conditions.

Effects of Water on Mechanics

Water content has a major impact on materials' mechanical properties and structure. We found that water acts as a plasticizer in the case of sucker ring teeth and this can be exploited to shape materials at very mild conditions (T below 100 C and high humidities). Once dried after shaping, the materials recover their original mechanical properties **[5].** Similarly, the same plasticizing effect in the interprismatic layer of Pinna nobilis makes water an essential player in determining explicit intrinsic and extrinsic toughening mechanisms of the mollusks' shell **[6].** If confined in small pores, water affects also the mechanics of harder inorganic materials. In collaboration with prof. P. Huber (TUH) we studied adsorption-induced deformation of mesoporous silicon and we developed a general model to relate the pore-load modulus to the porosity and to the elastic properties of materials **[7].**

3D Imaging of Organisms and Tissues

Lately, the activity of the group has been focussing on the imaging and 3D reconstruction with nm resolution of organisms and tissues in quasi-native hydrated conditions by means of FIB/SEM in cryogenic conditions. Using this technique, we could discover in the coccolithophorid alga Emiliania huxley a new Ca-rich cellular compartment likely involved in the biomineralization pathway **[8].** Also, we could determine the spatial relationships between the magnetosomes and the cellular membrane in magnetotactic bacteria **[9].**

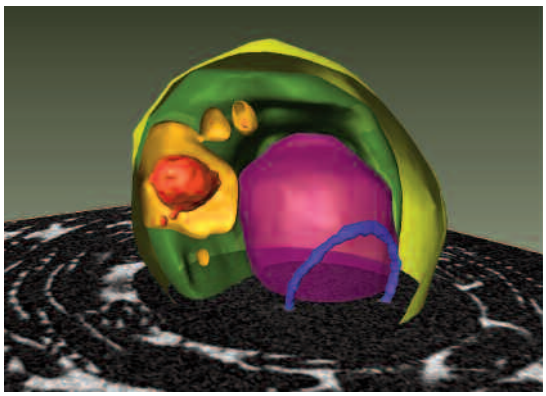

Fig. 1: 3D reconstruction of an E. huxleyi cell from a cryo-FIB-SEM image series, showing the nucleus (violet), chloroplast (dark green), plasma membrane (light green), a coccolith in statu nascendi (blue), Ca-rich bodies (red) and the membranes encompassing Ca-rich bodies (orange) .

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New Insights into Biological Mineral Formation

No chemical processes are more complicated than the ones that biology provides us. This is also true for mineral formation like bone, exoskeletons of crayfish and sea shells. In the last years we successfully discovered some of the underlying chemical and physical processes of biological mineral formation by selectively mimicking some properties of the biomineral and testing their effect using controlled synthetic crystallization experiments.

Amorphous Calcium Carbonate (ACC): Crystallization and Phase Behaviour

First the influence of particle size on ACC crystallization was investigated, resulting in an opposite behavior on crystallization in solution and upon heating **[1].** In the presence of water, crystallization is predominantly caused by a dissolution-reprecipitation behavior leading to the less stable polymorph with smaller nanoparticles, whereas upon heating the smaller spheres are more stable.

The dependence of ACC particle size on concentration and temperature was used to determine the phase behavior of ACC **[2].** This led to the formulation of a unstable ACC region with a maximum at higher temperatures, which showed a good fit with spinodal decomposition theory. Using this data we also investigated the effect of commonly found additives like poly(aspartic) acid (pAsp), magnesium (Mg) and phosphate (PO_4) on the phase behavior of ACC. Both pAsp and phosphate have the ability to decrease particle size dramatically, whereas Mg has no effect at all. Real changes in the phase diagram, however, were only observed with PO_4.

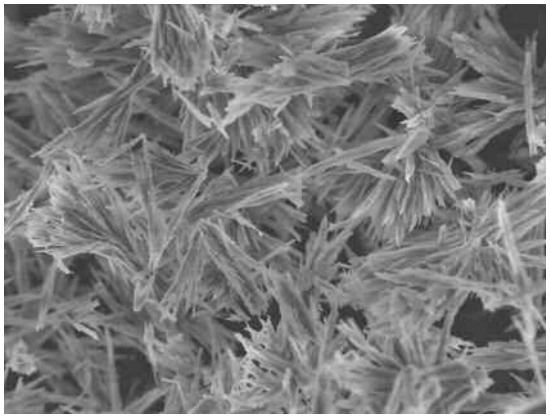

Figure 1: Golmite, A new Calcium Carbonate Phase

Also the behavior of these additives on the crystallization of ACC was investigated. It was observed that pAsp mainly influences the stability and polymorph selection of ACC by adsorbing to the ACC nanoparticles. Here, at high concentrations separate ACC nanospheres transformed directly to single vaterite spheres according to a pseudomorphic transformation mechanism.

Mg doesn't stabilize ACC very effective, though has a remarkable influence on polymorph selection. At Intermediate amounts of Mg and particle size we observed the formation of a new calcium carbonate-hemi-hydrate phase we named 'Golmite' (**Fig. 1**). The mechanism for the formation of such hydrated calcium carbonate phases from ACC is a nucleation at the surface of the ACC nanopheres, where the Mg prevents the dehydration of ACC structural units.

Structural Studies on Amorphous Calcium Carbonate

To Investigate the structure of amorphous calcium carbonate we focused on x-ray and neutron pdf-analysis. Neutron-pdf analysis allows us to look at the structural features of water, for which many speculations have been done.

In contrast to some studies we do not find any evidence for the presence of proto-structural features in any of the prepared ACC samples. The structure of ACC seems to be dominated by h-bonding between Ca and water, though above a certain water threshold we do see evidence for water clusters inside the ACC which are not h-bonded. More surprisingly, the local coordination of Ca with carbonates and water seems to resemble the arrangement of water molecules inside a saturated $CaCl_2$ solution.

Amorphous Calcium Phosphate and Condensed Phosphates

In contrast to ACC, amorphous calcium phosphate (ACP) has a much more variable composition that depends on the pH of the reaction solution. Next to that it can transform into different calcium phosphate crystals with changing composition, which makes studying its properties as well as its crystallization a much more tedious task **[3].** Additionally, especially in biology, also condensed phosphates like pyrophopshate and polyphosphate can be present, which are very poorly studied materials, and difficult to differentiate from amorphous calcium phosphate **[4,5].**

A common way of detecting condensed phosphates in Biology is by use of DAPI-staining. In a joint project with Sidney Omelon (Ottawa University), we discovered that the yellow staining is due to an autofluorescence effect upon concentration of DAPI **[5].** A consequence of this result is that every negatively charged surface that is able to attract DAPI will show this fluorescence, inclusive polyphosphate but also amorphous calcium phosphate, whose negative charge is at the base of bone mineral structure **[6].**

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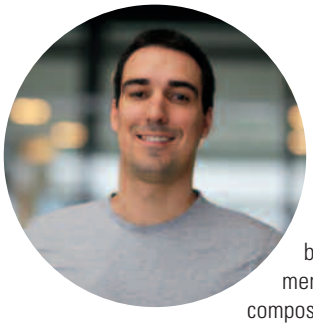
Physics of Biomolecular Interfaces



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Biological tissues and cells are composed of diverse functional units such as organelles, protein complexes, and carbohydrate assemblies. They are often organized as functional interfacial molecular layers, the prototypical examples being biological membranes. In the congested biological environment membrane functions are sensitive to the composition of the aqueous milieu and to their mutual interactions.

But soft interfaces constituted by molecular layers play important roles also in context with bio- and wet- technological processes, for instance, when resulting from adsorption processes.

In our Emmy-Noether research group, supported by the German Research Foundation (DFG), we study the interaction of biological and technologically relevant soft interfaces with solutes (such as proteins) in their aqueous environment and also their mutual interaction in the aqueous milieu, with a specific focus on interactions involving biological membranes (see **Fig. 1**). One of our main goals is to understand the relation between membrane interactions and the molecular composition of membrane surfaces. In this context we are also interested in Nature's strategies to control the interactions by adjusting membrane composition.

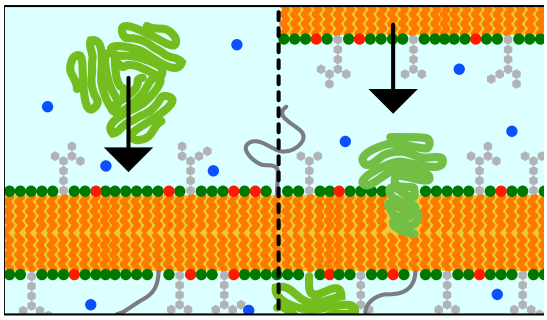


Fig. 1: Schematic illustration of a biological membrane interacting with a protein (left) and with the surface of another membrane (right).

X-Ray & Neutron Scattering Techniques and Complementary Computer Simulations

To address these questions, molecular-scale structural insight into the involved layers is required **[1].** In order to obtain such information we prepare model systems of well-defined (bio-)molecular composition at solid/air, solid/water, liquid-water, and air/water interfaces **[2-7]** and study them with various structure-sensitive techniques based on x-ray and neutron scattering **[2-6, 8].** In addition we employ complementary methods, such as ellipsometry, calorimetry, tensiometry, rheology, and spectroscopy. Finally, computer simulations carried out in collaborations provide a means to interpret experimental results on a mechanistic level **[9-13].** To this end we have developed a simulation method that accurately accounts for the chemical potential of water between interacting surfaces. The simulation results have recently led to a better understanding of the long-debated "hydration repulsion" between phospholipid membranes **[9-11]** and of the tight cohesion between glycolipid-rich membranes, which naturally occur in the form of multilamellar stacks **[13].**

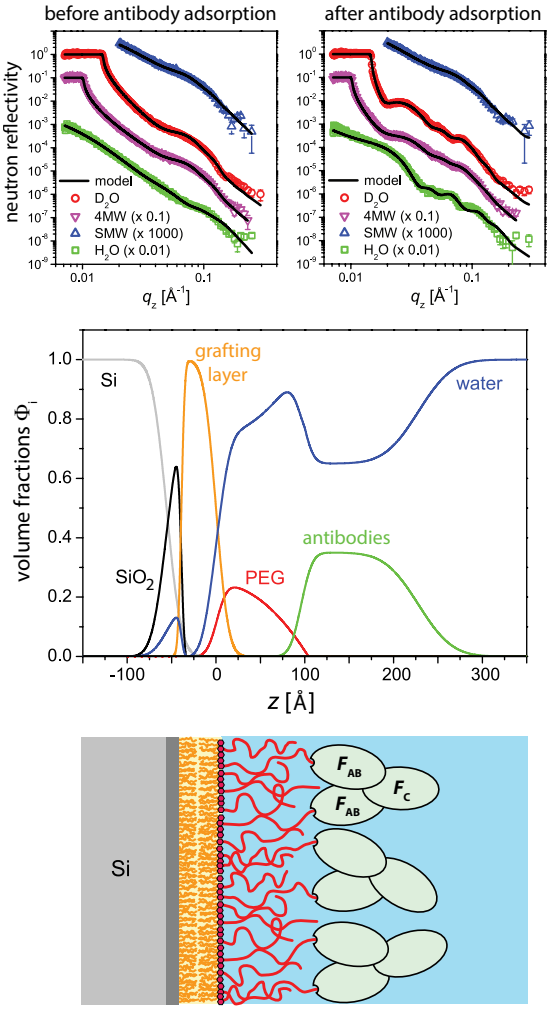
Protein Adsorption to Material Surfaces

Protein adsorption to material surfaces causes problems in medical applications such as implanted biomedical devices (e.g., catheters or stents), as it can promote foreign-body reaction. A common approach to prevent undesired protein adsorption is to functionalize surfaces with soft hydrophilic polymer brushes like poly[ethylene glycol] (PEG). However, the interaction of polymer brushes with proteins is not well understood. In particular, little is known about the mechanisms responsible for regularly observed „brush failure", where protein adsorption arises despite brush functionalization. We have fabricated PEG brushes of well-defined grafting layer chemistry, polymer length, and polymer grafting density, and structurally investigated different modes of undesired protein adsorption using neutron reflectometry with contrast variation. This experimental technique yields matter density profiles perpendicular to the interface with sub-nanometer resolution. Our results obtained after incubation with proteins highlight the importance of the brush parameters and the implications of PEG's reported but often neglected antigenicity **[2].**

Fig. 2 (top) shows a set of reflectivity curves from a PEG brush in aqueous solution before (left) and after (right) incubation with solutions of antiPEG IgG antibodies that can also be found in the human blood. The four curves in each panel correspond to four different "water contrasts" in neutron reflectometry, which are realized by mixing H_2O and D_2O in defined ratios. The adsorption of proteins leads to a number of additional features (in particular minima and maxima) in the reflectivity curves, from which the density profiles of the polymer brushes and adsorbed antibodies were reconstructed with the help of a suitable reflectivity model (solid lines in **Fig. 2** top). The reconstructed protein density profiles (**Fig. 2** middle) showed that the adsorption of antibodies occurred onto the brush itself (**Fig. 2** bottom), an adsorption mode termed "ternary adsorption" in the theoretical literature **[2].** In this configuration the antibodies display their F_c segment to the aqueous phase suggesting that foreign body reaction is promoted.

Depth Localization of Biologically Important Chemical Elements in Molecular Layers

In contrast to specular x-ray and neutron reflectometry, which reveal "global" matter density profiles perpendicular to soft interfaces and which today are widely used techniques, standing-wave X-ray fluorescence (SWXF) allows for the determination of density profiles specifically of chemical elements. The method is based on the standing wave (SW) created above a multilayered solid surface by interference of the



incident x-ray wave with the wave reflected from the periodic multilayers close to the Bragg condition.

Fig. 2: (top) Neutron reflectivity curves from a PEG brush in H_2O and D_2O as well as in H_2O/D_2O mixtures termed 4MW and SMW, before (left) and after (right) incubation with antiPEG IgG antibodies. Solid lines indicate the reflectivity model used to reconstruct the protein density profiles. (middle) Density profiles of antiPEG IgG antibodies (Abs), PEG, and other compounds in the vicinity of the silicon/water interface as reconstructed from the reflectivity curves. (bottom) Cartoon illustrating the interpretation of the density profiles.

During a scan of the angle of incidence Θ across the Bragg peak at Θ_B the maxima of the SW move along the surface normal and induce x-ray fluorescence with element-characteristic energies (see **Fig. 3 A** for a scheme of the experimental setup). The method thus allows reconstructing elemental depth profiles from the angle-dependent characteristic fluorescence.

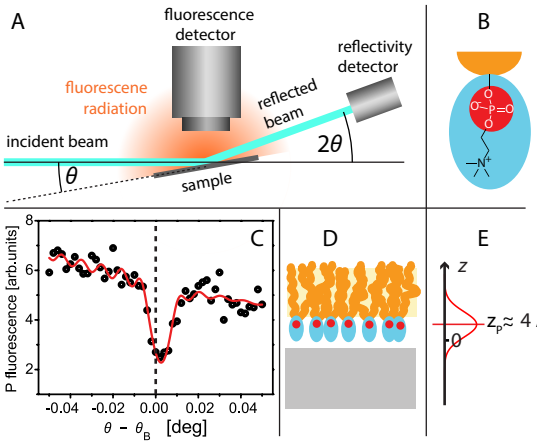


Fig. 3: (A) Scheme of the SWXF experimental setup. (B) Chemical structure of a phospholipid headgroup containing a P atom. (C) Angle-dependent P fluorescence (symbols) from a solid-supported phospholipid monolayer (panel D). Solid line: best matching modeled intensity. (E) Best-matching average height z_P of the P atoms above the solid surface.

While SWXF studies have so far dealt with relatively heavy elements, typically metal ions, as artificial labels for the molecular layers under investigation **[8],** we have made the technique applicable also to the comparatively light elements S and P, which are found in the most abundant classes of biomolecules, for example in the headgroups of phospholipids (**Fig. 3 B**). Our measurements yielded element-specific insight into the architecture of various lipid monolayer architectures and into the conformations of proteins adsorbed to surfaces under various conditions **[5]. Fig. 3 C** exemplarily shows the angle-dependent P fluorescence (symbols) from a solid-supported phospholipid monolayer (**Fig. 3 D**), together with the modeled intensity (solid line) corresponding to the best-matching average height z_P of the P atoms above the solid surface ($z_P \approx 4$ Å, see **Fig. 3 E**). More recently we have used the same approach for interacting model membrane surfaces, composed of lipids and lipopolymers, of which the interaction was adjusted via controlled dehydration **[6].**

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Adsorption of the Protein β-Lactoglobulin at Water/Air and Water/Hexane Interfaces – Effect of Solution pH and Ionic Strength

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In many modern technologies, proteins play an important role. In particular, for the production of various foodstuff, proteins are essential ingredients. For the tailored application of proteins and optimum solution conditions, fundamental knowledge is required. Although proteins do not decrease significantly the surface or interfacial tensions in foams or emulsions but rather the added surfactants, their presence is essential for the stabilization of these liquid colloidal systems. Due to the nature of foams and emulsions, knowledge not only on the equilibrium but also the dynamic interfacial properties of protein adsorption layers is of importance.

The adsorption of proteins at liquid interfaces is a process which does not only depend on the protein's bulk concentration. Due to their nature, protein molecules adsorb at an interface and upon contact with the hydrophobic phase they can change their conformation. These conformational changes can affect also the dynamics of the adsorption process, including the response of the interfaces to mechanic perturbations. The so-called induction time, for example, depends not only on protein bulk concentration but also on the pH and ionic strength of the solution **[1].**

The present work was dedicated to the surface pressure isotherms for BLG solutions at three different pH values (3, 5 and 7), different ionic strengths and at two interfaces: aqueous solution to air (W/A) and to tetradecane (W/TD), respectively. Based on the data of interfacial pressure isotherms, the dynamic surface pressure dependencies $\Pi(t)$ are analysed using a new theoretical approach recently derived in **[2].** The obtained adsorption parameters are discussed in terms of the pH effect and the particular impact of air **[3]** or tetradecane as the adjacent oil phase **[4],** respectively. In addition to the adsorption dynamics mechanism, also the relaxation mechanism due to compression/expansion perturbations was studied in **[3, 5].**

The interfacial tension isotherms of BLG adsorbed at the W/A and W/TD interfaces at the solution pH of 3, 5 and 7 can be well described by a thermodynamic model **[1, 4].** All model parameters obtained by fitting the experimental data to a thermodynamic model are more or less identical for the three pH values, except the surface activity parameter b, which increases with the pH.

When protein molecules adsorb at the interface, they are subjected to conformational changes. Protein molecules first adsorb at the interface in a folded conformation. At low bulk concentrations, they have sufficient space at the interface to unfold. Unfolded protein molecules occupy a much larger interfacial area. Moreover, at water/oil interfaces the hydrophobic parts of the protein molecules have the tendency to penetrate into the oil phase which is supported by the conformational change. The consequence of this changed conformation is taken into account in terms of a change in the adsorption parameter *b* in the corresponding adsorption model:

$$-\frac{\Pi\omega_0}{RT} = \ln(1-\theta) + \theta\left(1-\frac{\omega_0}{\omega}\right) + a\theta^2$$

$$bc = \frac{\omega\Gamma_1}{(1-\theta)^{\omega_1/\omega}} \exp\left(-2a\frac{\omega_1}{\omega}\theta\right)$$

where R is the gas law constant, T is the temperature, ω is the average molar area of adsorbed protein molecules, a is the protein intermolecular interaction parameter, ω_0 is the molar area of a water molecule, c is the subsurface concentration of the protein, and Γ_1 and ω_1 are the "partial" adsorption and molar area of protein in the state with the smallest molar area (native, folded).

The adsorption behaviour generally shows increasing interfacial pressure and dilational elasticity with increasing protein concentration. A comparison of the experimental data and model calculations of the adsorption behaviour of BLG at the W/TD interface with those at the W/A surface is presented in **Figs. 1 and 2.** The interfacial pressure of BLG adsorbed layers at the W/TD interface starts to increase at concentrations many orders of magnitude lower than that for the W/A surface. In addition, the isotherms at the W/A surface are much steeper as compared to the corresponding ones at the W/TD interface. While the adsorption isotherms at the W/A surface reach the critical point of secondary layer formation at rather low protein concentrations, at the W/TD interface the critical points are reached at much higher protein bulk concentrations. In addition, the corresponding interfacial pressure values Π^* at these critical concentrations (kinks in the isotherms) are larger at the W/TD interface than at the W/A surface by almost a factor of three. Hence, one could conclude that the adsorbed amounts of protein at the W/TD interface are much larger than at the W/A surface.

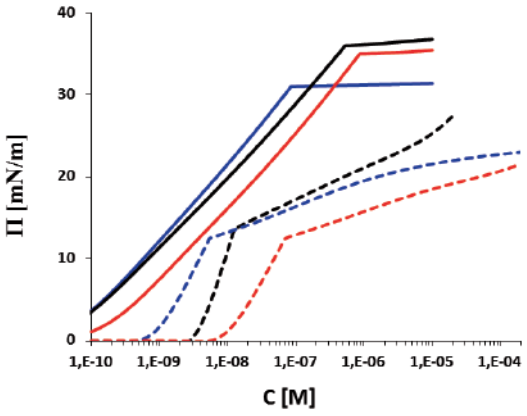

Fig. 1 Experimental interfacial pressure isotherms $\Pi(C_{BLG})$ of BLG at the W/TD (solid lines) interface and at the W/A (dashed lines) surface; blue lines - pH 7, black lines - pH 5, red lines - pH 3.

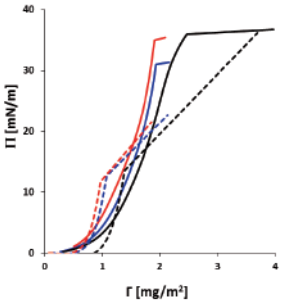

Fig. 2 Calculated dependence of Π as a function of the adsorbed amount Γ of BLG at the W/TD (solid lines) interface and at the W/A (dashed lines) surface; blue lines - pH 7, black lines - pH 5, red lines - pH 3.

However, the corresponding adsorption values Γ shown in **Fig. 3** are only slightly higher and the molar areas shown in **Fig. 4** slightly lower than those calculated for BLG at the W/A surface. Therefore, we must conclude that it is not the total adsorbed amount that leads to the high interfacial pressure values observed at the W/TD interface, but it is caused by the interfacial structure resulting from a strong interaction between the hydrophobic parts of the adsorbed protein molecules and the TD molecules as the oil phase.

Also a new diffusion controlled model to describe the protein adsorption kinetics was proposed to improve the agreement between theory and experiment. The classical diffusion controlled adsorption model with time-independent adsorption activity coefficients, referred to as the TIC model, fails to adequately describe our experimental results. As one can see in **Fig. 5,** the dashed lines calculated for different diffusion coefficients do not adequately describe the experimental data.

In contrast, the new model with a time-dependent (or surface-coverage dependent) adsorption activity coefficient *b(G)*, named as the TDC model, can be successfully applied to the dynamic interfacial tension data measured by drop profile analysis tensiometry PAT. The red line in **Fig. 5** represents an example for the excellent quality of data interpretation.

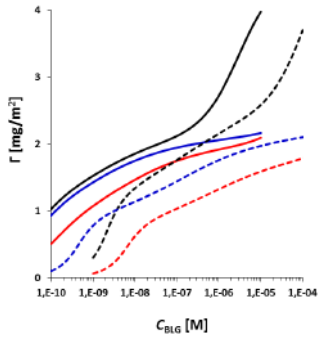

Fig. 3 Calculated dependences of the adsorbed amount on the BLG bulk concentration C_{BLG} at the W/TD (solid lines) interface and at the W/A (dashed lines) surface; blue lines - pH 7, black lines - pH 5, red lines – pH 3.

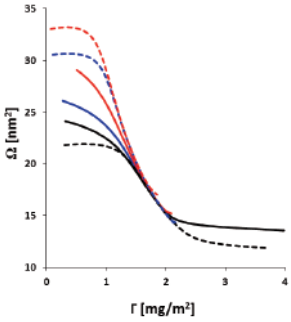

Fig. 4 Calculated dependences of the molar area Ω as a function of the adsorbed amount of BLG at the W/TD (solid lines) interface and at the W/A (dashed lines) surface; blue lines - pH 7, black lines - pH 5, red lines - pH 3.

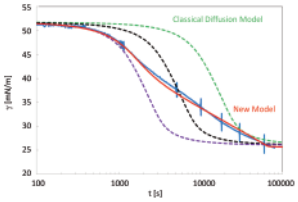

Fig. 5 Dynamic interfacial tension $\gamma(t)$ for a 10^{-7} mol/l BLG solution at pH 3 measured at the W/TD interface; blue curve – experimental data, dashed curves – calculations using the TIC model for different diffusion coefficients, red curve – calculated values using the TDC model and a fixed diffusion coefficient.

The results make clear that the measured dynamic interfacial tensions cannot be properly described by a pure diffusion controlled model. In contrast, the proposed combined model of diffusional transport and an additional time process for conformational changes can describe the experimental data properly. The model assumes that the conformational changes of adsorbed protein molecules can be reflected by changes in the adsorption activity coefficient *b*.

The rate (kinetic) constant k obtained by a best fitting of the experimental data using the proposed TDC model depends on the BLG bulk concentration and on the solution pH. The resulting kinetic rate constant for BLG solutions is the smallest at pH 5 (negligible net charge and compact molecular structure), which physically means that the protein molecules change their conformation at the interface to the smallest extent at these conditions. In contrast, it has the largest values at pH 3 (highest net charge and increased affinity to the adjacent bulk subphases) which means the conformational changes of the proteins are most considerable.

New experiments have been performed at a third interface, the solution surface to air saturated with alkane vapor. The presence of oil molecules adsorbed from the vapor phase, provide a special atmosphere that influences the protein adsorption process tremendously **[6]**. These effects will be further investigated in up-coming experiments.

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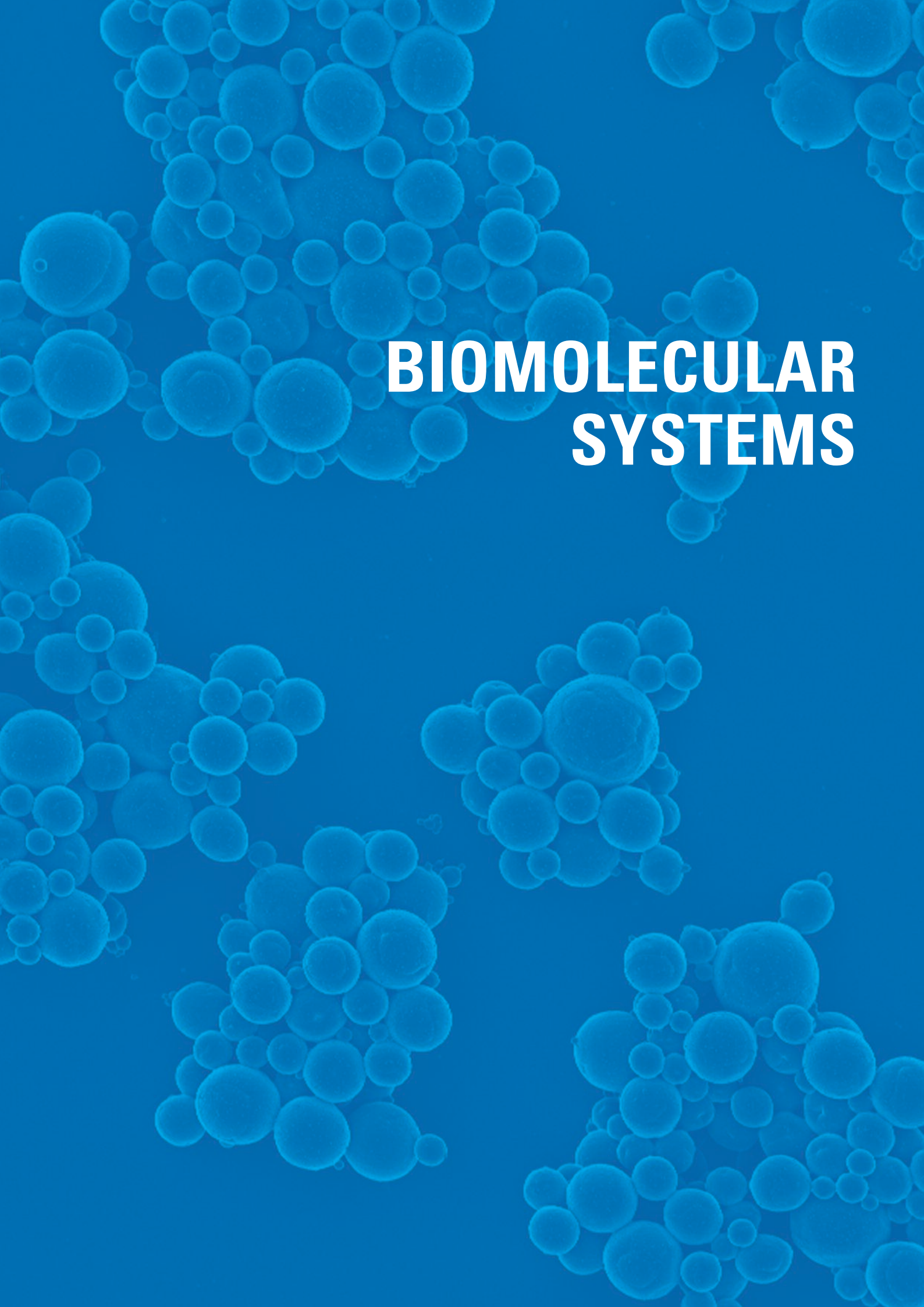
BIOMOLECULAR
SYSTEMS

Research in the Department of Biomolecular Systems

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The Department of Biomolecular Systems conducts research at the *interface of chemistry, engineering, biology, immunology and medicine*. The approach is trans-disciplinary and interactive between the groups in the department that cover different areas of expertise. The core focus are the glycosciences where the development of *synthetic methods* for the automated assembly of defined polysaccharides remains a key interest. The glycans serve as *chemical tools* that aid *biological investigations* into the fundamental roles complex carbohydrates play in biological processes of disease. Carbohydrate arrays are now a routine tool to advance our understanding of *immunological aspects* of various infectious diseases. Insights into how the mammalian immune system recognizes oligosaccharides laid the foundation for *vaccine development* efforts concerned with the glycan portion, novel carriers, and novel modes of presentation to the immune system.

In summer 2015, the department moved finally to the new building in Potsdam to be in close proximity to the other departments. In anticipation of the move the size of the department was reduced by 20% but has now reached steady state again.

In the past two years, three group leaders left the department. Dr. Bernd Lepenies who led the *Glycoimmunology* group for six years accepted a W2 professorship in Hannover in 2015. In the summer of 2015, Dr. Claney Pereira who led the *Vaccine Chemistry* group joined the spin-off company *Vaxxilon* that received €30 Mio in funding as head of research and was joined by six senior postdocs. Dr. Kolarich who had been in charge of the *Glycoproteomics Group* assumed an Associate Professorship at Griffith University (Australia) at the end of 2016.

To build strength on the technology front, Dr. Felix Löffler joined the department in early 2016 and already raised a large BMBF grant to build his *Synthetic Array Technologies* Group. During the past two years three Emmy-Noether Groups were associated with the department: Dr. Christoph Rademacher s group is concerned with questions relating to structural immunology and he received an ERC Starting Grant in 2016. Dr. Fabian Pfrengle has built a strong group concerned with the synthesis and study of plant glycans and Dr. Ursula Neu adds strength in X-ray crystallography studies. On the biophysical front, Prof. Gerald Brezesinski joint our department following his official retirement from the institute to maintain the strength in X-ray studies of glycolipids in membranes.

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. Over the past two years our efforts in creating and understanding novel carbohydrate materials have grown significantly. Fueled by our ability to prepare polysaccharides as large as 50-mers, collaborations with the *Biomaterials Department* as well as the MPI in Stuttgart for structural investigations were set up. Continuous-flow chemistry has benefitted from a close collaboration with the *Colloids Department*. Materials from our colleagues are key catalysts for efficient transformations in the context of the synthesis of active pharmaceutical ingredients.

Automated Synthesis of Carbohydrates

Automated glycan assembly (AGA), our core technology, has reached a new level of sophistication. After the synthesizer as well as most reagents were commercialized via the spin-off company *GlycoUniverse*, we are in the process of developing even better instruments and methods. Most types of linkages are now accessible selectively and using ever shorter coupling cycles that allow for access to polysaccharides as long as 50-mers have been drastically expanded. AGA is now a standard tool to prepare diverse sets of ever longer polysaccharides that enable investigations into new areas of biology as well as material sciences.

Synthetic Tools for Glycobiology

Access to synthetic oligosaccharides has given rise to tools such as glycan microarrays, glycan nanoparticles and radioactively labeled glycans. These tools are now commonly used by the glycobiologists in the department to elucidate fundamental processes such as the entry mechanism of parasites into host cells.

Synthetic Carbohydrate Vaccines

Our long-standing program to develop synthetic carbohydrate vaccines yielded more than ten vaccine conjugates that passed challenge studies in experimental animals. The team produced a host of antigens found on the surface of pathogenic bacteria. A major focus in the past two years was placed on emerging hospital acquired infections. Conjugations of these antigens with carrier proteins and with self-adjuvanting glycolipids performed extremely well in immunological and functional studies in several disease models, particularly in *Streptococcus pneumoniae*. Several glycoconjugate vaccine candidates are being readied for human clinical trials in the spin-off company *Vaxxilon*.

Carbohydrate-based Nanotechnology

The attachment of carbohydrates to the surface of nanoparticles continues also in close collaboration with material scientists and medical researchers from many collaborating laboratories. Silicon nanoparticles equipped with glycans have proven highly attractive and yielded interesting in vivo results.

Glycoimmunology

Several lines of immunological investigations are being pursued. Carbohydrate recognition by C-type lectin receptors influences key functions of dendritic cells such as antigen presentation, cytokine release, and the expression of co-stimulatory molecules. Even after the departure of the Lepenies group this area of investigation is seeing intense study mainly by the Rademacher group. Novel binding partners of CLRs were identified and used as delivery agents into dendritic cells.

The glycan array facility we have established over the past two years is now engaged in investigations into glycan antigens responsible for different types of allergies (*e.g.* meat allergies), autoimmune diseases and adverse responses to carbohydrate-based drugs.

Synthetic Plant Glycans

The Emmy-Noether research group, employs automated glycan assembly and chemo-enzymatic methods for the generation of plant carbohydrate libraries as a powerful means for investigating plant biology. The synthesized plant carbohydrates are applied in the characterization of monoclonal antibodies derived from cell wall polysaccharides and cell wall glycan-deconstructing enzymes. In addition, the polysaccharide fragments are evaluated for their immunostimulatory potential. The synthetic plant carbohydrates will provide a new toolbox for studying the role of carbohydrates in plant biology and their interaction with human health.

Structural Glycobiology Group

The group around Dr. Rademacher has made great progress in fragment-based drug design to develop novel glycan binding protein ligands. Small heterocyclic fragments of drug-like molecules are screened using NMR and SPR-based protocols as well as chemical fragment arrays on solid supports. Actives are identified and evolved to higher affinity ligands. These studies go alongside with virtual screening and molecular modeling techniques to complement our insights and yield a more comprehensive picture of the interaction. Highly interesting ligands have been identified that hold significant promise for pharmaceutical and drug delivery applications.

GPIs and Glycoproteins

Five years ago, the group developed a general synthetic strategy to obtain glycosyl phosphatidyl inositol anchors (GPIs). By using this strategy, GPI molecules from parasites (*T. gondii, T. congolense, T. brucei* and *P. falciparum*) and from mammalian cells have been prepared. The resulting molecules have given rise to diagnostics fort he parasitic disease toxoplasmosis. To create even more complexmolecules, the group is focusing on the synthesis of homogeneous GPI-anchored proteins and glycoproteins. New ligation strategies to conect synthetic GPI-anchors with expressed proteins and methods for the incorporation of carbohydrates into the side chains of peptides and proteins.

Multivalent Interactions

As part of the Collaborative Research Centre (SFB) 765 ("Multivalency as chemical organization and action principle"), we focus on the characterization of carbohydrate-carbohydrate interactions and on the use of multivalent carbohydrate display on graphene surfaces. A method for the selective killing of pathogenic E. coli bacteria was developed. Efforts to employ multivalent carbohydrate-protein interactions for cell-specific targeting and imaging are underway.

Continuous Flow Chemistry

The past two years have seen two major breakthroughs in long-running projects. For one, the automated reaction optimizer was completed and allowed for the reliable and reproducible screening of up to 48 reactions per day. The data obtained using this instrument has provided fundamental insights into the nature of the glycosylation reaction. The modular assembly of complex molecules has yielded several active pharmaceutical substances and has benefitted greatly from the inclusion of novel catalysts obtained from the Colloids Department. Dr. Kerry Gilmore obtained significant funding to expand the group and further deepen the collaboration with the chemical engineering colleagues at the MPI in Magdeburg with a major focus to implement continuous purification methods.

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Automated Glycan Assembly

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The main focus of the Seeberger group since its inception in 1998 has been the development of automated oligosaccharide synthesis. In order to more rapidly procure synthetic glycans as tools for the glycosciences, all aspects of the assembly process have been improved systematically.

Instrument Development

Since 2014 commercial glycan synthesizers (Glyconeer 2.1®) are marketed by the spin-off company *GlycoUniverse*. By now several instruments have been placed in Europe, Asia and North America.

At the same time, the group is continuously improving all aspects of the automation process **[1].** Three homebuilt synthesizers are used to incorporate novel means to more quickly adjust the reaction temperature and to shorten the coupling cycles. The novel designs and improvements are tested in the context of syntheses of complex glycans. The coupling cycles have been shortened from over three hours to about 45 minutes recently to greatly accelerate the assembly of longer sequences.

Rapid Quality Control of Synthetic Oligosaccharides by Ion Mobility-Mass Spectrometry

With a greatly improved AGA, the bottle-neck shifted to glycan analysis and quality control. Methods such as nuclear magnetic resonance spectroscopy, although capable of assigning linkages, requires milligrams of material while mass spectrometry on the other hand can provide information on glycan composition and connectivity even for small amounts of sample, but cannot distinguish stereoisomers. We demonstrated that ion mobility-mass spectrometry (IM-MS), a method that separates molecules according to their mass, charge, size, and shape, can unambiguously identify glycan regio- and stereoisomers.

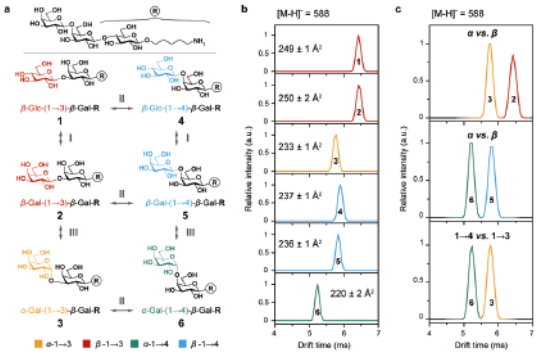

Figure. 1. Structure and IM-MS data of trisaccharides 1-6. (a) The synthetic trisaccharides 1 6 share the same disaccharide core and merely differ in the composition(I), connectivity(II), or configuration(III) of the last monosaccharide building block. (b) IM-MS arrival time distributions of 1-6 as [M-H]- ions. The number corresponds to the estimated CCS in the drift gas nitrogen. Although compositional isomers cannot be distinguished, connectivity and configurational isomers are clearly identified on basis of their CCS. (c) IM-MS arrival time distributions of isomeric mixtures show baseline separation between linkage- and stereoisomers.

Coexisting glycan isomers can be identified and relative concentrations as low as 0.1% of the minor isomer can be detected. In addition, the analysis is fast, requires no derivatisation and only small amounts of sample. IM-MS is an exceptionally effective tool for the structural analysis of complex carbohydrates that should become the standard for glycan characterization **[2].**

Incorporation of Sialic Acid Building Blocks

Over the past three years we have focused on extending the glycospace that can be prepared using automated glycan assembly.

The incorporation of sialic acid units via a sialic acid glycosyl phosphate building block was possible with high α-selectivity **[3].** The combination of automated glycan assembly (AGA) and enzymatic synthesis proved promising as five α(2,3)-sialylated glycans were prepared by rapid and high yielding assembly of the glycan backbones, while a sialyltransferase was used for high yielding and highly regio- and stereoselective sialylations **[4].**

Selective Incorporation of cis-Glycosidic Linkages

Previously, AGA was mainly employed to incorporate trans-glycosidic linkages, where C2 participating protecting groups ensure stereoselective couplings. Stereocontrol during the installation of cis-glycosidic linkages cannot rely on C2-participation and, anomeric mixtures are typically formed. We demonstrated that oligosaccharides containing multiple cis-glycosidic linkages can be prepared efficiently by AGA using monosaccharide building blocks equipped with remote participating protecting groups. The concept was illustrated by the automated syntheses of biologically relevant oligosaccharides bearing various cis-galactosidic and cis-glucosidic linkages.

Improvement of Overall AGA Protocols

After we had improved the automated assembly process in the past few years, a major focus was placed on creating an overall process involving the selection of building blocks all the way to purification and characterization. Using the commercial *Glyconeer 2.1* synthesizer we have been able to work out this.

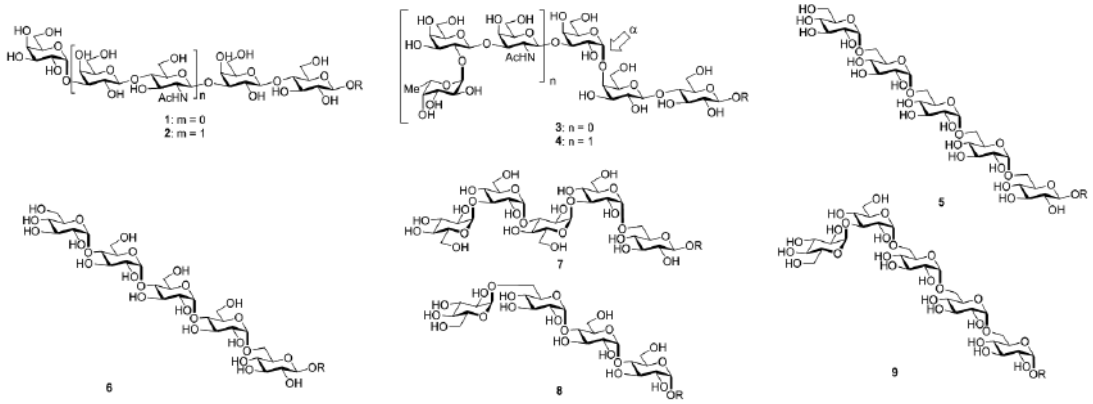

Figure 2. Oligosaccharides (1-9) containing different cis-glycosidic linkages were assembled by automated synthesis. OR = $O(CH_2)_5NH_2$

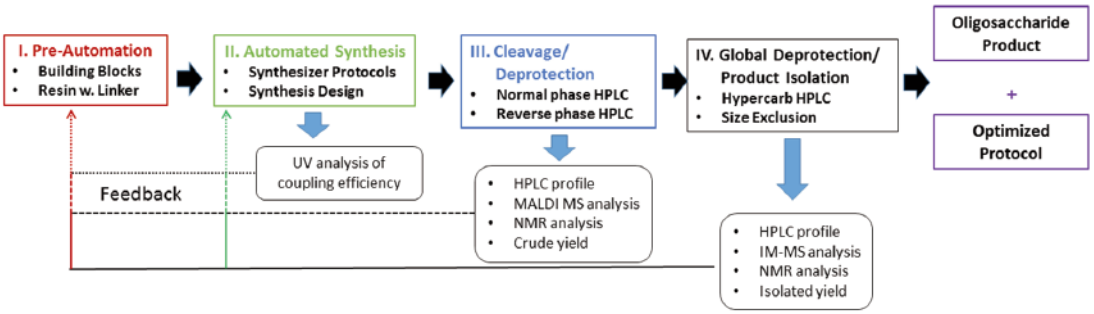

Figure 3. Work-flow for the automated synthesis, purification and analysis of complex glycans ***[13].***

AGA of Different Classes of Glycans

The AGA paradigm was challenged and expanded by assembly of different classes of glycans that served as synthetic tools or vaccine candidates for other groups in the department. Sulfated glycosaminoglycans remained of interest to us and the synthesis of chondroitin sulfate was further advanced **[6].** Streptococcus pneumoniae serotype 3 capsular polysaccharide antigens were prepared to assist the vaccine groups **[7].**The assembly of complex oligosaccharides related to blood group determinants was achieved to provide glycans for glycan array studies **[8].**

Oligo-N-acetyllactosamine glycan probes were prepared by AGA to help characterize adenovirus-glycan interactions as a basis for drug-delivery applications **[10].**

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Controlled Conditions, Controlled Chemistry

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Inarguably, the success of the vast majority of chemical transformations is reliant on the degree of control exhibited over a wide range of variables such as stoichiometry, temperature, reaction time, mixing, and exposure to light. Utilizing flow chemical techniques – where reagents are passed through a set of conditions via thin tubing as opposed to applying conditions to a round bottom flask – has allowed for achieving chemistries and efficiencies previously inaccessible. The modular nature of this technique has also facilitated the development of a novel means of chemical synthesis, which targets core functionalities as opposed to specific molecules, allowing for multiple derivatives to be produced with a single flow system.

At its core, the essential focus of an organic chemist's pursuits is control over molecules – whether this is expressed as regio- or chemoselectivity of functional group transformations, the formation and utilization of reactive intermediates, or precision in reaction conditions. For a number of applications, a significant increase in molecular and environmental (reaction conditions) control can be achieved using flow chemistry. This technique, where reagents are passed through tubing held at a precise set of conditions, is particularly advantageous in high temperature/pressure chemistries, multi-phasic systems (gas/liquid, liquid/liquid), very fast reactions, and photochemistry **[1].**

Flow chemistry is modular in nature, allowing for its components (pumps, mixers, reactors, etc.) to be arranged in any number of combinations. This built-in flexibility has allowed for a wide variety of applications. Recently, our group has utilized this technique to probe two major branches of organic synthesis: methodology (developing new reactions and studying their mechanisms) and multi-step synthesis (continuous and semi-continuous processes to produce active pharmaceutical ingredients (APIs)).

Methodology

Two areas of chemistry which are well suited for flow are the utilization of dangerous reagents and photochemistry. The reasons reactions using dangerous reagents are often converted to continuous flow processes are twofold: the amounts utilized at any one time are smaller due to the smaller volume of the reactor as compared to a batch process and the vastly-greater surface area that allows for excellent heat dissipation for exothermic reactions. One example is our recent work on the alpha-nitration of esters **[2],** where highly caustic fuming nitric acid and sulphuric acid are mixed to create a nitronium ion. By controlling the layout and the speeds which the reagents move through the modular system, this reactive intermediate can be trapped by a range of α-keto esters to give the desired product following treatment with methanol. The same reaction in batch was reported to "eject of the reaction material from the reaction vessel".

The second arena – photochemistry – is better suited for flow chemistry due to the limitations set by the Beer-Lambert Law, which describes the rapid decrease in the intensity of light when penetrating an absorbent medium. As such, by performing photochemistry in reactors thinner than this drop-off point (~1 mm), more rapid and efficient processes can be developed. Photochemistry is also reliant on a molecule being able to absorb light, generally through an extended π-system or a carbon-heteroatom double/triple bond. This limitation can be circumvented through the use of a photocatalyst, which is capable of utilizing photons to drive chemical transformations either through single-electron transfer (SET) processes or through energy transfer.

The first example of SET in flow was shown using a $Ru(bpy)_3$ catalyst **[3].** This simple flow set-up was shown to work for a range of both oxidative and reductive chemistries **(Fig. 1)**. Energy transfer processes nicely showcase the power of flow photochemistry, particularly for the generation of singlet oxygen. This allowed for the rapid examination of a variety of transformations and was utilized to provide the first continuous synthesis of the anti-malarial artemisinin.

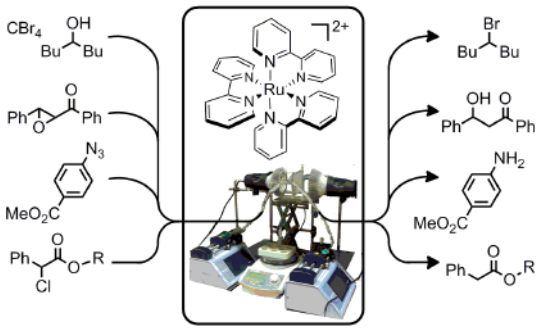

Fig. 1: The versatility of the photocatalytic SET reaction module, accessing both oxidative and reductive transformations.

The advantage of the flexible reactor module is the ability to control the temperature down to –80 °C, allowing for control of reactivity. This is critical in the singlet-oxygen-mediated oxidation of primary amines, where the resultant aldimine is immediately trapped by starting material to give the undesired secondary imine. However, at –50 °C the desired oxidation occurs cleanly, and can be trapped with a cyanide source to give the valuable α-aminonitrile functionality **[4].**

Coupled Modules

Molecular complexity can be quickly added by coupling two reactors together in either a continuous or semi-continuous process. This is advantageous when the product of the first reactor is unstable – as in the case of α-aminonitriles. One value-adding transformation is the hydrolysis of the nitrile portion of the molecule to give α-amino acids, achieved rapidly in flow (40 mins vs 48 h in batch) by reacting a concentrated HCl solution above its boiling point under pressure. A gas-liquid reactor can be exchanged for the HCl unit, allowing for carbon dioxide to react with the α-aminonitrile to give heterocycles called hydantoins **(Fig. 2) [5].**

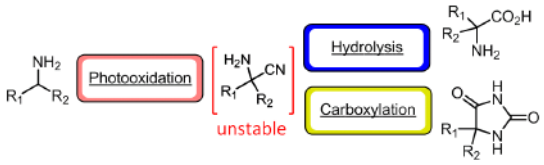

Figure 2: By coupling reaction modules together, molecular complexity can quickly be increased.

Target-Oriented Synthesis

Coupled reactors can also be used to design processes towards the synthesis of valuable small molecules such as APIs. For example, using precise control over reaction times, an ortho-lithiation of 1,4-dichlorobenzene using n-BuLi was achieved. This reactive intermediate was subsequently trapped by an acylating agent, and this serves as the first step in the shortest-ever (3 steps) semi-continuous synthesis of the HIV medicine Efaverinz **[6].**

Core-Functionality Targeted Synthesis

While processes can be developed to synthesize specific molecules, there exist a number of high-value molecules and APIs which share the same core functionalities. By coupling flexible, chemoselective reaction modules together it is possible that a multistep process can be created which targets structural cores – independent of the pendent functionalities. As these reaction modules are not dependent on the preceding or succeeding reactions, they can be interchanged to access different structural cores. This allows for an assembly-line approach to organic synthesis.

These chemical assembly lines can be arranged in in either a divergent or convergent manner. The first example is the extension of the artemisinin synthesis to yield all artemisinin-derivatives which serve as the WHO-recommended first-line treatments for Malaria. This three module process was further extended to include continuous purification, producing >99.5% pure material **(Fig. 3) [7]**.

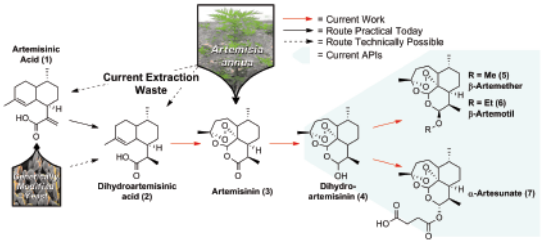

Figure 3: A divergent process accessing all four anti-malarial artemisinin derivatives.

The power of this approach was showcased in a series of publications utilizing a pool of eight reaction modules **(Fig 4) [8,9]**. These modules were arranged in divergent and convergent processes to produce five different structural cores and ten different active pharmaceutical ingredients. No intermediate purifications were used for any of the developed processes.

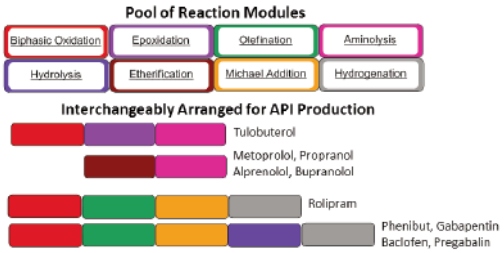

Fig. 4: A pool of reaction modules were utilized interchangeably to access five different structural cores and ten different APIs.

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The Glycome Represents a Largely Unmined Source for Disease Markers

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Cell surface and body fluid proteins are extensively modified with specific sugar moieties, so called glycans. These glycans build the basis for a universal language cells use to communicate, but it is also abused by cancer cells through specific glycosignature modifications. Though all cells in the body share one alphabet, different organs use different dialects, manifested by the individual glycosignatures that cells impose on the proteins they express. Changes in protein glycosylation are also a universal hallmark of cancer and in several examples, such as hepatocellular carcinoma, specific glycosignatures are already being applied in the clinic to improve diagnostic sensitivity and selectivity (**Fig. 1**) **[1].** However, to date the full potential embedded in glycosignatures to detect, subtype, classify and grade different types of cancer has not been exploited to its full potential. This has also been due to technical limitations hampering accurate translation of these glyco-languages from limited amounts of available clinical tissue specimens. We have recently overcome these issues and developed highly sensitive and selective glycomics tools that enable us now to translate these dialects from formalin-fixed, paraffin embedded (FFPE) histopathological slides providing hitherto unprecedented insights into disease specific glycosignatures from minimal amounts of clinical material **[2].**

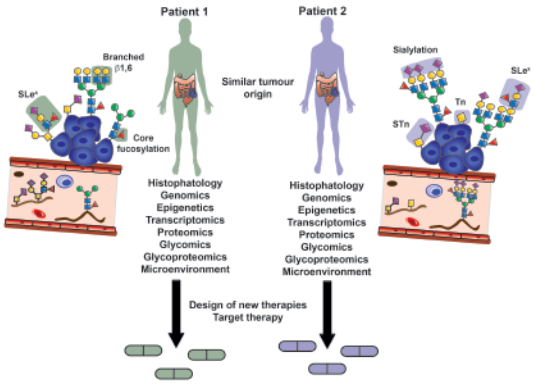

Fig. 1. Glycosylation signatures provide a global reflection on an individual's health/disease status and can function as predictive indicators for treatment success. A combination of different -omics strategies including glycomics & glycoproteomics will be essential for improving diagnosis and treatment personalisation. Figure taken from Almeida & Kolarich, BBA 2016 ***[1].***

The Technology behind PGC-nanoLC ESI-MS/MS Glycomics

Porous Graphitized Carbon nano Liquid Chromatography Electrospray Ionisation Tandem Mass Spectrometry (PGC-nanoLC ESI-MS/MS) based glycomics is a highly selective and sensitive technology that enables an exact glycan sequencing. Glycan structures are built up by similar building blocks, but in contrast to e.g. peptide or DNA oligomers there are numerous possibilities how these different glycan building blocks are linked to each other. The type of linkage and its position, however, influence the biological properties of glycoconjugates. Our technologies thus provide a key asset to sequence these molecules to better understand their functional relevance.

Many of these glycoconjugates exhibit an exact similar chemical composition, making it difficult to separate and distinguish them by simple tandem Mass Spectrometry (MS/MS) approaches. Within the glycoproteomics group we have been combining the selectivity benefits provided by PGC-LC ESI MS/MS detection to separate, detect, characterise and relatively quantify such isobaric structure compounds (**Fig. 2**) **[2].**

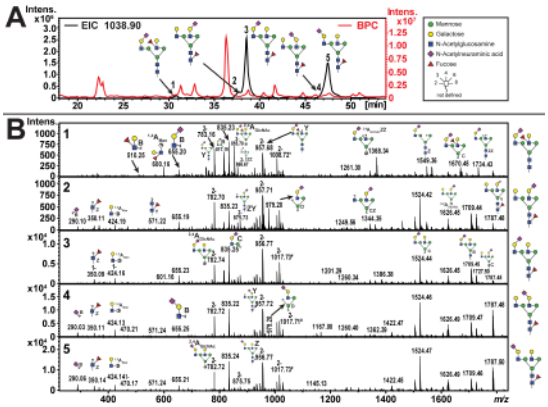

Fig. 2: Example for structure identification using PGC nano LC-ESI MS/MS. A: Base peak chromatogram (BPC, red trace) representing the N*-glycome obtained from FFPE preserved hepatic tissue. Extracted ion chromatogram (EIC, black trace) of an example* N*-glycan (Hex5HexNAc4NeuAcFuc, [M-2H]$^{2-}$ = 1038.9 Da) that is present in five different structure isomers. B: Individual product-ion spectra of the five Hex5HexNAc4NeuAcFuc isomers enabling differentiation and relative quantitation of the various N-glycan isomers. Figure taken from Hinneburg et al., MCP 2017* ***[2].***

FFPE Histopathological Tissue Slides can now be Used as a Source for Clinical Glycomics [2]

N- and *O*-glycans are attractive clinical biomarkers as glycosylation changes in response to diseases. The limited availability of defined clinical specimens impedes glyco-biomarker identification and validation in large patient cohorts. FFPE clinical specimens are the common form of sample preservation in clinical pathology, but qualitative and quantitative *N*- and *O*-glycomics of such samples has not been feasible to date. We have developed a novel approach to isolate and analyse the *N*- and *O*-glycome of FFPE clinical specimens that now allows a highly sensitive and glycan isomer selective characterisation of *N*- and *O*-glycans from histopathological slides. As few as 2000 cells isolated from FFPE tissue sections by laser capture microdissection were sufficient for in-depth histopathology-glycomics using porous graphitized carbon nanoLC ESI-MS/MS (**Fig. 3**). *N*- and *O*-glycan profiles

were similar between unstanined, hematoxylin and eosin stained FFPE samples but differed slightly compared with fresh tissue. With this method in hand we are now systematically investigating cancer glyco-biomarkers from FFPE histopathological tissues slides archived in pathology laboratories worldwide. The ability to investigate the differential glycome of disease and non-disease tissue of the very same patient from isolated tissues provides now unprecedented insights into disease associated glycan signatures.

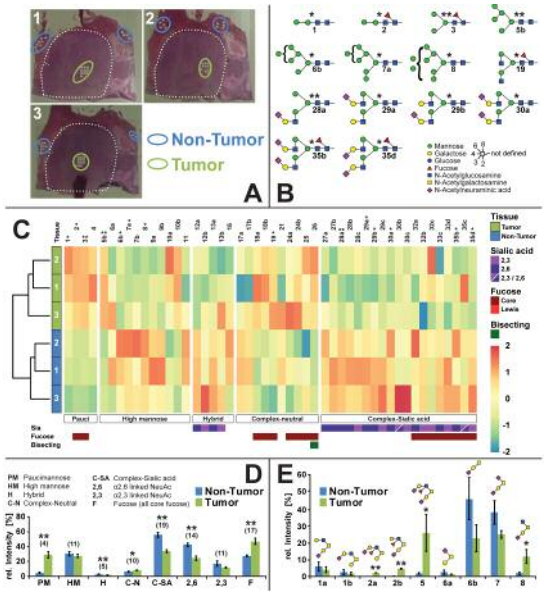

Fig. 3: N- *and* O*-glycome of hepatocellular carcinoma (HCC) and non-cancer hepatic tissue (NC). A: Representative image of FFPE preserved tissue sections of HCC used for isolation of HCC cells and surrounding non-cancerous tissue by laser capture microdissection. B:* N*-glycan structures exhibiting the largest expression level changes between HCC and NC tissue. C: Heat map obtained after unsupervised hierarchical clustering of the* N*-glycans detected from 2000 cells of HCC and NC hepatic tissue and sorted according to major structure categories, clearly showing the global changes present in the cancer cell* N*-glycome. D: Category comparison of the HCC and NC* N*-glycomes. The number of structures in each category is indicated above bars. E: Comparison of HCC and NC* O*-glycomes obtained from the very same material the* N*-glycomes were obtained. Sialyl Lewis X epitopes present on core 2 type* O*-glycans show a significant increase in HCC tissue, whereas core 1 type* O*-glycan levels are reduced. Figure taken from Hinneburg et al., MCP 2017* ***[2].***

Middle-down Glycoproteomics Uncovers the Specific Sites Preferred when Chemically Glycosylating Vaccine Proteins [3]

Production of glycoconjugate vaccines involves the chemical conjugation of glycans to an immunogenic carrier protein such as Cross-Reactive-Material-197 (CRM197). Instead of using glycans from natural sources recent vaccine development has been focusing on the use of synthetically defined minimal epitopes. While the glycan is structurally defined, the attachment sites on the protein are not. Fully characterized conjugates and batch-to-batch comparisons are the key to eventually create completely defined conjugates. We used a variety of mass spectrometric techniques to identify and characterise the specific sites modified during the conjugation process, showing that specific sites are preferred during the conjugation process. In particular regions close to the N- and C-termini were most efficiently conjugated (**Fig. 4**). These results help to ensure production consistency and provide better and safer products for the next generation of defined glycoconjugates vaccines **[3].**

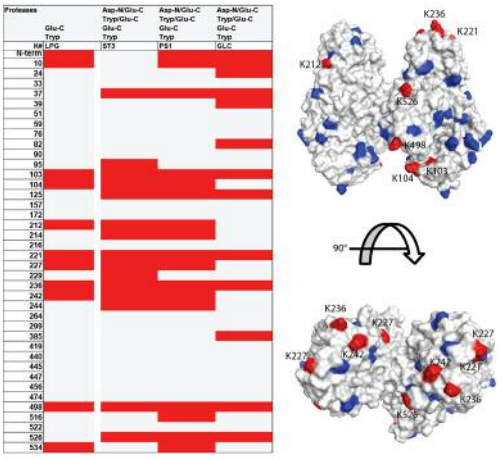

Fig. 4: Left: Heatmap showing the preferred lysine residues sites of CRM197 that are modified by chemical glycosylation (red). Right: 3D crystal structure of CRM197 dimer (PDB entry: 4AE0). Lysine residues are labelled blue. Lysine residues that were frequently found conjugated with a glycan in all the samples are labelled in red. Figure taken from Moginger et al., SciRep 2016 ***[3].***

In January 2017 the glycoproteomics group relocated to the Institute for Glycomics at Griffith University, Queensland, Australia

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C-type Lectin Receptors – from Glycan Arrays to Murine Models

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A main research focus of the Glycoimmunology group has been on pattern recognition receptors (PRRs) in innate immunity. PRRs recognize evolutionarily conserved pathogen- or danger-associated molecular patterns. They are predominantly expressed by cells of the innate immune system and provide a first line of defense in the body. Since PRRs trigger endocytosis and may also provoke signaling pathways that impact antigen presentation, the expression of co-stimulatory molecules, and cytokine production, PRRs are often essential to activate adaptive immune responses **(Fig. 1)**.

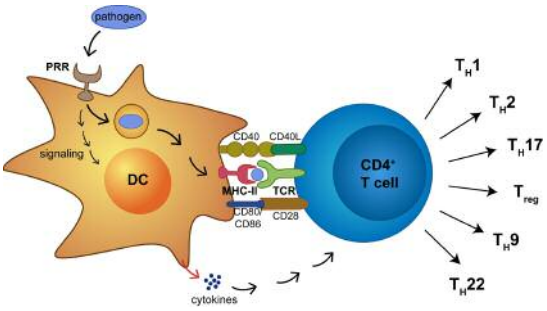

Fig. 1: Pattern recognition receptors (PRR) expressed by cells of the innate immune system such as dendritic cells (DC) bind to conserved pathogen-associated molecular patterns. This may lead to receptor-mediated endocytosis, antigen processing and presentation by major histocompatibility complex (MHC) molecules to T cells. In addition, signaling pathways are induced in DCs that induce the expression of the co-stimulatory molecules CD80/CD86 as well as cytokine production. Thus, subsequent T cell activation and differentiation may be influenced by signaling via PRRs. Figure designed by Dr. Julia Hütter.

Lectins represent a class of PRRs that are specialized to recognize glycan structures on pathogens and self-antigens. The Glycoimmunology group has been particularly interested in a large lectin superfamily called C-type lectin receptors (CLRs). CLRs often recognize carbohydrates in a Ca^{2+}-dependent manner and contribute to immunity by triggering a variety of cellular functions including antimicrobial responses, cytokine secretion, dendritic cell (DC) maturation, phagocytosis, antigen presentation, and T cell activation. Since some CLRs activate cellular functions whereas others inhibit intracellular signaling pathways, CLRs may be involved in both immune stimulation and immune suppression, thus they are promising targets for immune modulatory therapies **[1,2] (Fig. 2).**

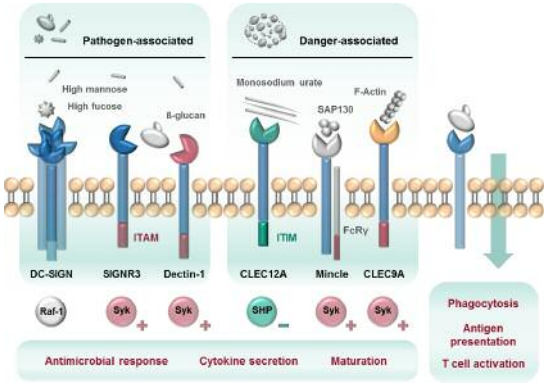

Fig. 2: Myeloid C-type lectin receptors (CLRs) in innate immunity. CLRs such as DC-SIGN, SIGNR3, Dectin-1, CLEC12A, Mincle, CLEC9A, among others, recognize pathogen- and also danger-associated molecular patterns. CLR ligation may trigger a variety of cellular functions including antimicrobial responses, cytokine secretion, phagocytosis, antigen presentation, and T cell activation. While some CLRs act as activatory receptors and stimulate cellular responses, others serve as inhibitory receptors, thus dampen immune responses. Figure designed by Dr. Timo Johannssen.

During the past years, we have generated and continuously extended a comprehensive library of CLR-Fc fusion proteins to identify yet unknown CLR ligands on pathogens and in libraries of synthetic glycans using ELISA-based methods, lectin arrays, and the glycan array technology. To this end, the extracellular part of the respective mouse CLR containing the carbohydrate recognition domain (CRD) was fused to the Fc fragment of human IgG1 molecules. The dimeric CLR-Fc fusion proteins were then transiently expressed in Chinese hamster ovary (CHO) cells, purified from the culture supernatant and used for comparative screenings.

A main focus has been on the role of innate immunity and in particular CLRs during infections **[3,4]**. With the help of the established CLR-Fc library, several previously unknown CLR ligands on bacterial pathogens or microbiota could be identified **[4,5]**. In one study, the CLR Macrophage-inducible C-type lectin (Mincle) was shown to bind to *Streptococcus pneumonia* in a Ca^{2+}-dependent, serotype-specific manner. Mechanistic studies using different Mincle-expressing cells as well as Mincle-deficient mice revealed a limited role of Mincle in bacterial phagocytosis, neutrophil-mediated killing, cytokine production, and antibacterial immune response during pneumonia **[4]**. However, this study demonstrates the utility of the generated CLR-Fc library to screen for novel CLR ligands on pathogens **(Fig. 3).**

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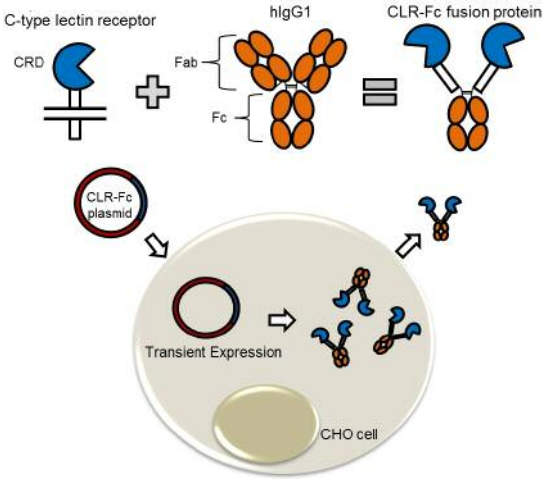

Fig. 3: Generation of the CLR-Fc fusion protein library. The extracellular part of the respective mouse CLR containing the carbohydrate recognition domain (CRD) is fused to the Fc fragment of human IgG1 molecules rendering dimeric CLR-Fc fusion proteins. They are transiently expressed in Chinese hamster ovary (CHO) cells and then purified from the culture supernatant. Figure designed by Joao Monteiro.

CLR Targeting for Drug and Vaccine Delivery

Since antigen targeting to DCs is a promising strategy to enhance the efficacy of vaccines, DC-expressed CLRs are attractive targets for cell-specific vaccine delivery. In addition, CLR targeting may be a means to enhance antigen presentation to T cells, thus promotes subsequent T cell activation. Numerous studies have focused on antibody-mediated CLR targeting, whereas glycan-based targeting approaches have only gained increasing attention during the last years. In fact, multivalent display of glycan CLR ligands on suitable carrier systems such as nanoparticles, dendrimers, polymers, or liposomes may have some advantages compared to antibody-mediated CLR targeting due to the easy tunability of ligand density and their spatial orientation on the carrier. Thus, glycan-based CLR targeting may indeed be a promising approach to manipulate cellular functions effectively **[6-8]**. Furthermore, various glycan ligands can be presented on one carrier to allow for targeting of different CLRs simultaneously. Interestingly, small structural glycan modifications have a marked impact on CLR binding, CLR-mediated endocytosis, and subsequent T cell activation. In a recent proof-of-principle study, glycoproteins displaying different biantennary *N*-glycans were analyzed for their binding to the previously established CLR-Fc fusion protein library **[6]**. Although both *N*-glycans only differed in the presence of an O-2 core xylosylation, they exhibited differential binding to selected CLRs which impacted targeting and uptake of the glycoproteins by DCs and also affected T cell activation in a DC/T cell co-cultivation assay. On the one hand, this study shows the utility of glycan-based DC targeting, but on the other hand it also highlights the marked impact of small differences in glycan structures on the targeting efficacy. Thus, glycan ligands of CLRs have to be tested in appropriate cell culture assays and *in vivo* models in order to evaluate their utility for targeted therapy and/or immune modulation **(Fig. 4)**.

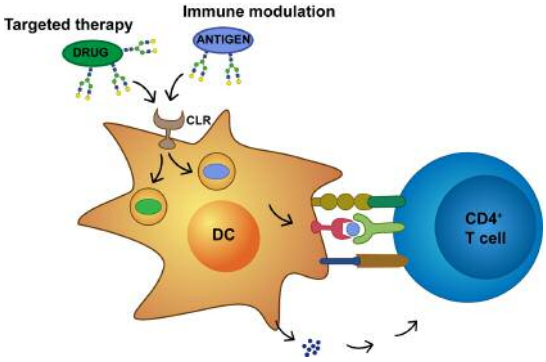

Fig. 4: Targeting of C-type lectin receptors (CLR) is a means to shape initiated immune responses. CLRs can be exploited for cell-specific drug and vaccine delivery into CLR-expressing cells such as dendritic cells (DC). Furthermore, signaling pathways may be provoked by CLR targeting that affect the expression of co-stimulatory molecules and cytokine production. As a consequence, T cell activation and differentiation may be influenced by CLR-mediated signaling. Thus, CLR targeting is a promising strategy to modulate immune responses. Figure designed by Dr. Julia Hütter.

Carbohydrate-carbohydrate Interactions

Glycan–lectin interactions are generally weak, thus multivalent binding is often crucial to exert biological effects. However, carbohydrate–carbohydrate interactions are even of ultralow affinity and are often difficult to detect. They are considered to be relevant during early embryogenesis as well as during the initial adhesion of melanoma cells to the endothelium thus contributing to metastasis formation. To analyze the function of carbohydrate–carbohydrate interactions more in depth, carbohydrate-capped silicon nanoparticles were used to measure the interaction between the cancer-associated glycosphingolipids GM3 and Gg3 **[10]**. Surface plasmon resonance experiments were performed to determine the binding affinity and cell binding studies revealed the relevance of this model carbohydrate–carbohydrate interaction *in vitro*. Thus, carbohydrate-capped silicon nanoparticles are useful tools for cell imaging and targeting and can be employed to analyze carbohydrate interactions of ultralow affinity in biophysical as well as cell biology studies.

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BIOMOLECULAR SYSTEMS

Synthetic Plant Carbohydrates

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Carbohydrates play crucial roles in the life cycle of plants, both as structural components and as important players in signaling events and energy provision **[1]**. As a food source, plant carbohydrates can provide beneficial effects on the human immune system, but constitute also abundant immune determinants on allergens. Despite the strong impact of plant carbohydrates on human health, their chemical synthesis remains largely unexplored compared to the synthesis of mammalian and bacterial glycans. Our aim is to explore automated oligosaccharide synthesis **[2]** and chemo-enzymatic methods **[3]** for the generation of plant carbohydrate libraries as a powerful means for investigating their application in plant biology and biomedical research. The synthesized plant carbohydrates are applied in the characterization of monoclonal antibodies derived from cell wall polysaccharides and cell wall glycan-deconstructing enzymes. In addition, the polysaccharide fragments are evaluated for their immunostimulatory potential. Together, the synthetic plant carbohydrates will provide a new toolbox for studying the role of carbohydrates in plant biology and their interaction with human health.

Automated Glycan Assembly of Plant Cell Wall Oligosaccharides

Automated glycan assembly is a technology that was introduced by Prof. Peter H. Seeberger in 2001 **[4]**. Using this technology, rapid access to collections of defined oligosaccharides is provided. We recently assembled structurally related fragments of different plant cell wall polysaccharide classes from a few monosaccharide building blocks **(Fig. 1) [5-8]**. These synthetic glycans were applied in the characterization of cell wall glycan-directed antibodies and cell wall-degrading enzymes.

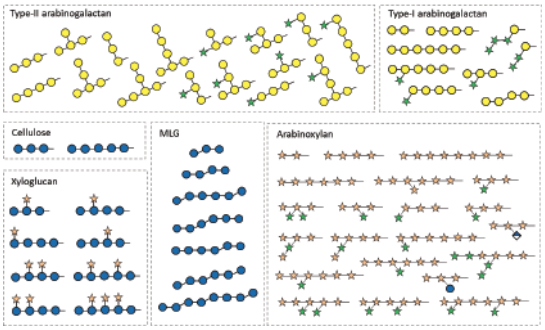

Fig. 1: Synthetic plant carbohydrates produced by automated glycan assembly.

Characterization of Cell Wall Glycan-Directed Antibodies with Synthetic Plant Carbohydrates

A large amount of plant carbohydrates are located in the cell wall, which consists of a complex mixture of polysaccharides and other biopolymers assembled into a highly organized network that surrounds all cells. Many genes responsible for the biosynthesis of cell wall polysaccharides have been identified and detailed insight into the structure and function of plant cell wall polymers has been gained by high resolution imaging of cell wall microstructures **[9]**. Monoclonal antibodies directed toward plant polysaccharide antigens are used by plant biologists as powerful molecular probes to detect the structural elements of glycans in the cell wall. However, the precise molecular structures recognized by the antibodies are unknown. The goal of the project is to synthesize plant carbohydrate libraries for a comprehensive epitope mapping of monoclonal antibodies.

One of the main components of plant cell wall polysaccharides is the hemicellulose xylan, the second most abundant polysaccharide in nature. Xylans are dietary carbohydrates in everyday food that can provide medicinal benefits including immunomodulatory, anti-tumor, and anti-microbial effects. In addition, xylans are potential resources for the production of food additives, cosmetics, and biofuels. Although the structure of xylans varies between plant species, they all possess a common backbone consisting of b-1,4-linked D-xylopyranoses. This backbone structure may be partially acetylated and substituted with L-arabinofuranosyl or D-(4-O-methyl) glucuronyl residues.

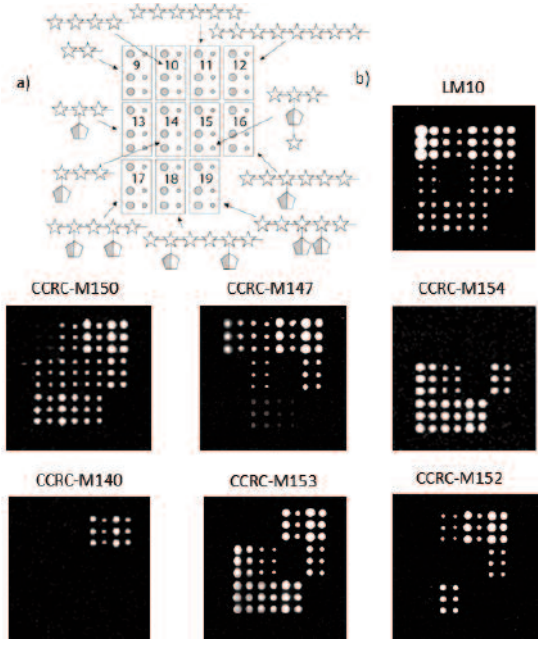

Fig. 2: Detection of oligoarabinoxylans by anti-xylan monoclonal antibodies (mAb): a) Printing pattern; b) Microarray scans. Representative scans of at least two independent experiments are shown. The intensity of the spots corresponds to the binding affinity of the respective mAb.

We produced a library of eleven oligoarabinoxylans of different complexity by automated solid-phase synthesis and printed the compounds as microarrays for probing a set of 31 anti-xylan monoclonal antibodies. We observed specific binding of the antibodies to the synthetic oligoarabinoxylans and the binding epitopes of several antibodies were characterized **(Fig. 2)**. This work will serve as a starting point for future studies where libraries of synthetic plant oligosaccharides are screened for the binding of cell wall glycan-directed antibodies, generating the essential information required for interpretation of immunolabeling studies of plant cell walls.

Active Site-mapping of Cell Wall-Degrading Enzymes Using Synthetic Plant Carbohydrates

Cell wall-degrading enzymes are essential in a variety of processes such as biomass conversion into fuels and chemicals and the digestion of dietary fiber in the human intestinal tract. We used synthetic plant carbohydrates to gain further insight into these enzymes by incubating the glycans with various glycosyl hydrolases followed by analyzing the digestion products by HPLC-MS. Synthetic arabinogalactan oligosaccharides enabled us for instance to determine the binding specificities of endo-galactanases **(Fig. 3)**. We discovered that the endo-galactanases recognize and hydrolyze arabinogalactan oligosaccharides of different lengths and arabinose substitution patterns.

Evaluation of the Synthesized Polysaccharide Fragments for their Potential as Immunomodulators

Plant cell wall polysaccharides are important dietary carbohydrates in everyday food such as fruits and cereals. They are believed to exhibit beneficial therapeutic properties through modulation of innate immunity **[10]**, but the molecular basis of their interaction with immune receptors remains largely unknown. We will evaluate synthetic polysaccharide fragments for their potential to stimulate immune cells. A long-term objective of the study is the identification of specific binding epitopes on immunomodulatory polysaccharides and of the receptors responsible for their recognition.

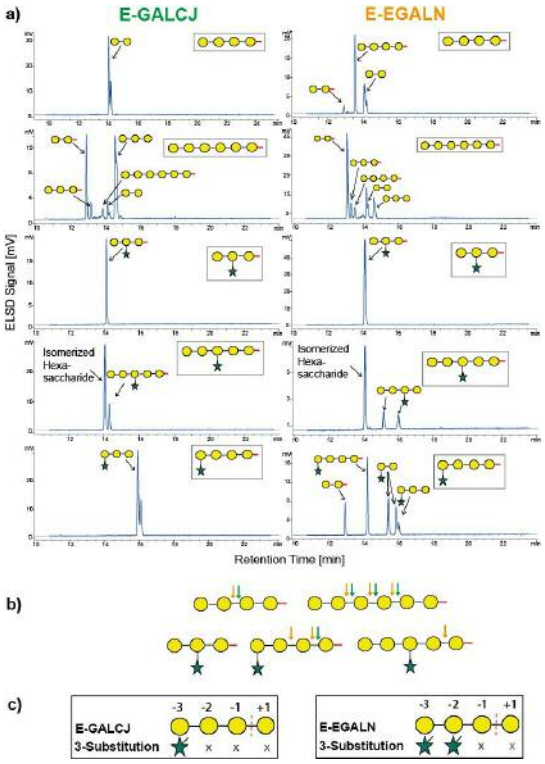

Fig. 3: Digestion of synthetic arabinogalactan oligosaccharides with the endo-galactanases E-GALCJ and E-EGALN and analysis of the resulting hydrolysis products by HPLC-MS. (a) HPLC analysis of the products after incubation of the respective oligosaccharides with the galactanases. (b) The cutting sites derived from (a) are summarized and indicated by arrows. (c) General requirements for arabinose substitutions relative to the cutting site of the galactanases. "X" denotes galactose residues that must not be substituted with arabinofuranose.

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Ligand-based Targeted Delivery to C-type Lectin Receptors

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Many pharmaceuticals are administered systemically and act on the diseased as well as on the healthy tissue. To reduce dosing and consequently the risk for side-effects, it would be highly desirable to enable tissue- or even cell-type specific delivery of pharmaceuticals. In particular, the specific modulation of immune cells in cancer immunotherapy has become an attractive route. To enable a cell-specific delivery of immunomodulatory agents, immune cell receptors have been identified as excellent entry points into these cells. More precisely, carbohydrate binding receptors, such as C-type lectins expressed on myeloid cells of the innate immune system, emerged as a prime target receptors. These receptors have a narrow expression pattern and promote uptake and processing of a variety of antigens. Classically, these receptors have been addressed using antibody-based delivery approaches. Stimulants are conjugated to an anti-lectin antibody and following injection, these antibodies deliver their payload to a defined subset of immune cells ultimately activating the immune system. Alternatively, carbohydrate ligands have been applied to enable uptake of nanoparticles making use of the pattern recognition function of these C-type lectin receptors. Glycosylated, particulate antigens are recognized by these lectins and initiate uptake and processing. Unfortunately, mammalian carbohydrate binding proteins typically bind their ligands with low affinity and the specificity for simple carbohydrates is often limited. Consequently, synthetic molecules mimicking the carbohydrate scaffolds may provide higher affinity and selectivity.

The development these so-called glycomimetics as targeting ligands to enable targeted delivery to cells of the innate immune system has been the prime goal of our research efforts and will be described in the following.

Druggability Assessment of C-Type Lectins

Before embarking on a small molecule discovery campaign, it is important to estimate the potential of the targeted receptor to interact with small drug-like molecules. This so-called druggability assessment can be conducted using several methods. First, computational techniques have been quite popular using pocket detection algorithms to find and score suitable binding sites available on protein crystal structures. We performed such analysis using DoGSiteScorer, analysing a larger panel of C-type lectins **[1]**. We concluded that the vast majority of these targets should be considered either challenging or undruggable owing to their shallow and hydrophilic binding sites.

In contrast, experimental druggability assessment of a set of C-type lectins using NMR-based fragment screening suggested the opposite **[1]**. Here, we applied ^{19}F NMR, as it is a sensitive method with limited sample consumption. A high portion of fragments bound to the lectins and strongly suggested these C-type lectins are druggable.

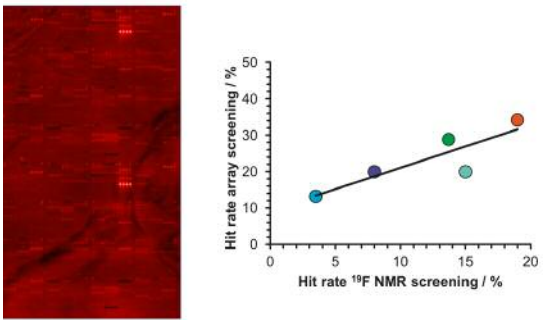

Fig. 1: Druggability assessment of C-type lectin receptors using chemical fragment arrays. Fragments of drug-like molecules were immobilised on a glass slide and probed with fluorescently labelled proteins (left). These data correlated well with previous findings of moderate to high hit rates for several protein targets including three C-type lectins (right). ***[1, 2].***

To further our insight into the druggability of C-type lectins, we developed so-called chemical fragment arrays. Small droplets containing fragments of are spotted on the surface of a glass slide and UV-activated, which led to covalent immobilisation of the fragment to the array **[2]**. Fluorescently labelled, multimeric and monomeric C-type lectin receptors bound to the immobilized fragments. As a result, the hit rates correlate with those found previously by ^{19}F NMR [1], which suggests that this fragment array method is well suited for druggability assessment with 1000-fold reduced protein consumption compare to NMR. Overall, these data suggested again a medium to high druggability of C-type lectins and initiated further research into the identification of targeting ligands.

Identification of Potential Targeting Ligands for Human Langerin

Experimental data from ^{19}F NMR and chemical fragment array screening during the druggability assessment provided enough evidence to continue our efforts to find targeting ligands for the human C-type lectin Langerin **[1, 2]**. For this, a suitable assay system had to be developed to guide the design process as the requirements for the identification of glycomimetic ligands for mammalian lectins are as follows: (i) a homogeneous assay is necessary, devoid of any washing steps as these might be too harsh and reduce reproducibility, (ii) such an assay has to provide binding site information, otherwise ligands binding to irrelevant sites might be identified, and (iii) the assay would preferentially yield thermodynamic information with high sensitivity. To this end, we have developed a ^{19}F NMR reporter displacement assay **[3]**. Here, a trifluoroacetamido mannose served as a sensitive reporter to probe for binding and competition with potential glycomimetics.

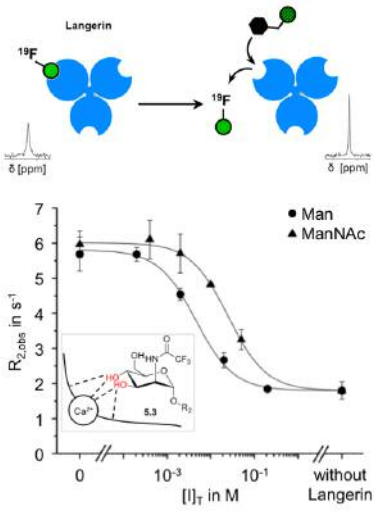

Fig. 2: ^{19}F NMR-based reporter displacement assay. Increased R_2 relaxation of a trifluoro group is measured upon binding to the C-type lectin Langerin. If the trifluoroacetamido mannose is displaced from the binding site by a competitor the R_2 relaxation decreases again. Titration studies using competitors yield thermodynamic inhibition constants. ***[3].***

Using this assay, two orthogonal screenings were conducted. First, an *in silico* screening was performed that evaluated a library of commercially available building blocks to increase the affinity of an existing carbohydrate ligand in the binding site of Langerin. Based on these insights, a selected panel of mannose derivatives was synthesized and tested. Ligands with 36-fold higher affinity than the natural ligand were identified. Second, 290 fragments were screened in cocktails of five and a fragment was identified to block the Langerin recognition site with millimolar affinity **[3]**.

An Allosteric Network Modulates the Calcium Affinity of Langerin

While the experimental druggability assessment suggested the availability of serval pockets that can harbour small molecule modulators of Langerin, our computational analysis did not **[1-3]**. Hence, we investigated the dynamics of the human Langerin **[4]**. Here, we focused on the molecular determinants of the affinity of Langerin for its cofactor Ca^{2+}. We expressed the carbohydrate recognition domain (CRD) in *E. coli* enabling ^{15}N and ^{13}C isotope enrichment, which allowed NMR resonance assignment. Following changes of these NMR resonances upon Ca^{2+} titration in a ^{1}H-^{15}N HSQC experiment, generated insight into a large network of amino acids involved in Ca^{2+} binding. Surprisingly, the network spans a large fraction in the protein, with many residues significantly distal from the Ca^{2+} site. Further analysis combining experimental mutagenesis and molecular dynamics simulations prompted us to propose an allosteric network modulating the function of Langerin. In particular, two single point mutations allowed to perturb the network, giving further insight into its function, which we concluded is to downregulate Ca^{2+} affinity. This modulation of the cofactor affinity by an allosteric network has important implication for the receptor function as the ligand and release under endosomal conditions needs to be tightly regulated. Overall, these data provided the first insight into such an allosteric network in a C-type lectin and opened new avenues to further development of potential drugs that modulate C-type lectins **[4]**.

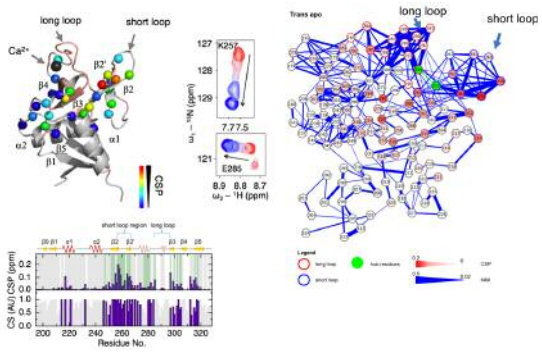

Fig. 3: The Ca^{2+} affinity of Langerin is modulated by an intradomain allosteric network. Binding of the cofactor Ca^{2+} to Langerin leads to chemical shift perturbation (CSP) of the backbone resonances of the carbohydrate recognition domain at several distal sites of the protein. Residues involved in this communication network are evolutionary conserved (CS). Analysing extensive molecular dynamics simulations using information theory yielded insight into the atomic details of this network (right). ***[4]***

Bacterial Polysaccharide Specificity of Langerin is Highly Species-dependent

Our insights into secondary sites being able to modulate the function of Langerin prompted us to look closer into the recognition of larger polysaccharide ligands. C-type lectin receptors such as Langerin are pattern recognition receptors that detect invading pathogens by carbohydrate patterns present on their surfaces. Therefore, these innate immune cell receptors are the product of a species-dependent evolutionary pressure. In this respect Langerin is of particular importance since it is conserved in many mammals with only moderate sequence variation. For example, humans and mice share 66% sequence identity. Based on our insights on the dynamics of the human Langerin and the observation that even single amino acid variations can potentially introduce significant changes in its biological function, we compared the human and the murine homolog side-by-side. We found that, while monosaccharide specificities remain almost unchanged between the two species, recognition of larger polysaccharides was significantly altered **[5]**. We solved the crystal structure of the murine Langerin to compare the molecular determinants and could deduce that minor changes at the trimeric interfaces might result in repulsion in the murine Langerin, which is not the case in the human homolog. At the same time a secondary binding site was proposed form our work explaining how the specificity might be altered for larger polysaccharides.

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Chemical Biology of Glycosylphosphatidylinositols

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Many eukaryotic proteins are anchored to the outer leaflet of the cell membrane using glycosylphosphatidylinositol glycolipids (GPIs). GPIs are characterized by a conserved core structure containing a glycan pseudo-pentasaccharide, a phosphoethanolamine unit, and a phospholipid tail. The GPI core is usually modified with additional phosphates, glycans and lipid chains in a cell type dependent form. The phospholipid moiety is highly variable and may contain a diacylglycerol (DAG), an alkylacylglycerol (AAG)or a ceramide (CER), with alkyl chains of different length and degree of saturation **(Fig. 1)**.

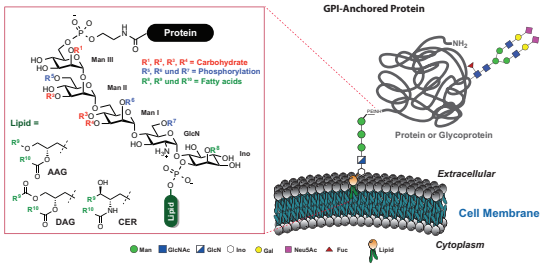

Fig. 1: Structure and possible modifications of GPIs

The primary and best known biological role of GPIs is to anchor the attached molecules to the cell membrane **[1]**. However, different studies show that GPIs play a role in the association of anchored proteins with lipid rafts and are, thereby, involved in diverse processes such as regulation of the immune system of the host during parasitic infections and protein localization, among others **[2]**.

Development of Strategies to obtain GPIs

To evaluate the role of GPIs and their structure-function relationship is necessary the availability of good amounts of homogeneous glycolipids. To address this need we developed a synthetic strategy to obtain well-defined GPIs **[3]**. This strategy was used to obtain different and structurally distinct GPIs and GPI derivatives that allowed biological and biophysical evaluations of these molecules. Various GPIs are characterized by the presence of unsaturated lipid chains and require special conditions for their synthesis. More recently, we developed a new strategy to obtain GPI molecules bearing unsaturations. The strategy is based on the use of the 2-(naphthyl)methyl (NAP), an acid labile group, for the permanent protection during the synthesis, the use of the allyl and PMB ethers as orthogonal protecting groups to mask the positions requiring late-stage phosphorylation, and the NAP easy removal using high concentrated TFA **(Fig 2) [4]**. To demonstrate the applicability of this strategy, we synthesized the pseudo-disaccharide GlcN-Ino 1 from the GPI of the Trypanosoma cruzi parasite **[5]**, which unsaturated lipid moiety has been associated with the strong proinflammatory activity of the GPI from this parasite.

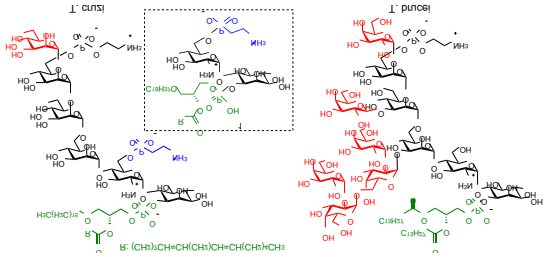

Fig. 2: Structures of the glycosylphosphatidylinositola from T. cruzi and T. brucei

GPIs as Vaccine Candidates for Toxoplasmosis

Protozoan parasites express high amounts of non-protein-linked, free GPIs, and GPI-anchored proteins (GPI-APs) that may participate in the regulation of the host immune response during infections **[6]**. However, in most cases, the heterogeneity and difficult isolation of pure GPIs have limited the evaluation of their function.

We investigated the immune response elicited in a BALB/c mouse model by two GPI glycans as vaccine candidates toward *T. gondii* using synthetic GPIs coupled to the carrier protein CRM197. We examined the generation of anti-GPI antibodies and the protective properties of the GPI-glycoconjugates in a lethal challenge study using the virulent *T. gondii* RH strain. Upon immunization, the mice raised anti-GPI antibodies that bind to the respective glycan structures on carbohydrate microarrays. **[7]** Unfortunately, these antibodies were mainly directed against an unspecific epitope of the glycocojugates including the cross-linker used for the attachment of the GPI to the carrier protein. Furthermore, antibodies *in vitro* binding studies suggest the lack of specificity toward cell surface exposed *T. gondii* GPI epitopes to be the reason for the failure of protection during the challenge studies. Consequently, future GPI-based vaccine candidates against toxoplasmosis, or any other disease, should rely on a conjugation without the use of immunogenic cross-linkers to generate a specific immune response against the desired carbohydrate antigens.

Structure of Glycosylphosphatidylinositols

NMR spectroscopy is a useful technique for the conformational analysis of carbohydrates in solution. However, it is not feasible to determine the dynamical conformation of carbohydrates solely on the basis of local conformational restraints derived from nuclear overhauser effects (NOEs) and scalar couplings. Recently, paramagnetic NMR techniques have been applied to provide long distance information for the characterization of carbohydrates conformations at the atomic level **[8]**. These techniques have been successfully applied to the conformational analysis of the disaccharides such as chitobiose, lactose, and also in breaking the pseudosymmetry of complex N-Glycans **[9]** .

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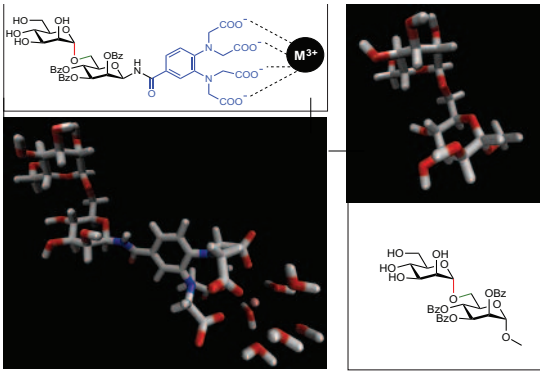

Fig. 3: Conformation of a dimannose with and without a TAG for the paramagnetic NMR.

To evaluate the effect of the core modifications in the structure and function of GPIs, we have applying this approach to perform conformational studies of GPI anchors fragments using lanthanides-assisted paramagnetic NMR spectroscopy in combination with molecular dynamics (MD) simulations. For this purpose, a metal chelating tag was synthesized and attached at the reducing end of different GPI glycan moieties of different length and carbohydrate constitution. We evaluated the effect of diverse paramagnetic metals (Dy^{3+}, Tb^{3+}, Yb^{3+}, Eu^{3+}) in paramagnetic tagged NMR spectroscopy, which in combination with molecular dynamics calculations deliver information about the conformation and flexibility of dimannose 1,2- and 1,6-linkages present in the glycan core structure of GPIs. These results confirmed the flexibility of the GPI structure around the 1,6-bond and delivered different conformations of GPIs for the elucidation of the structure-function relationship of GPIs, which may explain the formation of specific antibodies against the modifications on GPIs over other components of the GPI-core and help us to design GPI-based molecules for therapeutic applications.

Semi-Synthesis of GPI Anchored Proteins

To evaluate the effect of GPIs in the function and activity of GPI-anchored proteins, two ligation strategies have been used to attach synthetic GPIs to proteins: expressed protein ligation (EPL) and intein-mediated protein trans-splicing (PTS) **(Fig. 4)**.

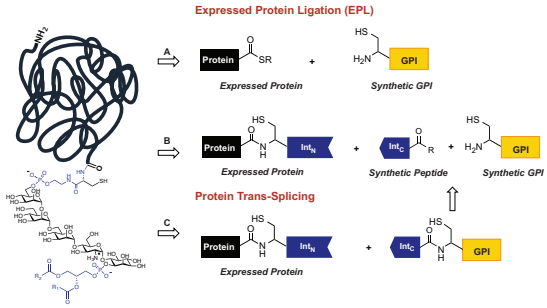

Fig. 4 Schematic representation for the semi-synthesis of GPI-anchored proteins

In the first strategy, GPIs containing a cysteine residue at the phosphoethanolamine residue were obtained using chemical synthesis. The active protein thioesters were isolated after folding an expressed fused protein of the protein of interest and an intein domain in the presence of thiols **(Fig 4,A)**, or they were generated in situ by the formation of an active intein domain using a mutated split-intein and the corresponding splicing reactions **(Fig 4,B)**. After establishing the best folding conditions, the desired protein thioesters were used in a EPL process with the Cys-containing GPIs to deliver the GPI-APs. In the second strategy, the proteins of interest are expressed as fusion proteins with the *N*-terminal fragment (Int^N) of the split intein from *N. punctiforme* **[10]**. The GPI molecules are ligated to a synthetic C-terminal intein fragment peptide by native chemical ligation. The GPI-APs are obtained by a trans-splicing process induced after folding the two split-intein fragments. With the established methods, we have synthesized diverse GPI-APs including the PrP, INF-α2 and GFP as well as some parasitic proteins containing mono- and bilipidated GPI molecules.

Besides the GPI-APs, we have also investigated the use of the NCL strategy for the synthesis of N-glycoproteins and for the synthesis of GPI-anchored glycopeptides. We evaluated different methods and established the combination of allyl / N,N-dimethylamino-phenacyl groups as suitable protecting groups for the side chain protection of aspartic acid and to obtain N-glycopeptides with variable glycosylation patterns. **[11]** The peptide thioesters were formed after cleavage of the glycopeptides from the resin. NCL has been applied to attach the glycopeptides to GPIs or to elongate the peptide chain to larger glycopeptides. Glycopeptides were obtained with small sugars and with complex N-glycans.

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Autoantigenicity Patters in Health and Disease

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Everybody has circulating self-reactive antibodies in the blood. Although these individual repertoires of autoantibodies can significantly overlap, they differ between healthy and diseased individuals. Therefore, we believe that differential analysis can lead to the identification of biomarker sets that can clearly separate different diseases or even allow subdiagnosis of patients within a certain disease.

Autoimmune disorders are characterised by the presence of antibodies against a number of self-antigens. In some cases, these autoantibodies have a known pathophysiological role and are explicit drivers of the disease leading to tissue destruction. However, in many autoimmune disorders, their role is yet not understood and their presence is seemingly without consequence. Our knowledge about their role in disease progression, whether being of significance or simply a bystander effect is rather vague.

The major interest of the Immunomics group centres on the investigation of antibody-antigen complexes in autoimmune disorders. The scientific focus is currently on the elucidation of autoantigenicity patterns in rheumatoid arthritis. The group is part of a consortium between a local small enterprise and the Charité and is financed exclusively by third party funding of the German Federal Ministry of Education and research (BMBF) and the Federal Ministry of Economic Affairs and Energy (BMWi). The aim of the work within this partnership is the characterisation of autoantibody profiles and the definition of patterns that can be used for differential diagnosis. The methodological portfolio includes primarily protein array and phage display technology, recombinant protein expression, as well as immunological methods.

Characterization of Autoantibody Repertoires in Rheumatoid Arthritis

Rheumatoid arthritis (RA) is a heterogeneous disease of presumably multifactorial but unknown aetiology. To date, the course of the disease as well as the response to specific treatment strategies is insufficiently predictable. RA cannot be cured, requires lifelong medication, frequently (>50%) causes work disability within the first ten years of disease and reduces life expectancy compared to the general population. Nevertheless, over the last years, the treatment of patients with RA has changed considerably. The new targeted therapies (biologics) can induce previously unachievable responses in subgroups of patients. Most recent studies suggest that especially "fast response" after initiation of treatment with biologics is an indicator of successful anti-inflammatory targeting. However, in long-term treatment relapses may occur and molecular mechanisms related to these flares are insufficiently understood. Furthermore, the goal of therapy is not only symptom relief, but in particular the prevention of long-term structural damage and functional decline. So far no personalized biomarkers exist, which can be used by the clinicians to decide which type of therapy shall be given, or which type of biologic drug in use is effective in an individual RA patient and can therefore be used to induce a fast remission.

A recent project in close collaboration with the Department of Rheumatology and Clinical Immunology of the Charité centred on the clinical validation of certain IgA autoantibody profiles, which can be used to identify TNFalpha inhibitor non-responders. We could show that measuring autoantibodies against a set of 5 autoantigens can identify 80% of therapy non-responders **[1, 2, 3]**. In another project, we used protein array technology to characterize autoantibody profiles in mouse models in RA **[4, 5, 6]**. We demonstrated, that the development of certain autoantibodies are toll-receptor dependent **[4]**. In yet another study, we looked into specific autoantibody profiles, which allow discrimination between early stages of RA and systemic lupus erythematosus (SLE). According to our current findings, the biomarkers may possibly also serve as prognostic marker, i.e. give clues about the progression of RA in those patients possessing such autoantibodies. We could show that detection of autoantibodies against certain heterogeneous ribonulceoproteins (hnRNPs) can be used to reduce the sensitivity gap of current standard biomarkers used in the initial serological diagnosis of RA **[7]**. We are currently finalizing a manuscript with our clinical partner where we have tested >1000 early RA patients with these markers. Another manuscript we are currently preparing shows that selected hnRNPs can distinguish between erosive and moderate forms of RA and therefore measuring autoantibodies against these markers can assist the clinician in his therapy decision.

The current research program is focussing on analysing the diagnostic potential of further hnRNPs for diagnostic purposes in the field of RA and their potential application as prognostic and predictive markers for therapy outcome. One major aspect is the investigation of (aberrant) post-translational modifications in this context. Within the project, we rely on our expertise in the production of recombinant proteins and antibodies in prokaryotic and eukaryotic hosts as well as the protozoan host *Leishmania tarentolae*. *L. tarentolae* is a promising host for the expression of recombinant proteins, as it has the ability to produce soluble proteins in the cytoplasm as well as glycosylated proteins utilising secretory pathways. We have explored this potential and could show for the first time, that O-glcosylation of a recombinant protein expressed in *L. tarentolae* can occur **[8]**.

The most recent project is devoted to the identification of autoantigenicity patterns that accompany therapy and therefore, might allow drawing predictive conclusions about therapy outcome **[9]**. Here, we apply two complementary screening technologies for the discovery of autoantigenicity patters, namely Protein Arrays and Phage Display. They comprise of different subsets of the human proteome and offer different means of selection. While most antigens on the array are denatured, the proteins on the bacteriophage surface are presented as folded structures. The used protein arrays consist of ~25.000 expression constructs of a human foetal brain cDNA library. For phage display screening, we will use various full-ORF libraries and peptide libraries available in our laboratory. While the identity of each spot on the protein array is known, the phage display libraries require downstream processing. Phage display selection is an iterative process based on affinity enrichment using patient-derived immunoglobulin fractions as selection targets over several rounds. The identity of the enriched clones is revealed by sequencing of the DNA inserts **[10]**.

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Rational Approach towards Glycoconjugate Vaccines

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Design of carbohydrate based glycoconjugate vaccine has not seen a huge change from its inception. Commercial vaccines are still rely on isolated natural capsular polysaccharide (CPS) present on bacterial surface. The vaccine subgroup is using a rational approach utilizing organic syntheses to identify key epitopes which are protective from these natural CPS. The approach relies on a library of oligosaccharides varying in length, type of monosaccharides at the reducing and non-reducing end, branching vs linear, frame shifts, neutral vs charged and many others. Using these unique set of glycans and employing glycan array and protective monoclonal antibodies for a given pathogen, we elucidate the most potent, immunogenic, antigenic and functional oligosaccharide that is then evaluated further using additional invitro and invivo experiments to identify a potential semi-synthetic vaccine candidate. The challenges associated in syntheses leads to further development of existing protocols or discovery of novel methods and reagents.

In an ongoing effort the ''vaccines'' research group is working on the chemical synthesis and biological evaluation of carbohydrates present on *Streptococcus pneumoniae, Yersinia pestis, Chlamydia trachomatis, Haemophilus influenzae type b, Leishmania donovani, Neisseria meningitidis, Salmonella typhi, Kleibsella pneumoniae, and Clostridium difficile.* Since carbohydrates are complex molecules the vaccine group is also refining the activators and glycosylation methods needed to put together these molecules using thier individual monosaccharides.

Streptococcus pneumoniae: The group is currently pursuing several serotypes and has finished the synthesis of a number of repeating units of the CPS of ST-1, ST-3 **[1],** ST-4 **[2],** ST-5, ST-8 and ST-12F (**Fig 1**). In all cases immunological evaluations have been followed up by functional evaluation either using the challenge studies or the standard surrogate opsonophagocytic killing assay (OPKA). This massive project opens up the possibility to better understand the roles played by various substituents like acetates and pyruvates (ST-4), rare sugars like pneumosamine (ST-5), conjugation methods, sugar loading, etc. on immunogenicity and antigenicity. We would like to address some key questions on glycoconjugate vaccine design so as to move away from empirical to rational way of designing glycoconjugate vaccines. The oligosaccharides also serve to evaluate potential stability issues, formulation development and to standardize the analytics needed to manufacture a glycoconjugate vaccine.

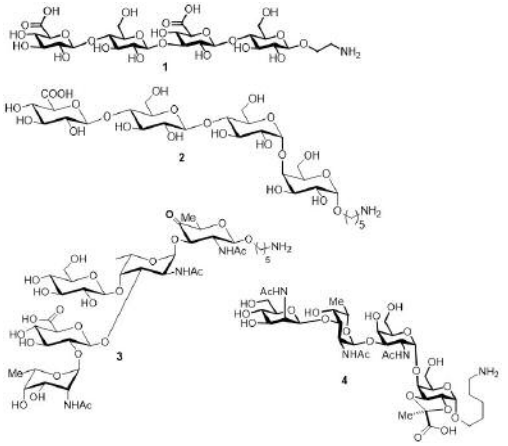

Fig. 1: Carbohydrate structures of S. pneumonaie that the ''vaccines'' research group has synthesized

Haemophilus influenzae: A library of synthetic oligosaccharides, based on the CPS repeating unit of Hibwere synthesized and subjected to immunological evaluation. The glycans were found to be immunogenic and showed cross reactivity to the natural CPS.

Clostridium difficile: Synthesis and immunological evaluation of the newly reported PS-III antigen wascarried out (**Fig 2**) **[3].** PS-III along with PS-I and PS-II antigens seem to be a promising vaccine candidate and would need to be further evaluated through an active as well as a passive challenge model using mAb specific for one of the three oligosaccharides.

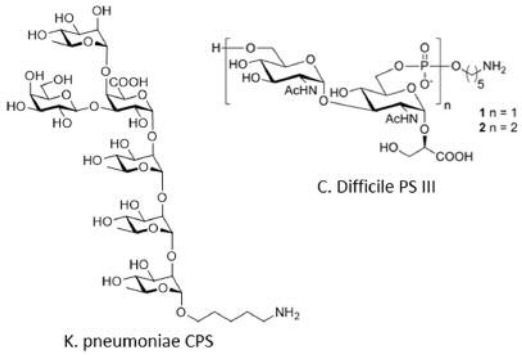

Fig. 2: Carbohydrate structures of pathogens that the ''vaccines'' research group has synthesized

Kleibsella pneumoniae: Infections caused by *K. pneumoniae* are becoming an important challenge due to the emergence of strains resistant to carbapenem antibiotics. Recently the CPS structure of ST258 clone was identified. Using this information the total synthesis of hexasaccharide repeating unit of the CPS of a carbapenem resistant *K. pneumoniae* was achieved (**Fig 2**). Immunization experiments and mAb generated cross reacted with the native CPS. In order to guage the potential as a vaccine candidate animal challenge models needs to be established and is currently underway for this very important medically unmet pathogen.

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b) Weishaupt, M. W., Matthies, S., Hurevich, M., Pereira, C. L., Hahm, H. S., Seeberger, P. H. *BJOC.* **2016,** 12, 1440-1446.
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[4] Schumann, B., Parameswarappa, S. G., Lisboa, M. P., Kottari, N., Guidetti, F., Pereira, C. L., Seeberger, P. H. *Angew. Chem. Intl. Ed.* **2016,** 55, 14431-14434.

Methodology: Glycosylation are still challenging reactions in oligosaccharide syntheses especially 1,2- cis. Given our interest to install an amine containing alkyl linker at the reducing end of an oligosaccharide, the selectivity and yield for such 1,2-cis glycosylations are governed by various factors that dictate the final steroselective outcomes. We developed a new methodology project using a unique fluorine containing linker that allowed us to get exclusive or better 1, 2 cis selectivity during glycosylations (**Fig 3**) **[4].** This approach is currently being tested on the syntheses of antigens using the automated glycan assembly were the 1,2-cis glycosylation are even more difficult to achieve.

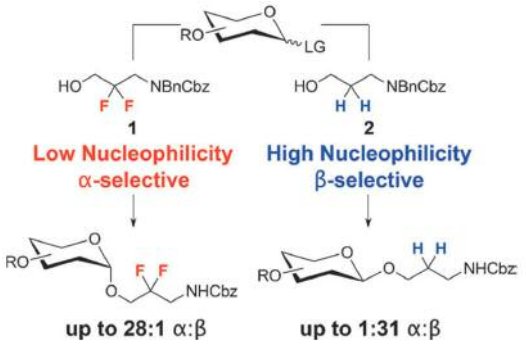

Fig. 3: Nucleophile directed stereocontrol in glycosylation

Other Projects: Along with the above mentioned work, we also are involved in methodology development for activation of glycosyl donors for glycosylation, mass based analysis of glycoconjugates **[5],** synthesis of glycans from lipopolysaccharides **[6],** modification of glycans to increase stability, syntheses of GSL based fully synthetic compounds and the syntheses of antigens from various other pathogens both in solution and using AGA.

Vaccine Chemistry:
C. L. Pereira, J. Y. Baek, M. Lisboa, S. G. Parameswarappa, B. Schumann, A. Calow, X. Fei-Fei, M. Emmadi, X. Guozhi, P. Menova, S. Awan. L. Lykke
claneylebev.pereira@mpikg.mpg.de

Vaccine Biology:
Peter H. Seeberger, F. Bröcker, A. Geissner, A. Reinhardt, P. Kaplonek, N. Khan, A. Wahlbrink.
peter.seeberger@mpikg.mpg.de

[5] Moeginger, U., Resemann, A., Martin, C. E., Parameswarappa, S. G., Govindan, S., Wamhoff, E.C., Broecker, F., Suckau, D., Pereira, C. L., Anish, C., Seeberger, P. H.; Kolarich, D. *Scientfic Reports.* **2016,** 6, 20488.
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Patents:

[1] Seeberger, P. H., Pereira, C. L., Anish, C., Schumann, B. "Synthetic saccharide structure of capsular polysaccharide of Streptococcus pneumoniae type 1 and glycoconjugate as vaccines against disease caused by Streptococcus pneumoniae type 1 or bacteria having such capsular polysaccharide" *PCT Int. Appl.* **2015,** WO 2015004041 A1 20150115.
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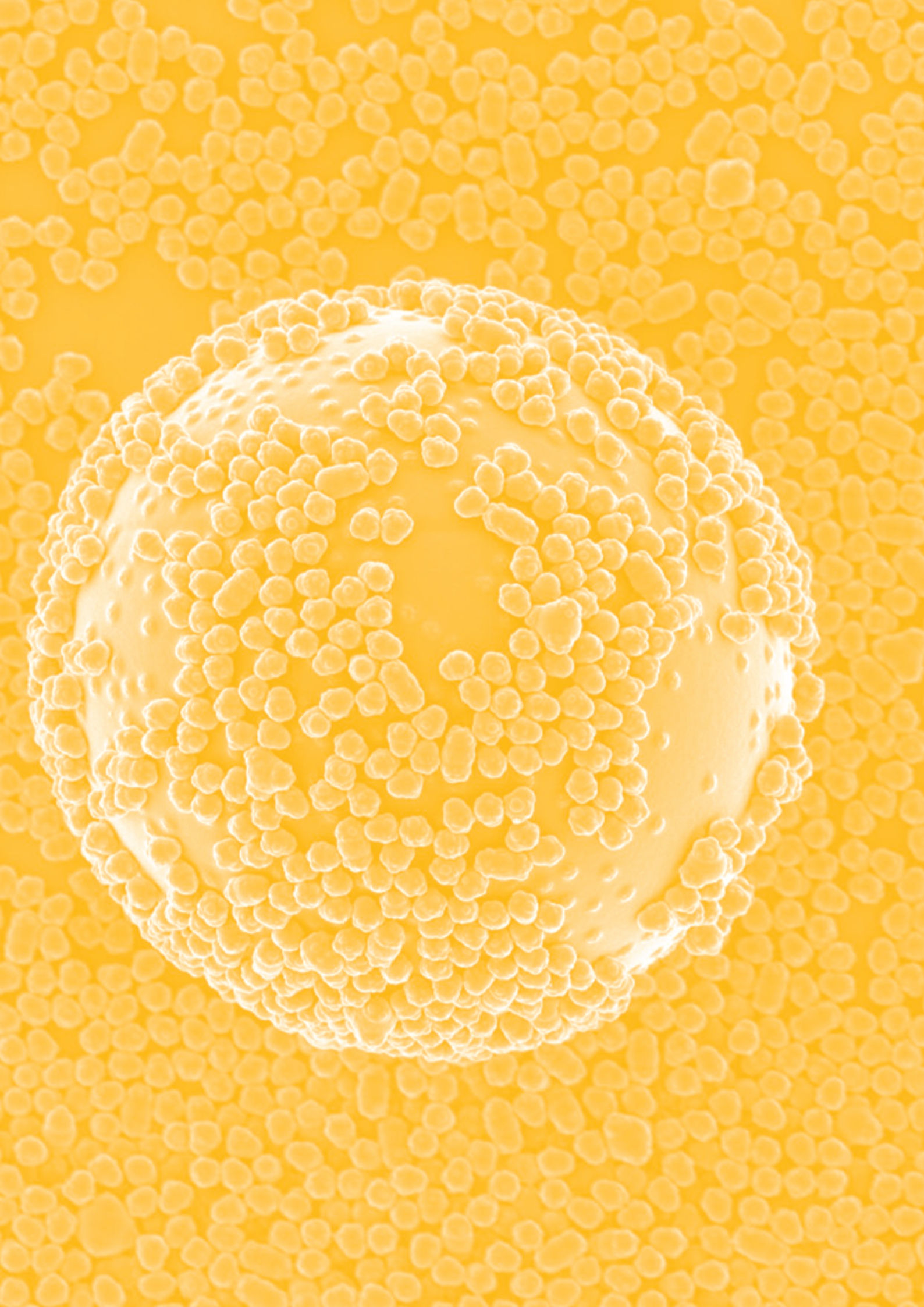
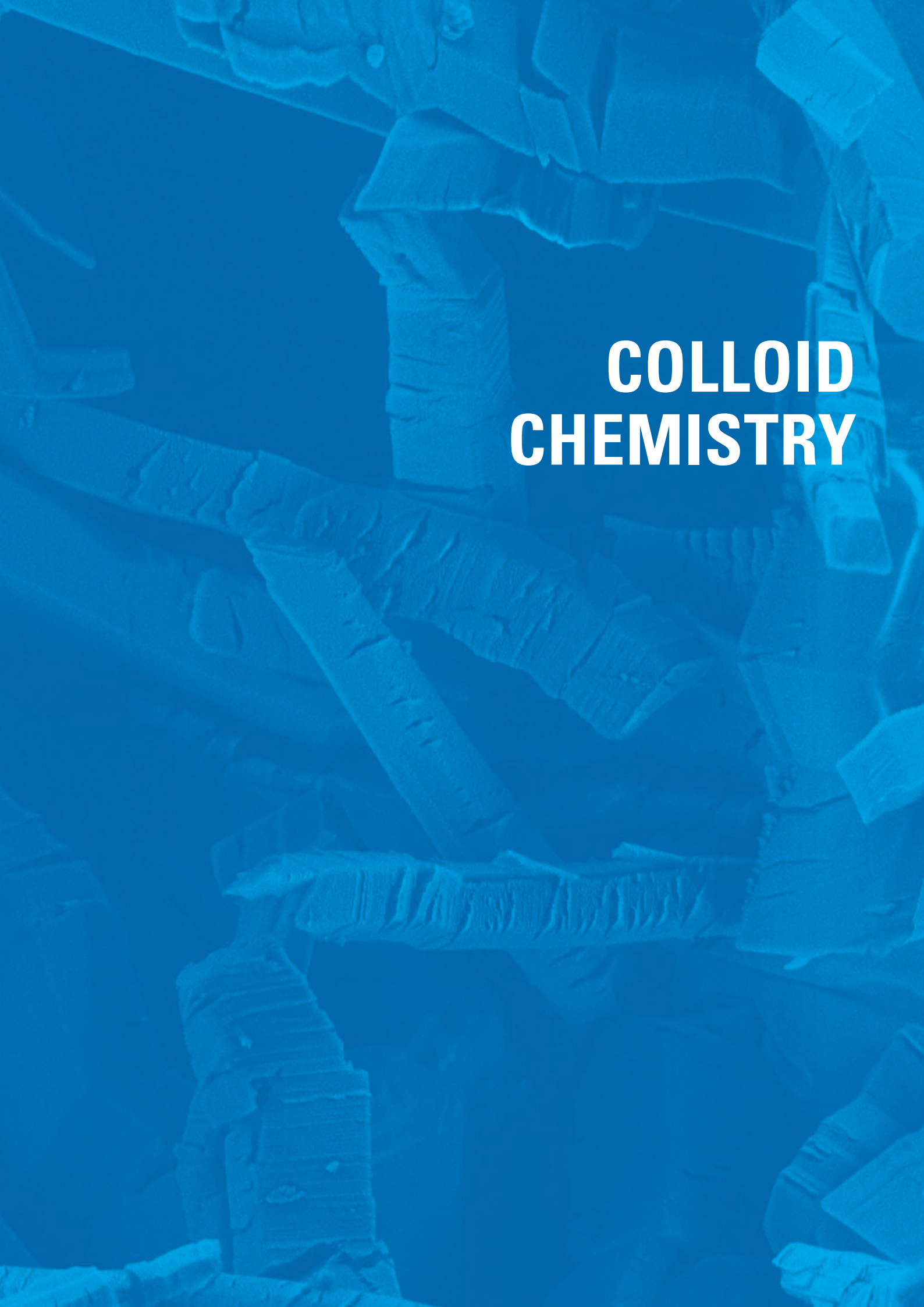
[5] Seeberger, P. H., Pereira, C. L., Anish, C., Schumann, B., Parameswarappa, S. G., Hahm, H. S., Govindan, S. "Synthetic vaccines against streptococcus pneumoniae serotype 8" *PCT Int. Appl.* **2016,** WO 2016046420 A1 20160331.
[6] Seeberger, P., Pereira, C. L., Xiao, G., Khan, N., Anish, C. "Vaccine against carbapenem-resistant Klebsiella pneumoniae" *PCT Int. Appl.* **2016,** WO 2016156338 A1 20161006.





COLLOID CHEMISTRY

Research in the Department of Colloid Chemistry

Markus Antonietti 06.02.1960
1983: Diploma, Chemistry (University of Mainz)
Thesis: Bestimmung der Diffusion von photomarkiertem Polystyrol: spezielle Systeme, chemische und physikalisch-chemische Aspekte
1985: Doctorate for natural science (summa cum laude, University of Mainz
Thesis: Diffusion in topological constraint polymer melts with Prof. Dr. H. Sillescu
1990: Habilitation, Physical Chemistry (University of Mainz) Thesis: Microgels – Polymers with a special architecture
02/1991: Associate Professor (University of Mainz)
09/1991: Full Professor (Philipps University Marburg)
Since 1993: Director (Max Planck Institute of Colloids and Interfaces, Golm),
Full Professor (University of Potsdam)

Scientific Profile

The overall size of the Department of Colloid Chemistry has decreased due to legal changes of employment contracts to about 65 people, however still covering a broad range of research topics. The effective constituting element of the scientific activities is the "project", a structure headed by a senior scientist involving a mixture of technicians, graduate students, and post-docs (3 – 10 people). Projects are related to scientists, but usually have a temporal character of about 5 years. After this time, permanent scientists (including the director) have to redefine their profile to justify the allocation of resources. In the case of non-permanent scientists, the projects usually leave the department with the promotion of the scientist, i.e. the group leaders can continue their specific research in their new academic environment (usually as professors) without competition of the institute.

In the time of this report and following those rules, the serious changes of my department already running in the last three periods continued to take place. Dr. Menny Shalom was promoted to Associate Professor at the Ben Gurion University/Israel, and the contracts of Dr. Dariya Dontsova and Dr. Davide Esposito which were bound to ternary funding operations were running out. Dr. Tim Fellinger accepted a junior guest professorship in Gothenburg and a Professor substitution for 6 months; Dr. Jiayin Yuan went out for an Associate Professorship at Clarkson University/New York. For those, Dr. Martin Oschatz moved in with a Liebig Stipendium, Dr. Ryan Guterman and Dr. Oleksandr Savatieiev accepted the duties to continue running operations and took responsibilities of left over groups. Dr. Valerio Molinari is now in the exploration phase of a novel science experiment, the so-called "kitchen lab". I am, however, happy to have won Dr. Marc Willinger as a Senior Project Leader for the new AC-HRTEM laboratory, a 5 M operation which came into completion in 2016.

It is fair to say that a majority of the group is now still in the early phase of higher academic profiling, making the following report more concept than result oriented. This turnover of leading junior scientists is beyond typical and easy, and I would opt for some more stability after so many changes.

The following topics are currently explored within the department:

- Heterophase Polymerization (until February 2016, then retirement)
- Novel Self Assembly Polymers
- Next generation Electrochemistry materials
- Modern Techniques of Colloid Analysis
- Energy and Environmental Utilization of Carbon Nanomaterials
- Colloid Chemistry for Green Chemistry, green polymers and Biorefining, Kitchen Lab
- Artificial photosynthesis

The projects behind the headers are briefly explained below:

Heterophase Polymerization
(Retirement of Klaus Tauer in February 2017)

The notation „Heterophase Polymerization" summarizes the techniques of suspension-, emulsion-, mini-, and microemulsion-polymerization as well as precipitation polymerization. Solvent is usually water. In all cases, the product is a polymer colloid or polymer nanoparticle This class of techniques, although one of the eldest in polymer science, is still most actual, as it allows the production of high polymer containing formulations in water as an environment-friendly solvent and to address nanoparticles and nanostructures on an industrial scale.

Central points of interest of the team working on heterophase polymerization are:

- Understand nucleation and particle formation for an optimal control of the particle; the experimental investigations are supplemented by theoretical and modelling descriptions *(Dr. Klaus Tauer).*
- Synthesis of complex polymer morphologies on a colloidal level (core-shell latices, hollow spheres, non-isometric particles) by a rational use of the particle interfaces and interface effects in heterophase polymerization *(Dr. Klaus Tauer).*

Novel Self Assembly Polymers

Amphiphilic polymers usually consist of components which dissolve in different media, e.g. a hydrophilic and a hydrophobic part, but this paradigm is proven to be incomplete. The newest observation in this direction is that also block copolymers without hydrophobic contrast can self-assemble to complex structures. Focal points of interest in this project group are:

- The micelle formation and lyotropic liquid crystalline phase behavior of double hydrophilic block copolymers is examined in dependence of the molecular structure, the relative amount of the different components, as well as the secondary interactions between the structure forming bio-like blocks *(Dr. Bernhard Schmidt).*
- Oligophenols are omnipresent in Nature, but less well used an examined in synthetic polymer chemistry. As polyphenols are strongly interacting with each other, with metals and with surfaces, we expect to discover "the fourth code" of polymeric secondary structure formation *(Dr. Bernhard Schmidt).* First amphiphiles with lignin fragments have been made.
- Polymer Ionic liquids represent highly polarizable surfactants which enable to solve very complicated dispersion problems, e.g. nanocarbons in water. The synthesis and self-organization of those PILs was systematically explored for the last four years *(Dr. Jiayin Yuan)*
- Polymer Ionic Liquids 2.0: Due to the promotion of Dr. Yuan, the activities are continued with *Dr. Ryan Guterman*. He is currently focusing on PILs as binders for electrodes as well as novel PIL chemistry to broaden the range of available polymer structures

Next Generation Electrochemistry Materials

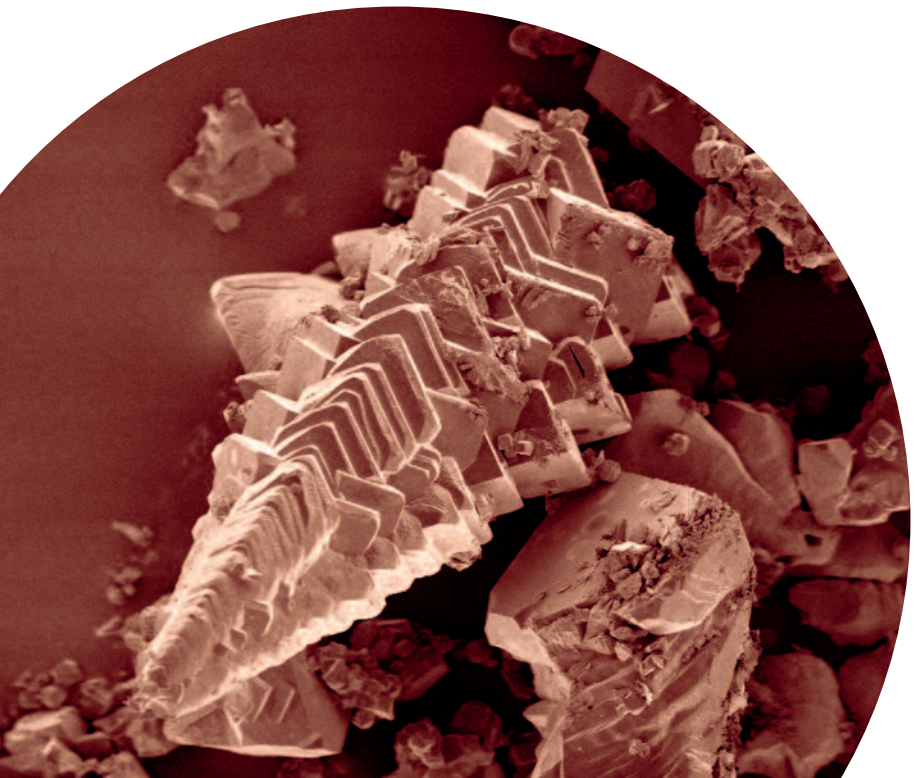
Following the project house ENERCHEM which has ran out, our department continues to take a leading role in the field of energy materials. This was also appreciated by the creation of the MaxNet, which has started in 2014 and host some of the activities described below. Hydrogen storage, better fuel cells, new energy cycles, new catalysts for more efficient processes, novel batteries, ultra-capacitors, remote energy storage, all these topics are intimately connected with the control and design of materials nanostructure. Activities based in Golm include:

- Metal free organocatalysis and photocatalysis with porous organic semiconductors: Novel synthesis schemes towards carbonnitrides *(Dr. Oleksandr Savatieiev).*
- Superhigh surface area carbons and their use for supercapacitors. Salt melt carbon synthesis and supramolecular approaches towards C_2N *(Dr. Nina Fechler)*
- New battery concepts such as the Magnesium battery rely on new solvent systems, new cathodes based on surface instead of intercalation, and of course novel solvent/ conducting salt systems. All this – with a physicochemical perspective – is handled within the new group of *Clemens Liedel*.

Modern Techniques of Colloid Analysis

All the work described above is necessarily accompanied by a considerable amount of colloid analysis which includes fully commercial techniques, but also relies on the development of new techniques or methods of preparation and data handling. The developments in this area are currently mainly focused on electron microscopy:

- Special techniques of transmission and scanning electron microscopy on soft, structured matter which are run on the base of a central service group *(Dr. Marc Willinger, Dr. Jürgen Hartmann).*
- Dynamics of growth and catalytic processes in time resolved electron microscopy *(Dr. Marc Willinger)*



Energy and Environmental Utilization of Carbon Nanomaterials

The group of *Dr. Martin Oschatz* is a rather recent addition and for the first 3 years placed by a Liebig-Fellowship. Dr. Oschatz will combine his longstanding experience on porous carbon materials from the Kaskel group with or own expertise in sustainable carbon synthesis. Projects include:

- Electrically induced gas sorption and gas separation. Similar to CDI in liquids, it is analyzed if gas adsorption can be biased by an outer potential. This should enable electro-swing processes
- Superstable and non-innocent catalytic supports for electrochemistry and classical heterogeneous catalysis.

Colloid Chemistry for Green Chemistry, Green Polymers and Biorefining: Kitchen Lab

Advanced materials chemistry is still mostly based on non-sustainable resources, leading to the so-called "element crisis", e.g. the global depletion of Co, Ni, Ta, or In. Based on previous projects on hydrothermal carbonization, we carefully analyzed hydrothermal processes for the generation of value chemicals from biomass. These projects were first driven by my ERC Advanced Grant but now have reached practical matureness. This project platform includes

- Valorization of lignin via reductive hydrothermal splitting (a joint Max Planck-Fraunhofer project,
- Conversion of carbohydrates into lactic acid and other platform chemicals (Dr. Valerio Molinari, Markus Antonietti)
- Next Generation Green Polymers based on sustainable monomers *(Markus Antonietti, Dr. Bernhard Schmidt)*

These projects move the department admittedly to upstream competence, but are expected to allow a new type of organic materials chemistry by new key components.

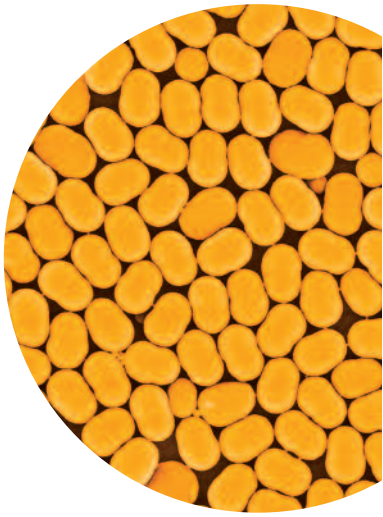
For outreach, but also for inner exploration, we just opened a so-called "Food-Lab" *(Dr. Valerio Molinari)* where typical cooking technologies are applied to the field of material synthesis. This is to be understood as the inversion of the principle of "molecular cuisine". Started as a safe place for school kids and candidates of temporal chemistry ban, it quickly turned out as a fountain of fresh processing ideas and materials. A first product is our so-called "wood remix", which is the base of a currently designed "flagship project" *(Dr. Nina Fechler)*.

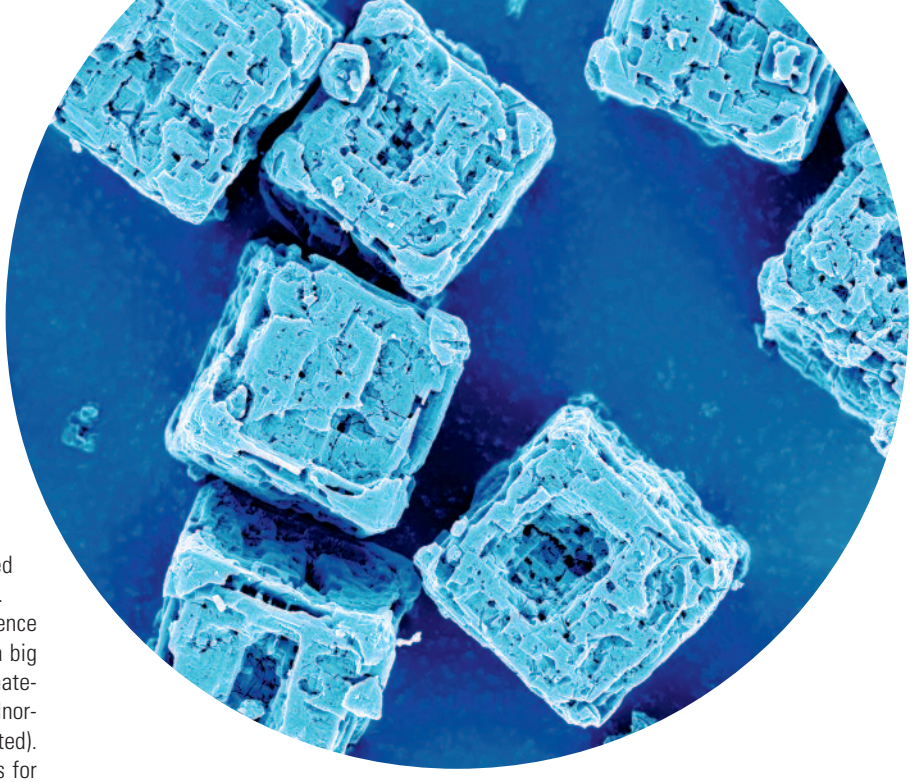
Artificial Photosynthesis

The international joint laboratory on Artificial Photosynthesis was established in July 2008 between the Max-Planck Institute of Colloids and Interfaces (Prof. Markus Antonietti) and Fuzhou University (Prof. Xianzhi Fu). The lab is now lead by Prof. Dr. Xinchen Wang, former group leader of the MPI-CI. Natural photosynthesis, the process by which green plants are converting solar energy into chemical energy, has inspired the development of artificial versions of photosynthesis, i.e. (1) the splitting of water into hydrogen and oxygen, and (2) the conversion of carbon dioxide into organics via sunlight. This was recently also successfully supported by a DFG-NSFC binational project

An important challenge in artificial photosynthesis is the development of catalysts that should be sufficiently efficient, stable, inexpensive, and capable of harvesting the abundant visible light in solar spectrum. There are many trials to establish stable systems for this purpose, mostly based on inorganic semiconductors with appropriately engineered bandgap. In our group we are investigating polymeric and organic-inorganic hybrid materials with controlled nanostructures as potential energy transducers for artificial photosynthesis for such applications as solar energy conversion, environmental purification, and organic synthesis.

- Melon, a carbon nitride polymer with graphitic structure, has turned out to be efficient for the direct splitting of water into oxygen and hydrogen. We improve the chemical structure of this polymer by copolymerization and textural control to improve light extinction and quantum efficiency of this process *(Dr. Darya Dontsova)*.
- Novel nanoparticles act as cocatalysts for both water oxidation and reduction to replace the non-sustainable Pt and Ru currently used. Functional carbon nanodots and carbon hybrids seem to be unexpected promising choices *(Markus Antonietti)*.
- New organic chemistry under photoredox conditions. A number of fellows are exploring the use of the as made catalysts for novel chemistry, such as photo-acetalization, Disulfide chemistry and thiamide synthesis. This is potentially to be integrated with the Seeberger department in a forthcoming joint project on the future of chemical fine synthesis.





Visions and Future Perspectives in the Director's View for the Next Years

After losing most of my more senior scientists for independent careers, I used the opportunity for a redefinition and reorientation of the department. I will have to continue the restructuration to enter a period with more coordinated research and longer term goals focused around the director and more tightly bound junior people.

Our trials to cooperate with the National Excellence Centre on Catalysis of the TU Berlin are to my opinion a big success, concerning the development of new catalytic materials and Solar Energy Usage Cascades (together with TU Inorganic Chemistry, 2 joint BMBF projects are now completed). The new projects on "Energy Materials" and "Processes for the Raw Material Change" turned out to be very timely and secured my department in the last two years a leading European role in these activities. This is also nicely reflected in many invitations for plenary and main lectures and the overall bibliometric performance. We are also seriously progressing with our activities to strengthen work projects between the departments, among them a "flow chemistry" project together with the Seeberger department, while also increased exchange on electron microscopy and mechanical testing is to be observed with the Fratzl department. Other potential projects which awaiting appropriate junior staff scientists are "carbon Q-dots" and "soil colloids".

Markus Antonietti
Director of the Department
of Colloid Chemistry

Novel Approaches to Carbon Nitrides Based Photocatalysts

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1999-2006: Bachelor and Master of Chemical Technology and Engineering (with Honours) (National Technical University of Ukraine "Kyiv Polytechnic Institute", Kyiv, Ukraine)
2006-2007: Research assistant, Department of Organofluorine Compounds Chemistry (Institute of Organic Chemistry, Kyiv, Ukraine)
12/2007-2011: Doctoral Thesis: Titania based photocatalytically active layer-by-layer coatings on model surfaces and textile materials (University of Strasbourg; Institut Charles Sadron, Strasbourg, France; Clariant Produkte (Schweiz) AG, Muttenz, Switzerland)
2011: Postdoctoral Scientist (Institut Charles Sadron, Strasbourg, France)
2012: Postdoctoral Scientist Department of Colloid Chemistry (Max Planck Institute of Colloids and Interfaces)
11/2012-6/2016: Research Group Leader Department of Colloid Chemistry (Max Planck Institute of Colloids and Interfaces)

In the last years, carbon nitride polymers with a stoichiometry close to C_3N_4 attracted remarkable attention as photocatalysts for water splitting, heterogeneous catalysts for various reactions, catalyst supports, etc. Still, typical representatives possess a number of drawbacks to be improved, such as low crystallinity, high charge carrier recombination rates, low surface areas or sophisticated synthesis procedures. Instead of improving the shortcomings of the existing polymers, we rather focus on design and preparation of novel materials originally free from drawbacks, as exemplified below by poly(heptazine imides) and hybrid metal atom/carbon nitride systems.

Poly(heptazine Imides) are Newly Discovered Members of the Family of Carbon Nitride Photocatalysts

The use of *more acidic*, compared to traditional ones (e.g. melamine, urea), carbon nitride precursors in the salt melt assisted synthesis results in the formation of potassium poly(heptazine imides) (PHIK) instead of conventional LiCl-intercalated poly(triazine imides). The increased acidity of the precursor strengthens interactions between condensation intermediates and K^+ ions, improves solubility of the former, and thus changes the reaction mechanism and the structure of the final reaction products. Originally, we used substituted 1,2,4-triazoles to access these fascinating materials **[1]**. Triazole-derived PHIK products displayed high activity in the visible light driven hydrogen evolution reaction (HER); still, the crystallinity of PHIK remained moderate.

Using 3-amino-1,2,4-triazole-5-thiol as a precursor, we developed a simple *one-step* procedure to prepare carbon nitride nanocomposites containing both water reduction (exemplified by MoS_2 nanoparticles) and water oxidation (exemplified by Co_2O_3 clusters) centers **[2] (Fig. 1)**. This was achieved by the salt melt assisted condensation of 3-amino-1,2,4-triazole-5-thiol that serves as C_3N_4 polymer precursor and sulfur source, and using small amounts of $MoCl_5$ and a reactive Co_3[3,5-diamino-1,2,4-triazole]$_6$ complex for the introduction of MoS_2 NPs and cobalt species, respectively. Under optimized synthesis conditions, poly(heptazine imide) phase is fairly crystalline, while 2H-MoS_2 NPs have the beneficial geometry for hydrogen evolution with an increased number of the active edge sites. The use of the *reactive* Co precursor results in homogeneous incorporation of Co_2O_3 clusters in the composite thus creating the active sites for oxygen evolution.

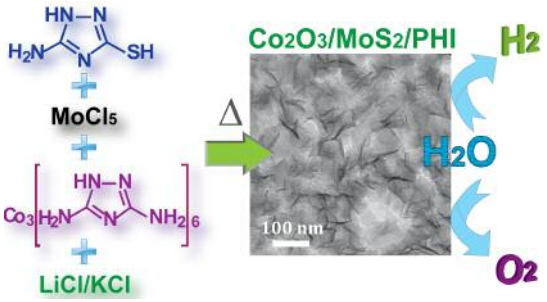

Fig. 1: Schematic of preparation and application of poly(heptazine imide) based composites in water splitting upon visible light irradiation.

More recently, we found that using the *more acidic* compared to 1,2,4-triazoles, amino-tetrazole as a precursor enables preparation of highly crystalline PHIK, in which the crystallinity extends over hundreds of nanometers enabling efficient electron/hole transport **[3]**. The crystal structure of products can be tuned by simple variation of the preparation conditions, leading to the alteration of their electronic properties (conduction and valence band positions). The poly(heptazine imide) works as a 'sponge' for K^+ ions enabling higher or lower ion intercalation. The conducted ^{13}C and ^{15}N SS-NMR and HR-TEM studies provided new insights into the PHIK structure depicted in **Fig. 2a** thus extending previous knowledge about this intriguing newly discovered class of materials.

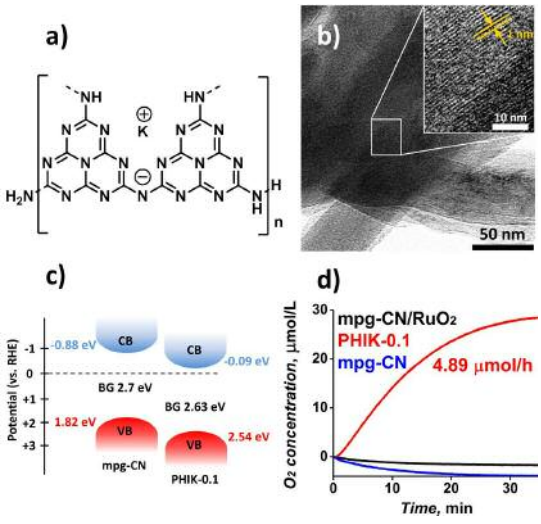

Fig. 2: Chemical structure of potassium poly(heptazine imide) (a); TEM image of a sample tetrazole-derived product (b); schematic illustration of the electronic band structures of conventional mesoporous graphitic carbon nitride (mpg-CN) and PHIK (c); visible light driven oxygen evolution by PHIK and reference materials (d).

The improvement of the structural order in PHIK resulted in much higher compared to known carbon nitrides, VB potentials in solids, 2.5 eV vs. 1.8 eV **(Fig. 2c)**. Thus, in addition to high activities in HER, tetrazole-derived PHIK are shown to photocatalytically liberate oxygen from water with high efficiency, without any metal co-catalysts **(Fig. 2d)**.

The aberration corrected high resolution electron microscopy studies of tetrazole-derived PHIK revealed that the nanostructure of the materials is represented by *columns* of heptazine units stacked on top of each other (stacking distance is ~0.3 nm) and *channels* occupied by potassium ions. The channels are located ~1 nm apart from each other **(Fig. 3a)**. The potassium ions in the channels can be easily exchanged by protons, or by a variety of alkali (Li, Na, Cs), earth alkali (Mg, Ca) and transition (Ni, Co, Ag, Zn) metal cations, keeping the stacked aromatic structure essentially intact, as illustrated in **Fig. 3b**. Such behavior is a typical feature of organic zeolites. The ion exchange causes alterations in the conductivity and electronic properties of the materials leading to increase or decrease of their photocatalytic performance, as it was exemplified by photocatalytic water reduction **[4]**.

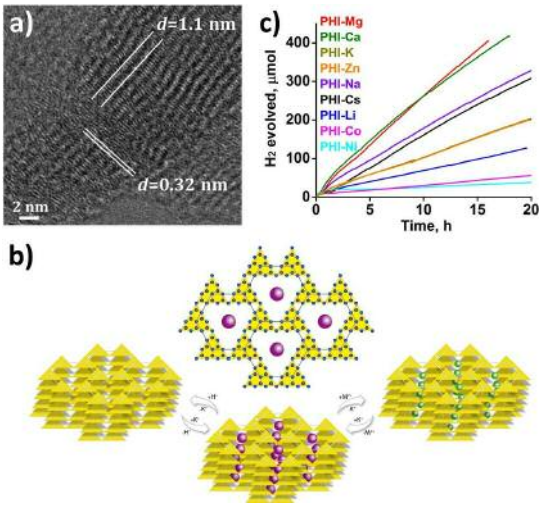

Fig. 3: HR-TEM image of tetrazole-derived potassium poly(heptazine imide) (a); idealized poly(heptazine imide) network structure illustrating proton–ion and ion–ion exchange (b); time dependent hydrogen evolution over poly(heptazine imide) salts upon irradiation with visible light (c).

The earth-alkali metal containing poly(heptazine imides) show a significantly improved activity and a more than twice higher hydrogen evolution rates compared to the pristine potassium salt **(Fig. 3c)**. The highest activity of 25.1 µmol H_2/hour is measured for *magnesium* salt that can be attributed to its high structural order and effective charge separation. The last example reveals the similarity of poly(heptazine imides) with chlorophylls where nature also uses magnesium ions to achieve the most efficient light harvesting. The ability of ion exchange positions poly(heptazine imide) as a solid state ion conductor further strengthening its application potential.

Single Metal Atoms/Graphitic Carbon Nitride Catalytic Hybrid Systems

In order to obtain functional carbon nitride-based composites for various catalytic applications, not limited to photocatalytic ones, we elaborated a general strategy to obtain a *joint electronic system with a shared electron orbital structure* consisting of atomically dispersed metal, here exemplified by silver, and carbon nitride polymer, by co-polymerization of the reactive silver tricyanomethanide with the carbon nitride precursor, cyanamide. This method avoids the drawbacks of the previously reported approaches of metal doping, but offers the advantage of extra-electron density present at carbon and nitrogen atoms resulting in the alteration of the semiconductor properties and the increase of the negative surface charge. The benefits of the developed doping method are illustrated in two applications: the photo-assisted water reduction (after further Pt NPs deposition) and the selective hydrogenation of 1-hexyne, where atomically dispersed Ag-doped carbon nitrides show an enhanced performance in comparison with other conventional Ag-based materials **(Fig. 4) [5]**. By optimizing synthesis conditions, Pd **[6]**, Ir, Pt and Au **[7]** were atomically doped into carbon nitrides, and the catalytic properties or the resulting materials were evaluated.

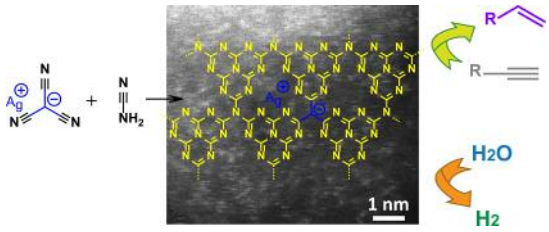

Fig. 4: Schematic of synthesis, structure and applications of a hybrid Ag@mpg-CN catalytic nanocomposite.

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BIOMASS CONVERSION INTO BUILDING BLOCKS FOR COLLOIDS

Biorefinery and Sustainable Chemistry

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Modern society is still heavily dependent on fossil resources for the generation of fuels, chemicals and pharmaceuticals. Unfortunately, the last decades have witnessed a constant depletion of traditional fossil feedstock. In addition, the global use of non-renewable resources has been responsible for a constant increase in environmental pollution. In this scenario, modern society is facing the challenge to provide solutions for a sustainable and environmental friendly development. In the last decades, the scientific community has identified biomass and food waste as promising feedstocks for the generation of fuels and commodity chemicals. The valorisation of renewable feedstocks in a biorefinery is analogous to that of classical refineries, which convert fossil resources (oil) into higher value products (fuels and chemicals). To date, examples of biorefineries for the production of energy (by thermal methods), or fuels (by biotechnological approaches) have appeared. Nevertheless, the *selective generation of bio-based fine chemicals and building blocks from biomass* using chemical strategies is still in its infancy, and its success will strongly depend on the development of efficient catalytic methodologies. *The main objective of our group is the development of successful strategies for synthesis of bio-active compounds and monomers using biorefinery-derived synthons as the starting materials.* We are currently articulating our research around three major thematic areas:

1 the development of solvo(hydro)thermal methods for biomass deconstruction, which enable the conversion of polysaccharides and lignin into an array of useful primary building blocks and platform chemicals;
2 the development of novel sustainable catalytic methods for the upgrade and functionalization in microfluidic reactors of primary biomass derived substrates;
3 the synthesis of value-added products on the basis of sustainable building blocks obtained through biorefinery conversion schemes.

1. Solvo(Hydro)thermal Deconstruction of Biomass

Lignocellulosic materials are rather heterogeneous in nature and are mostly composed of polysaccharides, usually accounting for 60-80% of the weight, and lignin (15-30%). The entry step in a biomass conversion scheme should enable the separation of the carbohydrate portion of the biomass from the lignin one. In this regard, organosolv methods, which consist in the treatment of biomass with organic solvents at elevated temperatures, have found broad application. Nevertheless, this approach has been aimed at the sole isolation of the lignin fraction. In order to improve the efficiency of these kinds of treatments, we design new methodologies that allow for the simultaneous isolation of an upgraded polysaccharide fraction. For example, we identified conditions for the alkaline hydrothermal treatment of sugars and biomass which are highly selective for the formation of lactic acid, a very important platform chemical for the preparation of biodegradable plastics **[1]**. This strategy has proven successful when applied to the conversion of raw biomass on a 40 grams scale. During the treatment of raw biomass, in addition to lactic acid, lignin can also be isolated, suggesting the possible use of this convenient method as entry point for new biorefinery schemes.

Besides alkaline treatments, complementary acidic hydrothermal methods, which usually results in the formation of C5 scaffolds, are also being explored. For instance, we optimized a method for the conversion of cellulose into levulinic acid, a very versatile platform chemical, which was subsequently hydrogenated with Raney-Nickel to afford γ-valerolactone **(Fig. 1) [2]**. The successive functionalization of γ-valerolactone via α-methylenation was also accomplished, in order to obtain a monomer suitable for radical polymerization. **[3]**

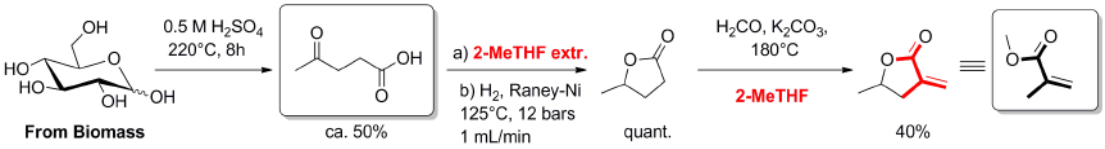

Fig. 1: Example of the synthesis of monomers from sugar via hydrothermal deconstruction and upgrade of primary building blocks.

Finally, the preparation of latex particles on the basis of such monomer was investigated as a proof of principle. The whole synthetic route showcases an example of integrated refinery scheme capable of converting lignocellulosic feedstock into value-added materials, as already shown schematically in **Figure 1**.

One of our future objectives in this area will be the screening of different solvothermal conditions in order to widen the spectrum of possible platform chemicals targets.

2. New Catalytic Continuous Flow Methodologies for the Upgrade of Bio-derived Molecules

Many of the primary products of the hydrothermal treatments of biomass can be conveniently upgraded into different platform chemicals by straightforward catalytic transformations. To reach this goal, we focus on the development of new continuous flow methodologies using supported catalysts. Traditionally, expensive and rare elements belonging to the platinum-group metals have been proposed as catalysts for such transformations. However, the use of inexpensive and abundant elements, for example iron and nickel, appears a good option to achieve the production of bio-derived chemicals in a more sustainable fashion. Carbon supported metals have been successfully applied as catalysts in the field of hydrogenolysis and hydrogenation. With this in mind, we prepared carbon supported Ni-Fe alloys by simple impregnation of cellulose from biomass followed by carbothermal reduc-

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tion **[4]**. This form of reductive treatment has proven ideal to generate carbon encapsulated nanoparticles characterized by high activity and stability. In particular, this material served as an optimal catalyst for the continuous flow reduction of a variety of biomass-derived compounds. More recently, we extended this approach to achieve the reductive amination of biomass molecules, as a general step for the preparation of intermediates in the synthesis of bioactive *N*-heterocyclic compounds **(Figure 2)**. **[5]**

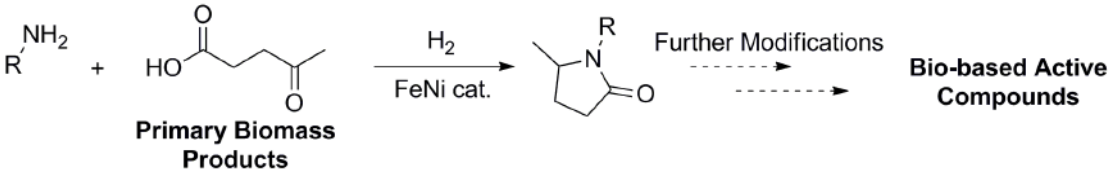

Fig. 2: Example of reductive amination as a key step for the preparation of bio-based active compounds.

In a complementary project we are pursuing the development of methodologies for the hydrogenolysis of aryl ethers, the most abundant type of linkages in lignin. We have recently showed how titanium nitride obtained as colloidal dispersion on amorphous carbon can be efficiently used as support for nickel nanoparticles,**[6]** leading to the preparation of a new composite with a high reactivity for the continuous flow hydrogenolysis of different aryl ethers and model lignin fragments. Currently, we are investigating in detail the hydrogenolytic depolymerization of lignin, which can afford a library of highly valuable aromatics scaffolds.**[7]** Lignin derived aromatics offer a unique set of functionalities (mostly polyphenols with a common phenyl propane backbone) that can give access to a well distinct chemical space upon functionalization, characterized by specific bio-activity (e.g. antioxidant activity).

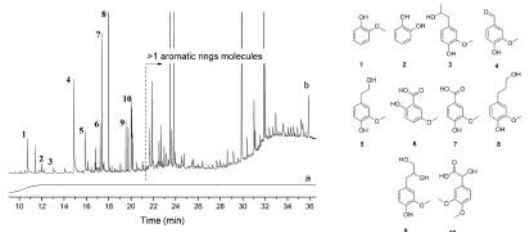

Fig. 3: Representative chromatogram of lignin hydrogenolysis over TiN-Ni for the preparation of bio-based aromatic compounds

In a series of different projects, we also exploited lignin fragments and oligomers for the preparation of porous carbons as support for heterogeneous catalysts **[8]** or nitrogen doped carbons as efficient electro-catalysts. **[9]**

3. New Value-Added Sustainable Chemicals

On the basis of the pool of molecules which can be obtained via biomass deconstruction, we design green strategies for the synthesis of sustainable building blocks and platform chemicals that can find application in polymer science and chemical biology. One of our areas of interest is the production of sustainable *N*-heterocyclic compounds. However, the synthesis of nitrogen-containing heterocycles from lignocellulosic sources remains elusive due to the lack of nitrogen in this row material. Complementing lignocellulose-derived molecules with other renewable *N*-containing precursors can sensibly increase the chemical space accessible in a sustainable manner. In this regard, amino acids have been evoked as interesting candidates. One of our first goals in this direction was the development of green synthetic methods to access sustainable imidazolium ions, which could be further transformed into ionic liquids. During the synthesis of lactic acid, pyruvaldehyde was identified as a valuable sustainable synthon **[1]**. This and other renewable dicarbonyl compounds were exploited to synthesize a library of disubstituted imidazolium ions in combination with natural amino acids by using a green modification of the Debus-Radziszewski synthesis **(Fig. 4) [10]**. The obtained compounds have proven as versatile building blocks for the preparations of ionic liquids by means of a new continuous hydrothermal decarboxylation method developed in our laboratory. This new method showed a great potential for the generation of a new family of ionic liquids that are derived exclusively from renewable precursors.

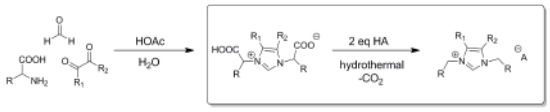

Fig. 4: Synthesis of imidazolium compounds from renewable starting materials.

Some of the so-prepared ionic liquids are under investigation as reaction media for cross coupling reactions as well as cellulose and biomass dissolution **[11]**. Recently, we employed a similar strategy also for the preparation of bio-based pyridinium zwitterions and ionic liquids using furfural (derived from sugars) and amino acids as the starting materials **(Fig. 5).[12]**

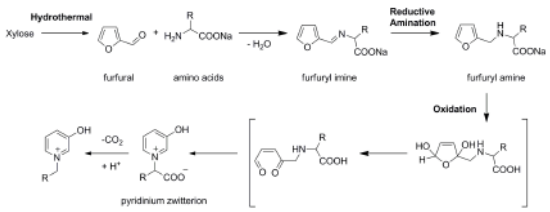

Fig. 5: Synthetic strategy for the preparation of pyridinium compounds from renewable starting materials.

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Supramolecular Porous Materials

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Scientific questions have become very complex and require close co-working of disciplines, research institutions and industry. However, such structures demand for careful communication and organization. Here, we believe that affiliation to both science and communications infrastructure is helpful to catalyse projects. Therefore, I decided to take the venture on this still emergent career path and operate as Research Coordinator employed by the MAXNET Energy.

Duties include the coordination of (internal) projects with the other partners of MAXNET Energy. Furthermore, in order to understand the needs and to stay active in the communication stream, I also work on my own research topics together with my small group, often in close collaboration with partner institutions. This allows me to further develop my scientific profile which is also a prerequisite for an effective coordination of research.

In this context, I complete my Master degree in Science Marketing at the TU Berlin.

A) Research Coordination

The MAXNET Energy pools knowledge and activities of eight different MPIs and tries to establish accelerated progress in the field of sustainable materials for energy conversion. Here, materials, measurement setups and theory for water splitting are the main focus.**[1]** Within these activities I'm responsible for the communication and matching of projects between the MAXNET Energy consortium and activities of our department.

B) Research Topics

In my group we aim to make use of rational and facile synthesis schemes towards functional porous carbon materials. **[2]**

On the one hand, salts turned out to be highly versatile alternatives for the generation of nanoporous structures. In this regard, we also develop methods to make the carbons more processable.

On the other hand, we follow the supramolecular approach where we currently make use of preorganization schemes mediated through strong but non-covalent and thus reversible interactions. Recent activities include:

- use of precursors with the ability to form hydrogen-bond structures resulting in eutectic mixtures or crystals. These intermediates can then form pre-defined, more ordered nanostructured carbons with unusual elemental composition and properties
- application of natural (poly)phenols in combination with soft-templating agents to form functional porous carbon monoliths and films
- coordination of phenols with a specific structure and metal ions to form crystalline oxocarbon metal complexes. These crystals can be further converted into porous carbons or metal-carbon composites with high degree of chemical surface functionality and preservation of the original crystal morphology such as micro cubes or small plates.

Nanoporous Carbons

Functional carbons and composites entered everyday life as they possess a variety of important properties while costs are rather low.

The final materials properties such as chemical and thermal stability, surface functionality or morphology are governed, besides others, on the molecular as well as mesoscopic level. The incorporation of heteroatoms such as nitrogen into the carbon lattice, metals or porosity turned out to be highly powerful.

However, opposed to inorganic systems the rational synthesis of functional carbons is still complicated. This is mainly related to the common necessity of high temperature treatments which essentially hinder external control during main phases of the synthesis. Therefore, approaches to circumvent this limitation are needed.

Here, we see one possibility in the "encoding of functionality" in the precursors, i.e. as much information as possible is already inherently present in the starting material. More specifically, the pre-setting/introduction of periodic binding motifs in the binding pool of carbon will lead to mosaic-like functional patterns. In this regard, dynamic processes such as (natural) assembly and bonding schemes offer internal control where especially hydrogen-bonds are convenient as they are strong but reversible at the same time.

Salts

In order allow reversibility also at higher synthesis temperatures, we invented a new tool called „salt templating".**[3]** The general concept is based on crosslinking of a precursor in the presence of a molten salt phase which simultaneously acts as solvent and template. Contrary to current methods, it is possible to proceed in a single-step synthesis, while the porogen can easily be removed by washing with water and in principal be recovered afterwards for further use.

Carbons from Eutectic Mixtures and Crystals

We found that complexation of quinones and phenols with urea leads to liquid monomer mixtures upon gentle heating with deep eutectic behaviour **(Fig. 1a)**. **[4]** These liquids can then be converted to carbonaceous nano architectures with well-defined nitrogen heteroatoms via condensation rather than pyrolysis, i.e. the formation of pyrazinic nitrogen sites in unusually high occurrence **(Fig. 1b)**. Due to the good processability and wettability of these liquid mixtures, this approach can furthermore be combined with various structuring methods such as templating, spin-coating and monolith formation **(Fig 1c)**.**[5]**

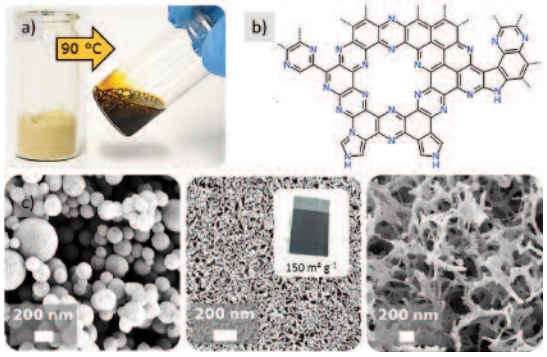

Fig. 1: a) Liquid eutectic carbon precursor mixture from heated phenol-urea powders, b) structure of the final carbon C_2N and c) Scanning Electron Microscopy images of differently processed carbons.

Additionally, depending on the quinone/phenol used we observe an ordering of the eutectic mixtures, i.e. liquid crystalline-like phases are generated which eventually contribute to the preservation of order and patterns in the final carbons. This can be pushed to the formation of actual solid crystals which then guide the final material morphology e.g. to sheets or hollow tubes **(Fig. 2)**.**[6]**

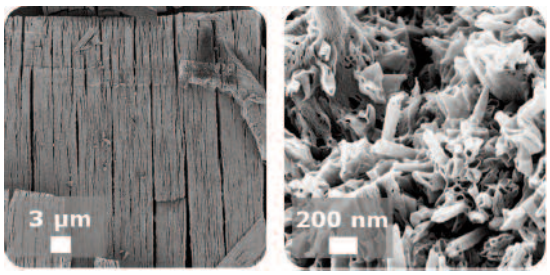

Fig. 2: Scanning Electron Microscopy images of C_2N carbons made from crystalline phenol-urea precursors.

When choosing educts without C-H bonds, the products can be generally described as a disordered version of "C_2N". It can be expected that the resulting family of N-modified carbons will effectively complement N-doped carbons and carbon nitrides in their electronic, (electro)catalytic, and sorption applications.**[7]**

Design of Oxocarbon Metal Complexes

In the case of metal coordination with ketones and organic acids, it is possible to first form macroscopic crystalline materials which can then be further converted to the respective carbon **(Fig. 3a)**.**[8]** Depending on the nature of the precursor, metal and reaction conditions, the morphology as well as porosity of the final material can be tuned. It is to be noted that the initial macroscopic structure of the crystal is retained in the final carbon which allows for convenient shaping and setting of materials properties, in spite of the applied high temperature process. It can be envisioned that structures like cubes can further orientate based on their shape to constitute network structures with hierarchical pores **(Fig. 3b)**.**[9]** This makes such materials attractive for applications where high surface areas and mass-transport in powders are important.

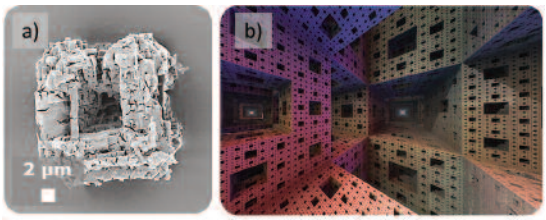

Fig. 3: a) Porous carbon cube made from an oxocarbon metal complex, b) sketch of potential 3D architectures built from porous cubes.

All these processes can be also extended to natural phenols and ketones broadening available structures while staying sustainable. With such methods in hand, it is our intention to establish a platform of facile, scalable and processable tools for the rational design of carbon nanostructures and composites.

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CARBON MATERIALS AND ELECTROCHEMICAL ENERGY APPLICATIONS

Novel Nanochemistry towards Improved Electrodes

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Introduction

The versatility of carbon materials in their physical and chemical properties together with the possibility to form and shape the morphology of carbon materials into 1D, 2D and 3D as well as micro-, meso- and macroporous structures make them indispensable for crucial technology related to new and sustainable energy schemes. Here the differentiation of physical effects (*e.g.* due to specific electronic properties) and chemical effects (due to specific surface compositions) is a difficult task. In electrochemical energy applications, where performances are often defined by accumulation or conversion of electroactive species, the influence of the morphology dictating the mass-transport properties additionally overlays such effects. The identification of the origin of performance variations is therefore even more difficult. In the "Carbon and Energy" group we are aiming to develop preparative methods to generate pores (porogenesis) and modify the porosity in carbon materials without affecting the surface chemistry and *vice versa* to elucidate structure-performance relationships in topical energy application such as fuel cells, lithium-sulfur (Li-S) batteries and lithium-oxygen (Li-O_2) batteries.

1) Salt-Templating to Ionothermal Carbonization: Carbons with Taylor-made Porosity

Recently the use of inorganic salt melts for the preparation of porous carbons has gained a lot of attention in the scientific community.**[1-4]** We previously reported on a novel one-step salt templating carbonization route using inorganic salt melts to prepare highly nanoporous nitrogen doped carbons (NDCs) from thermolysis of carbonizable ionic liquids.**[5]** The ionic liquids were used as precursors as they form homogeneous mixtures with the inorganic salt melts until the carbonization of the organic phase initiates nanoscopic phase separation (**Fig. 1a**). Aqueous removal of the inorganic salt phase after the carbonization creates nanoporosity. The actual size of the pores increased the lower the melting point of the used inorganic salts was. This trend was rationalized by separation kinetics *via* longer demixing times or lower viscosity, respectively. In a recent work we investigated the relation of the inorganic salt composition on the porogenesis in more detail for a biomass-derived nitrogen-rich carbon precursor adenine.**[6]** Stepwise increase of the NaCl fraction in NaCl-$ZnCl_2$ mixtures revealed a couple of interesting facts. 1) Very fine tuning of the pore size distribution could be realized by incremental changes in the NaCl fraction **(Fig. 1b)**. 2) The average pore size increases with increasing melting points of the inorganic salt mixture, and 3) for lower NaCl fractions a sudden loss of porosity is observed. The fine tuning of the porosity of carbon materials by simple means, like the precursor salt ratio, allows for simple access to taylor-made carbons, adapted precisely for the application addressed

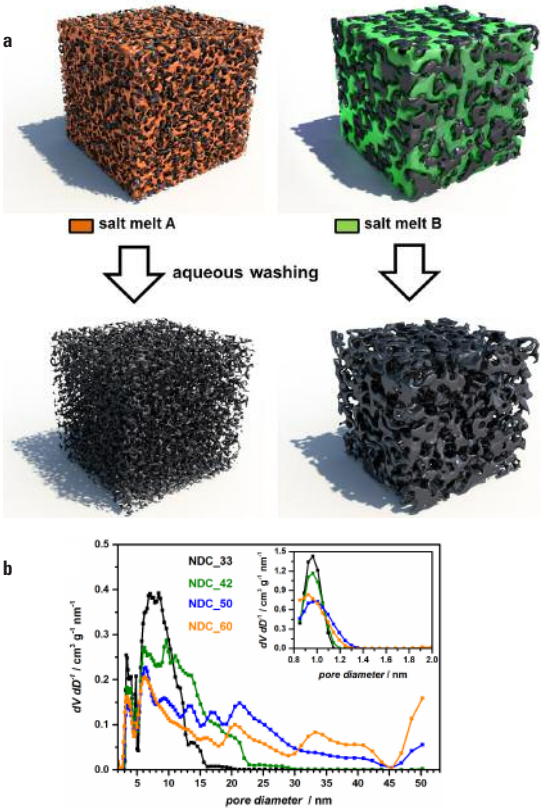


*Fig. 1: a) Scheme of the pore synthesis of carbon materials by carbonization of organic matter in presence different inorganic salt melt A and B (ionothermal carbonization). b) pore size distributions for adenine-derived carbon in NaCl-$ZnCl_2$ mixtures (in NDC-XX, XX stands for {mol%NaCl} (Fig. adapted from ref **[5]**).*

We extended the initial concept of ref.5 to glucose-derived carbon, where we obtained a linear relationship between specific surface area and fraction of KCl in KCl-$ZnCl_2$ mixtures.**[7]** In case of the adenine-derived carbons we discovered a strong pore size effect in the electrocatalytic activity of the obtained carbons **(see section 2)**. The other observations clearly point to an interplay of the inorganic salt with the organic precursor, which was previously "masked" by the very similar properties of the different ionic liquids. In fact the inorganic salt melt can be – in agreement with the original work, regarded as a high temperature solvent in the process. In this light pore generation can generally occur by means of dissolution/dispersion of the organic phase inside the salt melt or dispersion of the salt melt inside the organic matter. This insight improves the understanding of the sometimes more and sometimes less successful formation of biomass-derived activated carbons using $ZnCl_2$, that is a dispersion of nanoscopic $ZnCl_2$ droplets inside the carbonized biomass precursor. **[8]**.

Improvement of current "activation" protocols can therefore be expected from adaption of the salt composition to the biomass properties and *vice versa*. Together with the "Biorefinery and Sustainable Chemistry" group we optimized the introduction of porosity and surface area throughout car-

bonization of the highly abundant natural biopolymer lignin.**[9]** The carbonization of nitrated lignin (NL) in a 1:5 weight mixture with eutectic KCl-$ZnCl_2$ at 850 °C under inert gas flow lead to a nitrogen doped micro and mesoporous carbon (NL-C) with 4.8 %N and 1600 $m^2\ g^{-1}$ specific surface area. The cheap, biomass-derived material performed comparable to state-of-the-art metal-free (NDCs) and iron-containing carbon (FeNDCs) electrocatalysts in the important oxygen reduction reaction (ORR), which for instance restricts today's fuel cell performances **(Fig. 2)**.

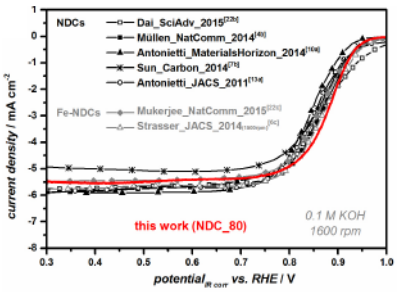
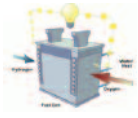


*Fig. 2: Comparison of the rotating disk polarization curve (ORR in O_2 saturated 0.1M KOH) of NL-C with different literature benchmarks for non-noble metal catalysts (Fig. adapted from ref. **[9]**).*

2) Mass-Transport Conditions are Crucial in Many Energy Applications

In electrochemical energy applications very challenging morphological electrode conditions are faced. In context of fuel cell electrodes this is typically named as three-phase boundary problem, due to the necessary spacial coincidence of the solid electrode/catalyst, the gaseous reactants and the solid electrolyte. The mechanistically related next generation battery concepts of Li-S batteries and Li-O_2 batteries even show additional deposition of the solid products on top of the electrode/catalyst (Li_2S or Li_2O_2), *i.e.* a four-phase boundary. The deposition of discharge products is herein blocking the active site and limits performances. Moreover the reaction kinetics are strongly affected by the mass transport properties of the electrode, e.g. the delivery of reactants. In our research in 2016 we came up with a few concepts on how to improve the device performances with morphologies for improved mass-transport characteristics, shown in examples for 1) fuel cells, 2) Li-S batteries and 3) Li-O_2 batteries.



The previously mentioned fine tuning of pores of ionothermal NDCs (see section 1) revealed a strong limitation of ORR performances due to the presence small bottle-neck pores. Chemically identical carbon materials showed clearly improved performance *via* opening of nanoscopic bottle-neck pores despite a clear reduction of active surface area **(Fig 3.)**. These results motivate the revisiting of the pore systems of the currently best electrocatalysts with a potentially large space for improvement of ~100 mV (*i.e.* ~8 %).**[6]**

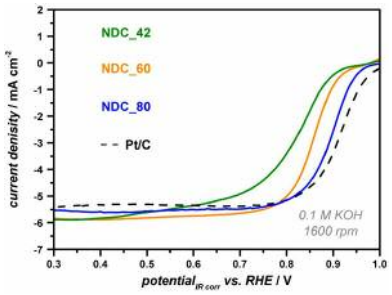


*Fig. 3: Comparison of the polarization curves (ORR in O_2 saturated 0.1M KOH) of adenine-derived NDCs with different pore size distributions **(see partly in Fig. 1)** and with the platinum on carbon benchmark catalyst. The respective active surface areas in $m^2\ g^{-1}$ are ~2800 (NDC_42), 2550 (NDC_60) and ~1750 (NDC_80). (Fig. adapted from ref. **[6]**.)*

Limited ion wiring due to reduced electrolyte wetting in Li-S batteries was shown to allow for the direct conversion of Li_2S to S_8, bypassing the formation of parasitic polysulfides that cause the most severe downside of this technology – the strong capacity fading. The supply of ions was limited by a nitrogen doped carbon layer surrounding the Li_2S particles. A peculiarity here is that the carbon layer was also used as a high temperature reducing agent of lithium sulfate nanoparticles in the synthesis to obtain the desired Li_2S nanoparticles **[10].**

Vertically aligned carbon nanosheets (CNS) display advantageous mass-transport properties due to their open card-house structure.**[11]** The material can act as an efficient ORR catalyst *e.g.* in Li-O_2 batteries. Electrodeposition of transition metal hydroxide ($M(OH)_x$) nanoparticles creates a nanocomposite with bifunctional catalytic properties, because the $M(OH)_x$ act as catalyst for the reverse reaction (oxygen evolution) that is crucial for the recharging of the battery (Fig. 4). A very interesting effect herein is that the polar discharge product (Li_2O_2) is deposited directly on the hydroxide particles, *i.e.* the catalyst for the recharging, instead of blocking the active discharge sites.

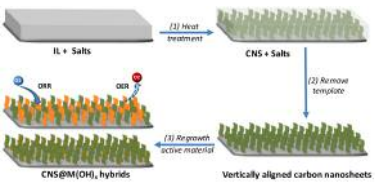


Fig. 4: Scheme of the bifunctional nanocomposits of vertically aligned CNS with $M(OH)_x$ with enhanced mass-transport properties and selective deposition of the discharge product (Li_2O_2) on the $M(OH)_x$ catalyst for the recharging.

The possibility for the discharge product to form hydrogen bonds with the transition metal hydroxides mediates nucleation directly on the recharge catalysts leading to very high capacities because of the "clean" catalyst surface.**[12]**

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Electron Microscopic Studies of Colloidal Systems and Interfaces

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The study and the understanding of struture/property, structure/function and chemical synthesis/structure relations of both synthetic and biological colloidal materials are important for the development of new technologies and materials.

Synthesis of bio-inspired particles, inorganic nanoparticles and organic-inorganic hybrid materials, nano-porous carbon, functional carbonaceous materials, the preparation of polymer particles, biomimetic materials and hybrid materials, membranes, emulsions, active coatings and interfaces and functional supramolecular organizates are in focus on the interdisciplinary research in the institute.

Transmission electron microscopy, high-resolution scanning electron microscopy and environmental electron microscopy are suitable techniques to determine the characteristic structural parameters such as the shape, size and size distribution of colloidal particles and the pore size of mesostructured networks, the diameter of nanofibrills, the spatial arrangement of nanoparticles with a high electron optical resolution.

Using cryo-scanning electron microscopy the internal morphological structures of aqueous systems like concentrated oil/water emulsions can be characterized. The combination of energy-dispersive X-ray spectroscopy and high-resolution scanning electron microscopy is a powerful analytical tool to determine the local chemical composition and the spatial elemental distribution on surfaces and interface structures of solid materials.

As a central service lab the electron microscopy group performs scientific routine measurements for the whole institute, which are demonstrated in different reports of this issue. Because of the organization of the institute, there is a close collaboration with other departments of our institute, but also with the Max Planck Institute of Molecular Plant Physiology and the University of Potsdam.

Some of the interesting results of electron microscopic investigations are presented here.

In general the aqueous hetero-phase polymerization is used to form stabile solid colloidal polymer particles as single spheres. The free radical polymerization variant allows the synthesis of block copolymers. Thus, both hydrophilic N-isopropylacrylamide (NIPAM) and hydrophobic monomers styrene can be added in subsequent polymerization steps offering a wide variety of possible block copolymer structures and particle morphologies **[1]**. A peculiar particle morphology was obtained if instead of a hydrophilic polymer, hydrophilic molecules such as β-cyclodextrin (β-CD), sucrose, glycerol, and other low molecular weight alcohols (ethanol and 1-pentanol) are used as reductant. Electron microscopic investigations revealed the fine grained morphology of stable colloidal clusters (multiple suspension particle (MSP) morphology) with subtle differences depending on the particular molecular structure of the reductant **(Fig.1. a,b)**.

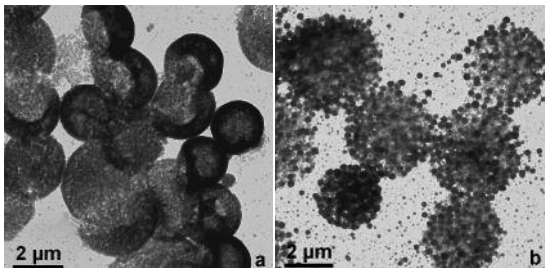

Fig. 1: MSP morphology of PNIPAM–PS block copolymer particles prepared with a) ethanol, and b) 1-pentanol as reductant.

Each MSP has a size of up to few micrometers (1–4 µm) and contains few hundred polystyrene (PS) particles with a diameter smaller than 100 nm which are evenly dispersed in a PNIPAM matrix. It is to emphasize that the numerical data refer to the visible particles in the 2D projection of the electron microscopic images and these quantitative data hold for the particular clusters under consideration but nevertheless, these values illustrate the generally observed trend. The MSP formation is not restricted to styrene as second stage monomer **[2]**.

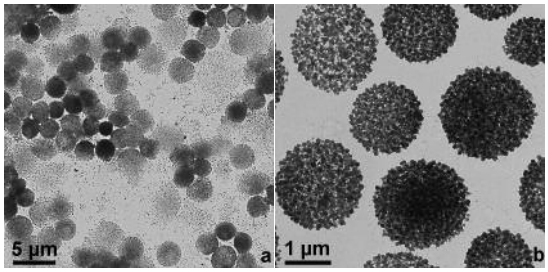

Fig. 2: MSP morphology of a) PNIPAM–PBMA with complex of PEG in α-CD and b) PNIPAM–PVAc–PS block copolymers with β-CD as reductant.

The MSP morphology also has been observed for other monomers such as butyl acrylate (BA), butyl methacrylate (BMA) **(Fig. 2)**, and vinyl acetate (VAc). The lower film formation temperature of poly-VAc, poly-BMA, and poly-BA causes the indistinct appearance of these particles. Sequential addition of VAc and styrene leads to triblock copolymer MSP (PNIPAM–PVAc–PS). PS is the outermost layer and prevents film formation of the nanoparticles **(Fig. 2 b)**.

The morphology of the block copolymer particles generated via redox-initiated aqueous heterophase polymerization with NIPAM depends on the nature of the reductant **[2]**. Using α-CD as reductant leads to stable MSP too. The polymer aggregates are a physically cross-linked and the size of the aggregates is smaller than 4 µm.

Not only in polymer synthesis but also in inorganic aqueous dispersions the stability of colloidal metal oxide nanoparticles is of our research interest.

In combination of dynamic light scattering and transmission electron microscopy the aggregation behavior of hematite and hematite-akageneite composite nanoparticles stabilized with alkyl sulfates was studied in dependence of the pH in the range of 3–11 **[3]**. The iron oxide nanoparticles were dispersed in an ultrasonic batch at solid-to-liquid ratio of 1:5000 by mass in aqueous solutions.

Whereas the ζ potential decreases continuously from lower to higher pH-values, the size of the aggregated particles shows a maximum at the isoelectric point (IEP). The maximum in the level of aggregation matches the minimum in the stability condition of the dispersion.

Typical primary nanoparticles in hematite dispersions are nearly spherical and are 20–80 nm in diameter **(Fig. 3a)**. Most of the particles are in the range 40–70 nm in diameter, and the fraction of particles smaller than 40 nm or larger than 70 nm is low.

Primary particles in hematite-akageneite composite dispersions show two different shapes. On the one hand we found nearly spherical particles similar in shape to those presented in **Fig. 3a,** but considerably larger (80–120 nm in diameter). On the other hand we found lath-shaped akageneite particles of about 100 nm wide and 400–500 nm long **(Fig. 3b)**.

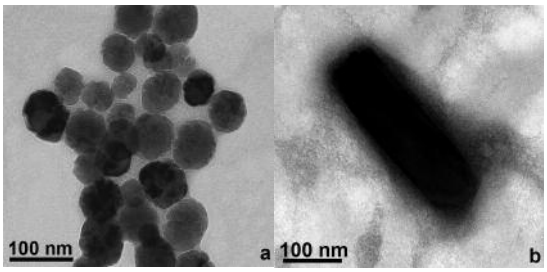

Fig. 3: Primary hematite nanoparticles a),and primary lath-shaped akageneite particle b)

In dispersions of hematite stabilized with C12, C14 and C16 (concentrations in the range 0.1–1 mM) the mean particle diameter of aggregates are pH-independent **[3]**. Typical hematite aggregates are presented in **Fig. 4a.** The dispersion contains different structures, which consists of smaller and bigger aggregates of primary particles, as well as single primary particles. In hematite-akageneite composite dispersions practically all primary particles are aggregated. Even relatively small aggregates contained both lath-shaped particles and spherical particles as illustrated in **Fig. 4b.**

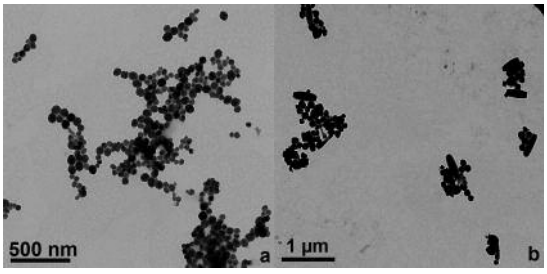

Fig. 4: Aggregates: (a) in dispersion of hematite in 0.1 mM sodium hexadecyl sulfate, pH 9.5, ζ-potential -54 mV; (b) in dispersion of hematite-akageneite composite in 0.1 mM sodium hexadecyl sulfate, pH 4.28, ζ-potential -61 mV.

Apparently heteroaggregation involving both spherical and lath-shaped particles in hematite-akageneite dispersions is preferred over homoaggregation.

All of the electron microscopic investigations confirm the presence of aggregates in dispersions of iron oxides stabilized with alkyl sulfates originally found by light scattering. These are the first experimental results, which directly shows formation of mixed aggregates in dispersions composed of particles having similar chemical compositions (iron oxides), and different morphologies.

Both the colloidal stability and the interfacial morphology of oil/water (O/W) Pickering emulsions play an important role within the development of functional micro- and nanocontainers.

The application of the Layer-by-Layer assembly approach for Pickering emulsions not only stabilizes the emulsion particles, but also closes the interstitial pores of the emulsion nanoparticulated shell thus providing its controlled permeability and release of the materials dissolved in the oil core.

Here, the weak polyacid poly(methacrylic acid sodium salt) (PMAA, Mw~9500g/Mol) and the polybase poly(allylamine hydrochloride) (PAH, Mw~17000g/Mol) were selected for the surface modification of oppositely charged alumina (Al_2O_3) and silica (SiO_2) nanoparticles. The size of the stabile core/shell dodecane/water emulsions droplets are in the range of 500 nm to 2 µm.

There are different shell morphologies of oil/water/silica and oil/water/alumina emulsion droplets in dependence of the chemical surface modification of the silica nanoparticles with PAH and the alumina nanoparticles with PMAA.

The narrow distributed silica nanoparticles with a mean diameter of about 20 nm covers the oil phase by a closed packed mono layer (pH=8.5) **[4]**, whereas the alumina nanoparticles with a mean diameter of about 4 nm form a dense and complete layer of a thickness of about 30 nm (pH=5) consists of aggregates of alumina nanoparticles **(Fig. 5)**.

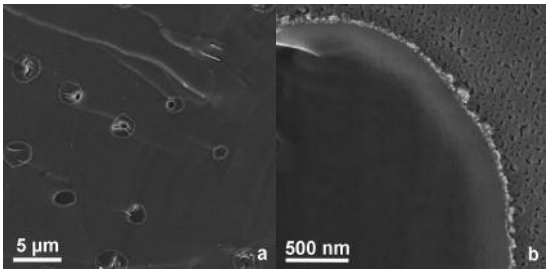

Fig. 5: Dodecane emulsion droplets stabilized with surface modified alumina nanoparticles (a,b)

Above pH > 9, flocculation of silica nanoparticles takes place **[5],** consequentially, the dodecane droplet shell consists almost entirely of particle aggregates. The know-how acquired during development of particle stabilized nano- and microcontainers is applied for encapsulation of different active chemical and biological components.

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Materials for Photo and Electrochemical Reactions

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One of the promising technologies for future alternative energy sources is the direct conversion of sunlight into chemical and electrical energy by using photocatalysis or photoelectrochemical cells (PEC), respectively **[1]**. The greatest challenge in these fields is to develop new types of advanced materials with the desired electrical and optical properties that will replace the conventional raw materials that are currently used. Photocatalysis has attracted great interest over the last decades, especially for its potential to produce clean and cheap renewable energy without dependence on fossil fuels and without carbon dioxide emission. Photocatalysis applications span from many fields such as: solar fuel production, water splitting, photo-degradation of pollutants, and catalysis of other chemical reactions, e.g. for the production of fine chemicals. The photocatalytic operation usually involves photoactive semiconductors, mostly the ones which consist of metal-based semiconductors like TiO_2, ZnO, Fe_2O_3, and many more. For efficient photocatalysis, the internal recombination rate of the charge carriers should be sufficiently low to allow electron/hole migration to the surface of the catalyst, in order to perform the desired reaction. In this system, the photocatalyst is dispersed within the desired solution, and under illumination the charges transfer to the solution and start the desired reaction **(Fig. 1)**.

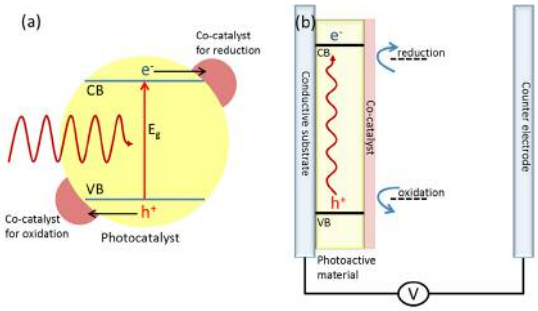

Fig. 1: Illustration of two photocatalysis systems.

The second system is based on photo electrochemical cell (PEC) which is based on semiconductor-liquid junctions which can be relatively efficient with respect to the first system, due to improvement of charge separation under illumination. The PECs can be used in order to convert the solar radiation into chemical energy (i.e. water splitting) or to electric energy (i.e. solar cells). Typically for efficient photo (electro) catalysis, an additional co-catalyst, which is currently mostly based on noble metals, is needed in order to increase the wanted reaction activity and rate. Although in the last years a significant progress has been made in this field, it is still an essential task to find efficient and low cost materials as photoactive materials and co-catalysts. More importantly, it is necessary to gain a basic understanding of the physical properties and the fundamental operation mechanisms in this field.

Metal Free Carbon Nitride-Based Materials

While most of the research in this field is focused on metal based semiconductors (metal oxides, sulfides and nitrides) as photocatalysts, in the last years metal-free graphitic carbon nitride (C3N4) materials have attracted widespread attention due to their outstanding (electro)catalytic and photocatalytic activity.

Despite of the great progress in C_3N_4 synthesis, it is still a standard problem of C_3N_4 chemistry that only rather disorganized textures with small grain sizes are obtained. Therefore, it is essential to find new and simple synthetic pathways to form highly ordered structures of carbon nitride with controlled electronic, optical and catalytic properties.

Recently, this group used the supramolecular chemistry approach to synthesize well-defined structures of C_3N_4 such as hollow boxes, spheres and spherical macroscopic assemblies **[2-4]** with the possibility to control their photophysical and photocatalytic properties **(Fig. 2)**. Supramolecular chemistry provides a great opportunity for the synthesis of nanostructured materials without any further templating techniques. The supramolecular approach includes the use of non-covalent interactions such as hydrogen bonding to form order between building blocks for the desired synthesis. Hydrogen bonds are very useful for controlling molecular self-assembly thanks to the reversibility, specificity, and directionality of this class of interactions. The structure of the final products can be controlled by choosing the appropriate monomers and solvents for the synthesis. The starting monomers will organize into different structures according to their ability to form hydrogen bonds in the given solvent and form ordered and stable aggregates which consecutively define the resulting materials.

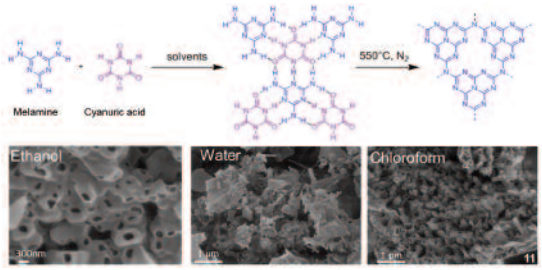

Fig. 2: A graphic presentation of hydrogen-bonded supramolecular complex and the resulting carbon nitride materials in different solvents.

However, for photoelectrochemical applications a direct connection between C_3N_4 and the conductive substrates is needed. Due to the large particle size and the insolubility of C_3N_4 in most solvents, the use of common deposition techniques such as spin-coating and screen-printing results in poor coverage and conductivity. Therefore it is essential to find a new and simple synthetic pathway to grow C_3N_4 on different substrates. Using the supramolecular approach we were able to grow highly ordered carbon nitride structures on different substrates both in solid state and liquid-based growth **[5-6]**.

Thanks to the new deposition methods we were able to show, for the first time, the reduction of water to hydrogen using a metal-free C_3N_4 electrocatalyst. Moreover, we found that the C_3N_4 can act as an absorber and electron accepting layer in polymer solar cell which exhibits a remarkable open circuit voltage of 1 V.

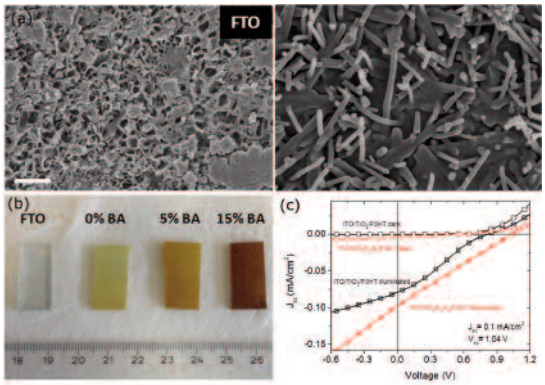

Fig. 3: (a) SEM images of carbon nitride deposited on FTO and glass. (b) Photograph of bare FTO and FTO with C_3N_4 films modified by different amounts of carbon. (c) J-V curves of TiO_2/C_3N_4/P3HT and TiO_2/P3HT solar cells measured in darkness and under 100 mW/cm^2 AM 1.5G illumination.

Carbon Nitride Based Hydrogels

In our lab we synthesize carbon nitride hydrogel with good mechanical properties, high selective pollutants adsorption capacity and photodegradation. Moreover, carbon nitride hydrogel show very promising activity as photocatalyst for the water splitting applications. The synthesis of the carbon nitride hydrogel, with adjustable shape, i.e. cylindrical and tube-like, is acquired through photo-polymerization of poly(N,N-dimethylacrylamide) (DMA) in the presence of well-dispersed highly photoactive carbon nitride as initiator in aqueous solution. In our current research we synthesize new carbon nitride hydrogels toward their utilization as catalysts for various reactions.

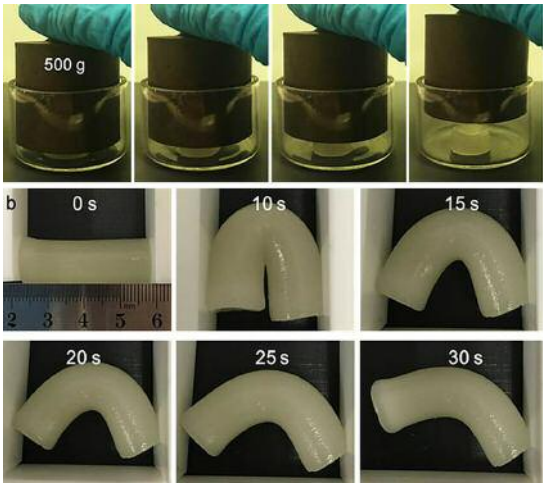

Fig. 4: Carbon nitride based hydrogel.

Ceramic Metals as Water Splitting Electrocatalysts

An important topic of our group is the development of new, low cost and efficient materials as electro and co-catalysts for energy related applications (i.e. water splitting). Electrochemical water splitting to hydrogen (HER) and oxygen (OER) plays a growing role in the fabrication of alternative energy devices due to the need of clean and sustainable energy. Nickel-based materials have attracted enormous attention because of the flexible catalytic properties, along with low price and high abundance when compared to noble metals.

We developed a facile and easy synthesis of large- scale nanoporous, nickel based materials (Ni, Ni_5P_4, Ni_3N and Ni_3S_2), partly embedded in an amorphous matrix of a carbon-nitrogen material or directly grown on Ni substrates. The obtained materials show remarkable performance in the electrochemical production of hydrogen and oxygen both in terms of low overpotential and high current densities. In sum, the activity of these materials results in a high overall water splitting efficiency.

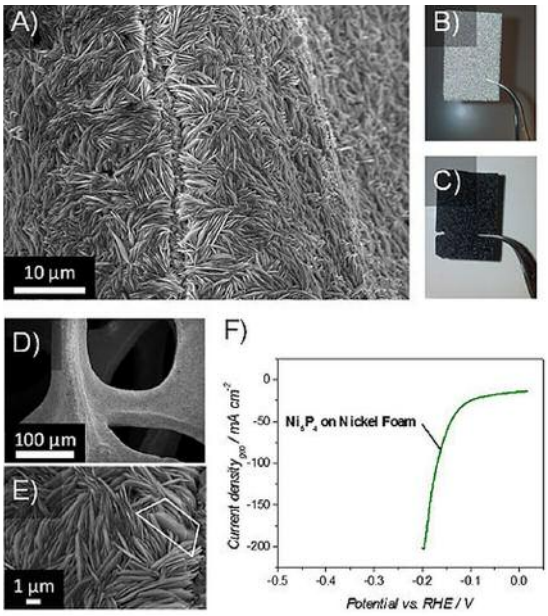

Fig. 5 (a) SEM image of Ni_5P_4 on Ni foam (b) picture of Ni foam and (c) modified Ni_5P_4/Ni foam and the corresponding SEM image of (D-E) the modified foam. (f) Linear sweep voltammetry of Ni_5P_4/Ni foam which shows the hydrogen evolution reaction activity.

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Polymer Dispersions / Heterophase Polymerizations

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Heterophase polymerization (HP) is a centennial technology and the base for producing a great variety of polymer dispersions in both laboratory and industrial scale. Better understanding of the basics of HP and educating students on this topic is of general scientific and economic interest and a goal in the very core of the activities of our research. Amongst others the following results have been published 2015-16.

Swelling of Latex Particles and the Role of Monomer Drops during Heterophase Polymerization

The role of monomer drops went unnoticed for many decades. It is state of the art to consider the monomer drops play an only passive role as storehouse for the monomer since the 1940-ies of the last century. Accordingly, the monomer molecules enter the polymer particles from the drops via diffusion through the aqueous phase. However, these state of the art concepts are challenged by new experimental and simulation results **[1, 2]**. Taking advantage of an experimental method which was previously developed in our group **[3]** we were able to prove that fast swelling of polymer samples cannot occur via diffusion of individual molecules of the swelling agent through the aqueous phase but requires direct contact with drops of the swelling agent **(Fig. 1)**.

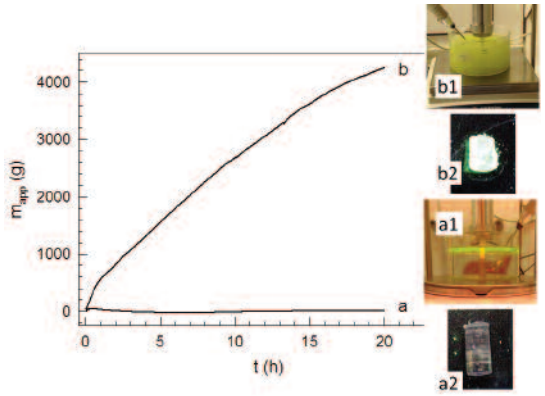


Fig. 1: Influence of the stirring rate on the swelling of crosslinked polystyrene with ethyl benzene labeled with water-insoluble fluorescence dye; the graph shows the temporal development of the swelling pressure (expressed as apparent mass, m_{app}); curve a – unstirred (only diffusion, image a1), b – vigorous stirring (drop formation and advection, image b1); fluorescence of the polymer sample (image b2) proves successful swelling in contrast to image a2

The conclusions drawn from these non-polymerization experiments for the conditions during HP are impossible directly to prove in polymerization experiments. However, simulation results using Fick's laws support the necessity of direct contact between monomer droplets and latex particles for a sufficiently high monomer concentration inside the particles as observed during emulsion polymerization **(Fig. 2) [4]**. For monomer concentration $C_{M,P} \geq 2.6$ M which is in accordance with Fick's law also necessary at the particle – water interface, the monomer diffusion is faster than propagation ($f^2_{Th} < 1$) and equilibrium swelling is maintained. If however, $C_{M,P} < 2.6$ M the replenishment of monomer via diffusion is not fast enough and the particle, with respect to monomer, starves out.

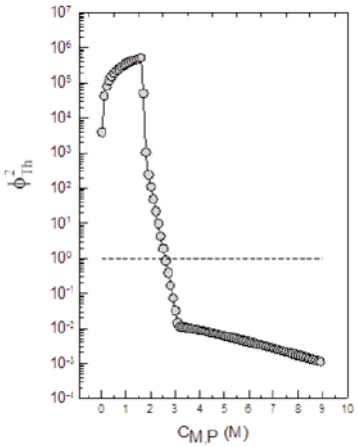
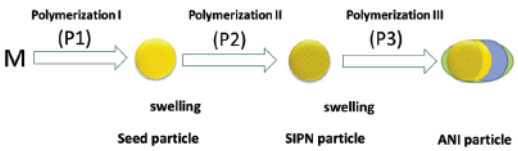


Fig.2 Correlation of the Thiele modulus (f_{Th}) with the monomer concentration inside a 100 nm particle ($C_{M,P}$) containing one polymerizing radical; the calculation was made with assuming an equilibrium situation with respect to $C_{M,P}$ at the particle interface and inside $\Phi^2_{Th} = \frac{k_p C_{M,P} \cdot r_0^2}{\tilde{D}}$

Swelling-Induced Formation of Anisotropic Latex Particles

The mass production of non-spherical latex particles directly via aqueous heterophase polymerization is quite a tedious process **(Fig. 3)** and requires more than one subsequent polymerization step, typically three with additionally repeated purification stages in between **[5]**.



Fig, 3 Illustration of the procedure for the synthesis of anisotropic particles via the direct polymerization route comprising three consecutive polymerizations (P1 – P3) and two swelling steps; typically but not necessarily the monomers for P1 and P2 are the same, however, P2 is carried out in the presence of a crosslinker and leads to the formation of a semi-interpenetrating network (SIPN), and for P3 a different monomer can be chosen; the different colors sketched in the anisotropic particles represent different polymers assumed to be in the final particles; yellow – SIPN portion, blue – portion of the polymer generated during P3, green – mixed portion of polymer (mainly due to chain transfer to polymer)

In addition, the last polymerization step requires SIPN particles. The experiments described so far in the public scientific literature seemingly are in agreement with the mechanistic idea based on elastic network relaxation by increasing temperature.

Here we communicate experimental results proving that the swelling of SIPN seed particles is the crucial step for the synthesis of anisotropic polymer particles via seeded heterophase polymerization but not the increase of temperature **(Figure 4) [5]**.

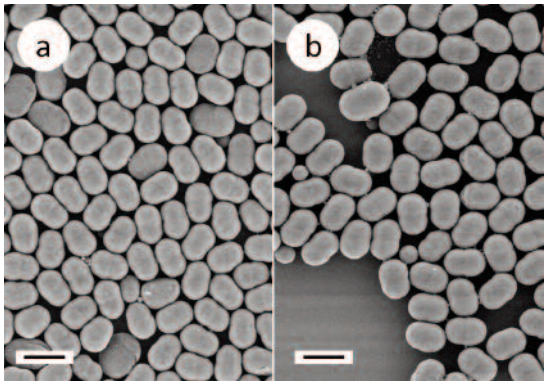


Fig. 4. SEM micrographs of anisotropic particles obtained with V65 at 70 °C (image a) and with Irgacure® 819 at room temperature (image b); styrene as monomer during P1 and P2, methyl methacrylate as monomer during P3; scale bar 2 µm

The isothermal deformation of micrometer-sized spherical SIPN particles due to swelling can be directly observed with light microscopy **Figure 5**). The degree of deformation depends on both the time after addition of the swelling agent and the distance of the particles from the swelling agent – water interface.

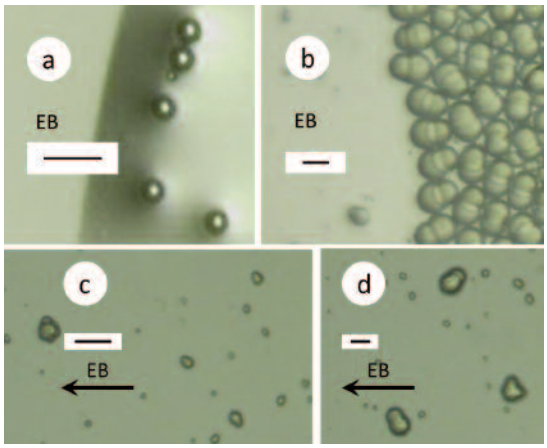


Fig. 5. Optical micrographs illustrating the development of polystyrene-SIPN particles' morphology during swelling with ethyl benzene (EB) over time; a – before, b – 12.5 h, c – 12 min, and d – 44 min after the addition of EB to the cuvette

The experimental data show that the direct formation of anisotropic colloidal polymer particles via aqueous heterophase polymerization is essentially controlled by the entropy gain of the linear fraction in the semi-interpenetrating network of the seed particles during swelling. This conclusion is supported by simulation results with a thermodynamic model. The larger compartment of the anisotropic particles contains the linear polymer chains and exhibits a volume-based swelling ratio of about 130 compared to about 7 of the smaller section containing the crosslinked polymer fraction.

Ionic Liquids Can be Used to Make Durable Wood Connections

The weighing method as described recently **[3]** is an easy to use and versatile tool to study also the swelling behavior of wood. The measuring system is open and hence, during the measurements the composition of the swelling agent can be changed without interrupting the data recording. This feature allows transient measurements, i.e. following uptake and release of volatile swelling agents. Studying the swelling of wood samples with a mixture of ionic liquids and water revealed a particular behavior **[6]**. On the one hand water swells wood much faster and stronger than the ionic liquid alone and on the other hand it facilitates the uptake of the ionic liquid. Transient studies have shown that water evaporates alone but the ionic liquid remains in the wood causing a sustained swelling. The durable swelling with the ionic liquid is useful for the construction of permanent joints in wood-containing assemblies. To detach the beech cylinder from the aluminum ring **(cf. Fig. 6)** requires 270 N. Another benefit for the application of wooden construction can be expected with respect to antifouling and antibacterial protection because it is known that ionic liquids are effective in this sense.

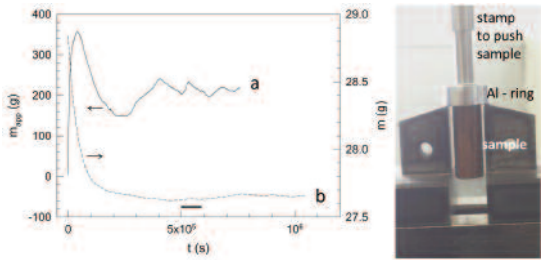


*Fig. 6. **Graph:** following the swelling of a cube of spruce wood (edge length 20 mm) with water (1.1 g) added 4 days after the addition of ionic liquid (1-hexyl-3-methylimidazolium chloride) (m_{app}, solid line a, left y-axis) and the weight loss (m, dashed line b, right y-axis); the short solid line parallel to the x-axis represents 24 hours; **Image:** beech wood cylinder (outer diameter in dry state of 8 mm) connected to an Al ring (inner diameter of 8.3 mm) by swelling with ionic liquid (ethylammonium nitrate) prepared for measuring the force to detach*

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Poly(ionic liquid)s as a Multifunctional Materials Platform

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Poly(ionic liquid)s (PILs) are polymers produced *via* polymerization of monomeric ionic liquids (ILs).**[1]** The marriage between ILs and polymers combines synergistically some unique properties of ILs with the general processable and mechanically stable profile of polymers. Thus PILs possess an unusually broad spectrum of properties and functions that attract tremendous interest in the fields of polymer and materials science. The aim of the current study on PILs is generally to understand their fundamental physics and chemistry, as well to realize their numerous materials applications, which are preferentially energy and environment-oriented. Our group is pioneering the PILs research, and devotes itself to discovering new science and practical usage of PILs in membrane technology **[2-3]**, colloidal science **[4-5]**, responsive materials **[6-8]**, innovative stabilizers **[9]**, and carbon nanostructures **[10]**.

PILs for Nanoporous Carbon Membranes

Freestanding nanoporous carbon membranes hold great promise in catalysis, water treatment, biofiltration, gas separation and optoelectronics, just to name a few, because of their structural integrity, continuity, and purity. When they are used as an electrode in electrochemical energy conversion/storage or nanoelectronic devices, precise control over key structure parameters and synthetically easy access to membranes of large size and large surface area, is highly relevant but cannot be fully met by the state-of-the-art synthetic protocols. These structure parameters include the atomic order, local chemical composition, nanoscale morphology and complex pore architecture. In this context, the PILs group reported recently a bottom-up approach to fabricate hierarchically structured, nitrogen-doped, graphitic nanoporous carbon membranes (termed HNDCMs) *via* morphology-retaining carbonization of a porous PIL membrane precursor (**Fig. 1a**) at low-pressure under N_2 atmosphere **[2]**. This is a joint project with Professor Tom Wu in the King Abdullah University of Science and Technology (KAUST).

The HNDCMs produced at 1000 °C, are conductive (200 S/cm at 298 K), N-doped (5.7 wt%), and graphitic (single-crystal-like). In addition, the HNDCMs bear a hierarchical porous structure with two sets of pores: a set of large pores of 30nm - 2μm (pore set I) and a set of small pores of < 30 nm (pore set II). A unique feature of the HNDCMs is the presence of a pore size gradient of pore set I across the membranes, with large pores on the top and small ones at the bottom (Fig. 1B-1E). Gradient property in materials science is exotic and useful to tailor materials property, where high-energy interfaces in multicomponent systems can be avoided. Gradient property is a core difference between HNDCMs and powderous carbons, as well as common porous carbon membranes. The HNDCMs are appealing as binder-free electrodes to be used in electrochemical energy devices due to the high electron conductivity, catalytically active sites stemming from nitrogen-doping, and hierarchical pore architecture. As a proof-of-concept, Co nanoparticles could be loaded in these membranes and served as high performance electrocatalyst for H_2 evolution in alkaline condition at low overpotential. In the future, HNDCMs might have the potential to be further used to replace the powderous carbon electrodes in many other electrochemical energy devices, such as batteries and fuel cells, to improve long-term electrochemical stability.

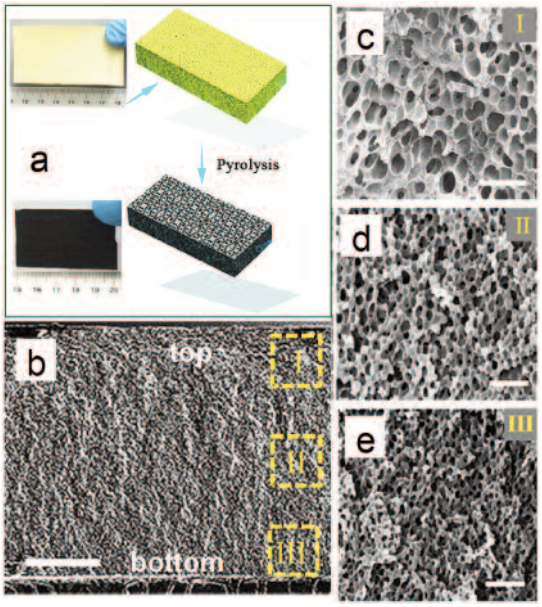

Fig. 1: a) Synthetic scheme towards nanoporous N-doped gradient carbon membranes. The paragraphs on the left are a freestanding porous PIL membrane before (top, 7.2 x 3.3 cm^2) and after carbonization (bottom, 5.2 x 2.5 cm^2). b) SEM cross-sectional view of the carbon membrane. Scale bar 20 μm. c-e) Enlarged SEM images of the local cross-sectional areas (boxes I, II and III). Scale bar: 500 nm.

PIL ellipsoid-like Nanoparticles

Both the surface and the inner morphology of polymer nanostructures are crucial to define their properties and functions, and require precise control. Versatile techniques and methods have been devoted to this endeavor, which are dominated by manipulation of their shapes, surface functionalities or dimensions, leaving their interior rarely addressed. The capability to tailor not only the overall shape but also fine interior represents a high-level of control over characteristics of polymer (nano)particles that is inevitably required for task-specific functions and applications. When particles are downsized to <50 nm, *i.e.* approaching the size of some individual polymer chains, suitable synthetic approaches or fabrication techniques are missing in polymer science. This piece of knowledge is now harvested in our investigation of 1,2,4-triazolium PIL nanoparticles, which is a joint project with the Schmidt group in the Colloidal Chemistry department **[4]**. In these extremely small nanoparticles (below 50 nm and bearing sub-5 nm domain size), we identified and analyzed an unusually striped ellipsoid-like morphology **(Fig. 2)**. The chem-

ical structure of the PIL is shown on the left in **Figure 2**, which contains a long hydrophobic dodecyl alkyl chain and a hydrophilic ionic backbone. In the cryogenic transmission electron microscopy (Cryo-TEM) image **(middle in Fig. 2)**, the dark lamellae represent the PIL backbone because of the high electron density of bromide anions, while the gray zones are from the alkyl chain domain. The ellipsoid- instead of onion-like morphology is a balance of the surface energy among the hydrophobic dodecyl domain, the hydrophilic backbone domains, and the surround water. The ellipsoid-like nanoparticles are structurally complex and well ordered, yet synthetically easy-to-make in a one-pot dispersion polymerization process.

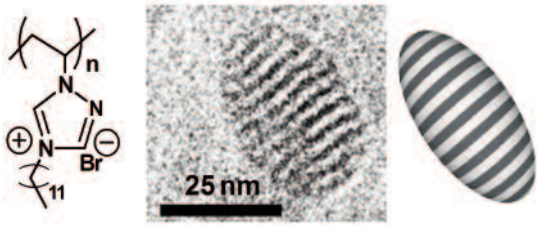

Fig. 2: Left: chemical structure of the 1,2,4-triazolium PIL nanoparticles. Middle: Cryo-TEM image of a single ellipsoid-like PIL nanoparticle. Right: a cartoon illustration of the PIL nanoparticle.

PILs as Innovative Stabilizers

The creation of inorganic materials with tailored structures and morphologies has continued advancing materials chemistry by offering new properties and applications. Previous synthesis using polymers as stabilizers and crystal growth modifiers has achieved substantial success in making systems with targeted properties. In PILs, the structural synergy coupling with their good solubility in organic solvents can create newly structured materials, which has remained unexplored. Our latest progress demonstrated PILs as additives for the morphogenesis of transition metal chalcogenides **[9]**, here exemplified by a highly photoconductive semiconductor, bismuth sulfide (Bi_2S_3) with a direct band gap (Eg) of ~1.3 eV. Current approaches for making Bi_2S_3 described overwhelmingly one-dimensional (1D) structures, because of its highly anisotropic crystal structure consisting of infinite chains of covalently bound atoms. When PILs were used, we could modify the nucleation and growth of Bi_2S_3 materials in organic solvents, which leads to unique crystals with highly tailored sizes, dimensions and architectures, and in consequence a tuneable Eg owing to the quantum-size effect.

As shown in **Fig. 3,** commercially available or readily synthesized PILs, including poly(1-methyl-3-(4-vinylbenzyl)-imidazolium chloride) (PIL-1), poly(diallyldimethylammonium bis(trifuoromethane sulfonyl)imide) (PIL-2), and poly(3-ethyl-1-vinyl-imidazolium bromide) (PIL-3), are applied as exemplary additives. All these PILs are soluble in N,N-dimethylformamide (DMF), a polar organic solvent used here. The syntheses were performed in a simple solvothermal system, composing of mixtures of DMF, $Bi(NO_3)_3$, CH_4N_2S and PILs in appropriate ratios, which were then heated at desired temperature to induce crystallization **(Fig. 3)**. Notably, the three PIL additives resulted in significant morphological diversity of the achieved materials, owing to their different cations, anions, and backbone architectures that selectively couple with specific crystal faces, to modulate and even template consecutive growth, strongly evidencing the effective role of PILs in modifying the crystal growth pattern.

A broad set of characterization techniques confirms that the participation of PILs in the synthesis of Bi_2S_3 can not only control the synthesis, but also enable surface electronic structure modulation, endowing the resultant Bi_2S_3 with enhanced catalytic performance. This was illustrated by an important but notoriously difficult reaction, *i.e.* the anodic water oxidation reaction of water electrolyzers, where it can compete with the reference RuO_2 catalyst, while its commercial counterpart is almost catalytically inactive.

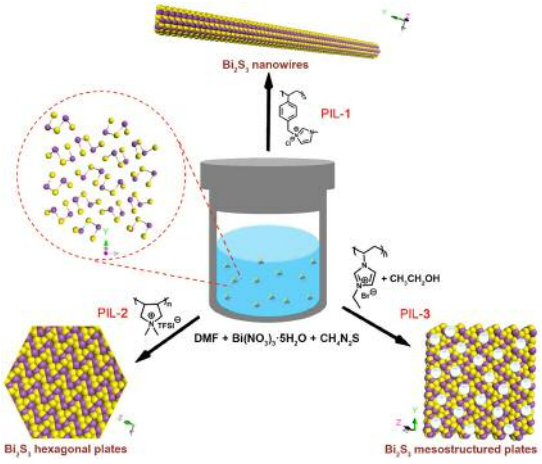

Fig. 3: Schematic illustration of the PIL-controlled synthesis of Bi_2S_3 crystals. High-quality Bi_2S_3 crystals with significant morphological diversity are created by using various PILs as synthetic additives. Inset in red dotted circle shows the crystal structure of Bi_2S_3 projected on the (001) plane. Purple and yellow balls indicate Bi and S atoms, respectively.

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Using Polymers and Ionic Liquids for Next Generation Energy Storage Devices

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Lithium ion batteries are ubiquitous in today's society due to their high energy density and rechargeability. Applications which require less energy often utilize cheaper batteries based on zinc, cadmium, lead, or nickel. All of them however pose dangers regarding flammability, corrosivity, or toxicity of electrodes or electrolytes if handled incorrectly or malfunctioning. Reports of burning laptops and cell phones (usually caused by malfunctioning lithium ion batteries) or skin burns and deformities (often caused by exposure to heavy metals or battery acids) are reoccurring on a regular basis. Apart from their dangers, metals as currently employed in batteries have a significant negative environmental impact during mining (since many of them are rare) or insufficient recycling.

For next generation energy storage devices, other metals like magnesium or aluminium might be a safe alternative since even in their elemental form they will not overheat or catch fire when exposed to humidity, in contrast to lithium. The environmental impact is also lower since there is 1000 times as much of these metals in the earth crust compared to lithium. Because of their multivalency, ion radius, and, especially in case of magnesium, electrochemical potential, batteries based on such metals will still have higher energy densities when compared to current lithium batteries. Reactivity and fast passivation however currently hinder widespread application, and prototypes only work in combination with selective electrolyte compositions. One approach in our group is to develop ionic liquid electrolytes to be used in future magnesium batteries. In addition to their electrochemical stability, such electrolytes will decrease the risk of explosion of electrical devices since they are not volatile.

Another approach to reduce the environmental impact of energy storage devices is to use organic molecules as electrodes instead of metals or metal oxides. Polymers with redox functionalities are especially interesting since they are more difficult to dissolve in electrolytes, and charge transport between active groups is facilitated compared to low molecular species. Both natural and synthetic polymers may be used, and disposure is much more benign since incineration of waste electrodes after usage will prevent hazardous refuse while not producing more dangerous gases then when incinerating other plastics. We research the possibilities of using synthetic and natural polymers as electrode material in batteries and supercapacitors.

Sustainable Ionic Liquid Electrolytes for Battery Applications

Ionic liquids are considered a safe and electrochemically stable alternative to chemical solvents and may find applications in a multitude of fields, amongst others in battery electrolytes. By introducing functional groups, a plethora of so-called task-specific ionic liquids is available. For applications in electrochemistry, amongst others a large electrochemical stability range and liquidity at low temperatures are desirable. Applications which involve ionic liquids often comply with green chemical principles such as waste prevention, benign reaction conditions, reduced toxicity, efficiency, and minimized hazard and accident risk. In most cases, however, synthesis of ionic liquids is neither "green" nor cheap since usual reaction routes include expensive and harmful chemicals like alkyl halides.

We used the modified Debus-Radziszewski reaction and reagents which are potentially derived from renewable resources to synthesize task-specific ionic liquids for applications as possible electrolyte in magnesium batteries. By introducing tetrahydrofurfuryl side groups, we may exchange the common solvent in prototype magnesium batteries, THF, by a safe, non-volatile, non-flammable, and electrochemically stable alternative, gained from cheap and potentially renewable resources. Reaction conditions were benign, and the products exhibited a large range of liquidity and electrochemical stability (**Fig. 1**) **[1].**

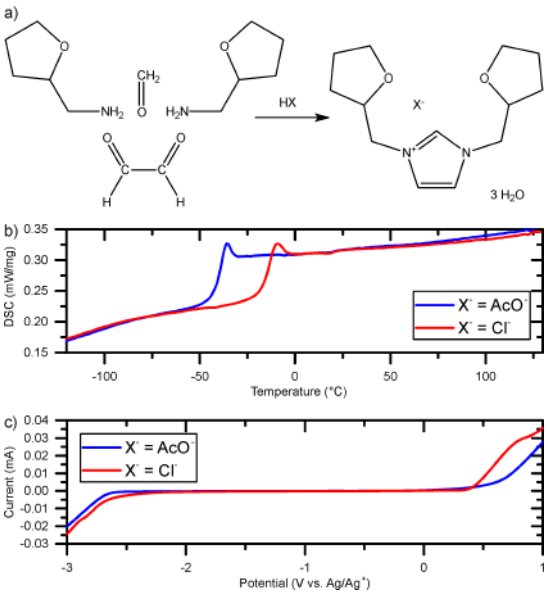

Fig. 1: (a) Schematics of the modified Debus-Radziszewski reaction yielding substituted imidazolium ionics in a simple one-step reaction without using alkyl halides. (b) DSC thermogram demonstrating low glass transition temperatures (well below 0 °C) of the imidazolium products shown in (a) with different counter ions. (c) Linear sweep voltammograms of the imidazolium ionic liquids. The sample with Cl^- counter ion can also be obtained by metathesis of the sample with AcO^- counter ion; the graphs in (b) and (c) derive from a product obtained by metathesis ***[1].***

Redox Active Polymers as Electrode Material

To reduce cost, hazards, and environmental impact, electrode materials in future energy storage systems might derive from organic molecules with redox functionalities. Easy and large-scale synthesis, a suitable electrochemical potential of the redox reaction, and reversibility of oxidation/reduction are some of the most important properties. To prevent dissolution in the electrolyte, polymers with pendant redox active groups may be advantageous, and blending the polymers with high surface area carbon leads to synergistic double layer capacitance with redox processes. Binders like fluorinated polymers also help preventing dissolution.

Redox functionalities may derive from, e.g., nitroxyl radicals or quinones. Synthetic polymers have the advantage that functionalized units are defined and can be adjusted. Mixing in other polymers to include different tasks like conductivity or non-solubility and patterning surfaces with redox functionalities is possible by synthesizing block copolymers. **Fig. 2** shows the surface structure and corresponding cyclic voltammogram of a synthetic block copolymer featuring one redox active nitroxyl containing block and a polystyrene block **[2].**

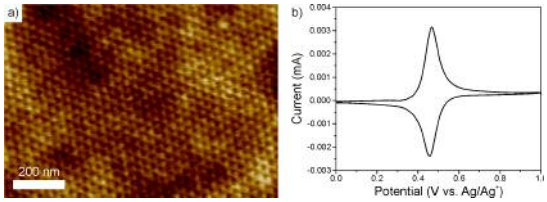

Fig. 2: (a) AFM topography image of a polystyrene-block-poly(2,2,6,6-tetramethyl-piperidinyloxy-4-yl methacrylate) block copolymer synthesized by anionic polymerization featuring a majority block with stable nitroxyl radicals. The AFM image after solvent vapor annealing on a patterned surface shows upright-standing polystyrene cylinders in a matrix which contains redox active stable radical groups. (b) Cyclic voltammogram showing the reversible redox activity of this block copolymer ***[2].***

Ordered structures like in **Fig. 2** are possible only because the polymer has a very low dispersity of 1.06. While synthetically this is challenging (here: anionic polymerization), natural monodisperse polymers exist and might be available in large scales. Natural monodisperse polymers with redox active groups, however, do not feature a high density of redox functionalities. In contrast, lignin, which is one of the main constituents of all plant material, is a biopolymer with a high density of redox active hydroquinone functionalities (after demethylation of methyl ethers) but rather polydisperse. We investigated its application as electrode material after blending with high surface area conductive carbon and some binder. Resulting organic electrodes are cheap and environmentally friendly. For charge storage, they combine electric double layer capacitance at the high surface area conductive carbon with redox reactions in the reversible quinone-hydroquinone redox couple (**Fig. 3**) **[3].**

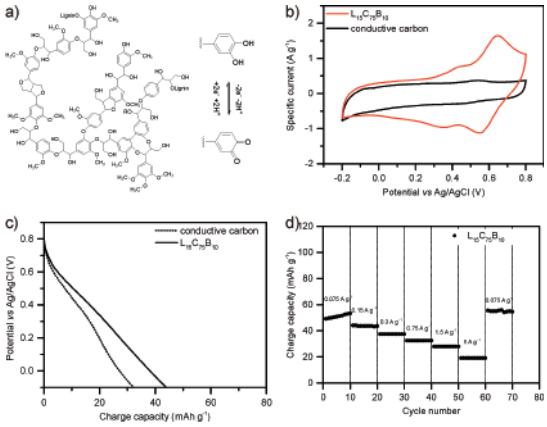

Fig. 3: Electrochemical behaviour of lignin-based organic electrodes. (a) Schematical structure of lignin and the respective redox reaction. (b) Cyclic voltammograms of electrochemical cells with lignin-based working electrode and platinum counter electrode. Compared to carbon electrodes, redox reactions contribute to additional charge storage. (c) Galvanostatic discharge measurements at a current density of 0.15 A g^{-1}. (d) Rate capability by stepwise galvanostatic cycling of the composites from lignin and conductive carbon.

Carbon Nitrides for Photocatalytic Hydrogen Evolution

A different path towards sustainable energy is the photocatalytic production of hydrogen gas to be used in fuel cells. Energy from sunlight is converted to chemical energy which can later be used for powering cars, for example. While conventional catalysts for the hydrogen evolution reaction are often based on platinum, development of suitable carbon nitride catalysts will greatly decrease their costs and contribute to economical and ecologically benign energy storage in form of chemical energy. The morphology and texture of carbon nitride greatly influences performance, and studies of carbon nitride formation are hence crucial for developing highly active materials.

Via supramolecular self-assembly, cyanuric acid-melamine complexes were formed. Sequential treatment with different solvents led to formation of core-shell particles, and calcination resulted, depending on the solvents, in hollow structures and structures with platelet-like surface structure. The formed carbon nitrides showed significantly higher activity for the hydrogen evolution reaction (depending on the morphology up to 10 times as high) compared to bulk carbon nitride **[4].**

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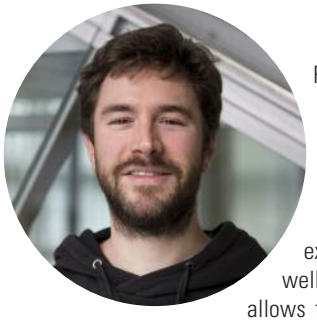
Polymer Synthesis and Self-Assembly for Novel Soft Materials



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Polymers offer a plethora of available structures from the nano- to micrometer range and self-assembled structures from polymers find various applications, e.g. in biomedicine or organic electronics. Moreover, the polymer properties depend to a great extent on polymer microstructure. Therefore, well-controlled synthesis of polymer materials allows for the formation of materials with tailored properties and research on synthetic polymer formation procedures offers the opportunity to generate polymer materials with novel or enhanced properties. Especially, when complex self-assembly processes are targeted, efficient synthetic tools are needed, e.g. reversible deactivation radical polymerization or modular ligation chemistry. In such a way, complex polymer materials can be designed and utilized for self-assemblies that feature specific properties. In this group two topics regarding self-assembly of polymers and synthetic polymerization methodology are investigated. On one hand self-assembly of double hydrophilic block copolymers (DHBCs) in aqueous solution is investigated with the aim to obtain drug-delivery vehicles for complex drugs. On the other hand metal-organic frameworks (MOFs) are utilized as catalysts as well as reaction environment for polymerization reactions.

Double Hydrophilic Block Copolymer Self-Assembly

Unlike the well-known self-assembly of amphiphilic block copolymers, self-assembly of DHBCs in aqueous media is not based on interactions of hydrophobic blocks. Taking a step back looking at water-soluble homopolymers, aqueous biphasic systems can be generated from water-soluble homopolymers, where each homopolymer type is present in one of the aqueous phases. Such a phase separation is possible, when the concentration of the polymers is high enough and significant differences in the hydrophilicity of the homopolymers are present. In the case of a covalent connection of both homopolymers as a block copolymer demixing on the microscopic scale is possible.

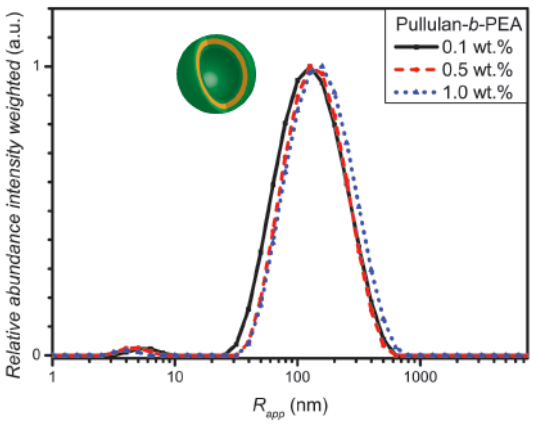

*Fig. 1: Self-assembly of pullulan-b-poly(N-ethyl acrylamide) in water observed via DLS at 25 °C **[1].***

In order to obtain DHBC-based self-assemblies, polymer synthesis has to be performed at first. A suitable tool is reversible deactivation radical polymerization that allows the formation of well-defined polymers, e.g. block copolymers or polymers with specific endgroups. In principle it is possible to form DHBCs from a macroinitiator **[2]** or to conjugate two distinct blocks with specific endgroups.**[1]**

In a subsequent step self-assembly of the formed DHBCs in water can be probed via dynamic light scattering (DLS) (**Fig. 1**), e.g. for the polymer system pullulan-*b*-poly(*N*-ethyl acrylamide).**[1]** Particle size distributions generated from DLS show the formation of particular structures with radii around 200 nm. Moreover, imaging with cryo scanning electron microscopy shows spherical structures that can be attributed to the formation of self-assembled hollow structures (**Fig. 2**).

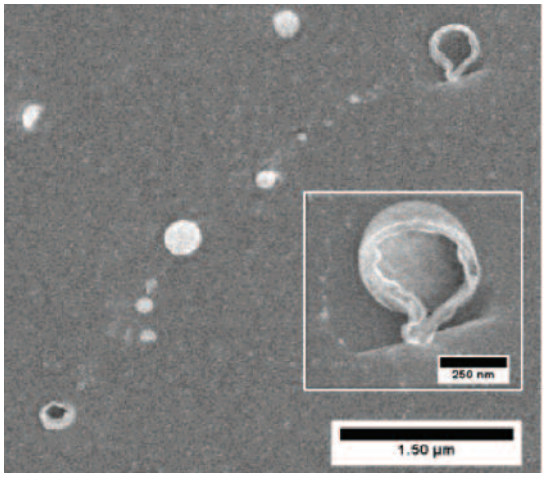

*Fig. 2: Self-assembly of pullulan-b-poly(N-ethyl acrylamide) in water: Cryo SEM imaging **[1].***

One drawback of DHBC-based self-assemblies is their instability in diluted solutions, which poses a significant problem with respect to applications in biomedicine. In order to overcome this problem, a crosslinking strategy was developed. Therefore, the block copolymer poly(ethylene oxide)-*b*-poly(*N*-vinylpyrrolidone-co-*N*-vinyl imidazole) was synthesized.**[2]** The vinylimidazole units allow the formation of crosslinks via nucleophilic substitution reaction with dihalogenide molecules. In such a way the formed particular structures could be preserved even in high dilution and in organic solvents (**Fig. 3**).

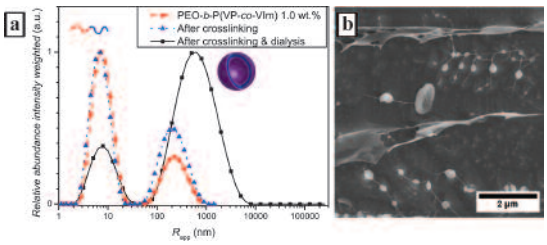

*Fig. 3: Self-assembly of poly(ethylene oxide)-b-poly(N-vinylpyrrolidone-co-N-vinyl imidazole) in water: a) DLS at 25 °C before crosslinking at 1.0 wt.%, after crosslinking and at 0.06 wt.% after dialysis, b) cryo SEM of the crosslinked particles **[2].***

Metal-Organic Frameworks as Polymerization Catalyst and Reaction Environment

MOFs provide porous networks with defined pore sizes and architectures. Moreover, the incorporation of carefully chosen metal ions endows MOFs with catalytic properties.

One of the most frequently used reversible deactivation radical polymerizations is atom transfer radical polymerization (ATRP) that is a Cu(I) catalysed process. More recently activators regenerated by electron transfer (ARGET) ATRP was developed, which is based on Cu(II) reduction to form the catalytic active species. To catalyse polymerizations a Cu(II)-based MOF was formed via complexation of Cu(II) ions, terephthalic acid and 1,4-diazabi-cyclo[2.2.2]octane (DABCO) as a 3D crystalline porous network. In a subsequent step, MOF, monomer, reduction agent (DABCO) and initiator were mixed and heated to start the polymerization. Monomers like styrene, benzyl methacrylate, isoprene and 4-vinylpyridine could be polymerized that way in a controlled fashion as shown via chain extension experiments and narrow molecular mass distributions (**Fig. 4**). More importantly, MOF catalyst could be removed easily via centrifugation and recycled several times.

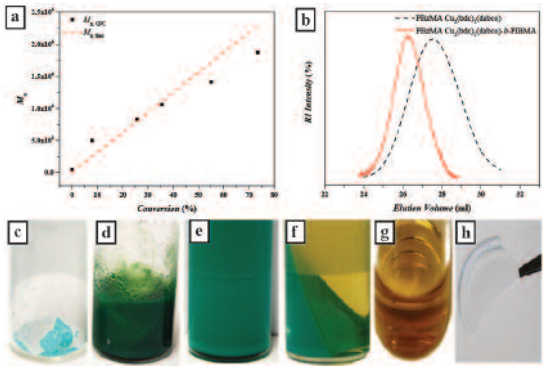

Fig. 4: a) Kinetic plot for the MOF catalyzed polymerization of benzyl methacrylate, b) chain extension, c) MOF catalyst, d) polymerization mixture, e) polymerization mixture after termination, f) centrifugation, g) solution after removal of catalyst and h) final polymer material ***[3].***

After studying the polymerization outside of MOF crystals, polymerization in porous frameworks of MOFs was investigated. The pore diameters of MOFs can be adjusted via utilization of defined precursors in the range of 1–2 nm. Thus, monomer molecules can be introduced into the porous structure that provides a confined environment for the small monomer molecules. That way molecular movement during the polymerization of the monomers is significantly hindered, which should lead to improved stereocontrol/tacticity during polymerization. Again ARGET ATRP was chosen as polymerization technique to conduct polymerizations in controlled fashion. Polymerizations inside of MOFs led to polymers with narrow molecular mass distribution and chain extension proved the controlled character of the polymerizations (**Fig. 5**). Interestingly, studies on the tacticity of the obtained polymers showed a significant effect of monomer size. Methyl methacrylate led to slightly increased isotactic polymer structures compared to the bulk without MOF, while benzyl methacrylate led to significantly increased isotactic fractions (**Fig. 4**). Moreover, the very bulky monomer isobornyl methacrylate did not form any polymer in the MOF as it does not fit into the porous framework. Thus, a significant effect of the confined porous environment on polymer tacticity is indicated.

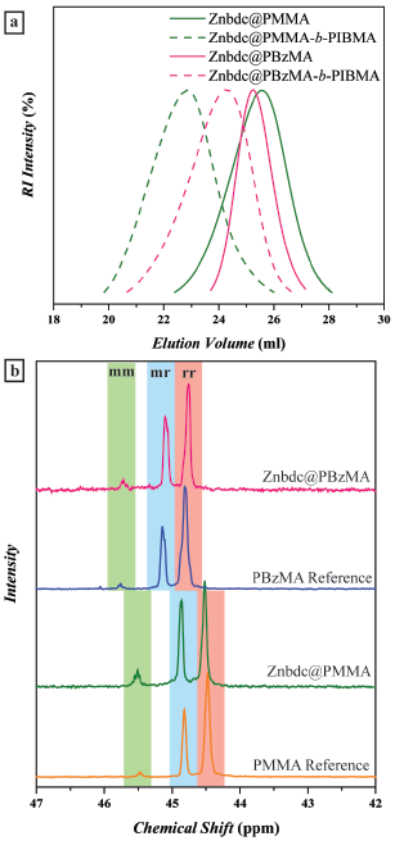

Fig. 5: a) Chain extension of poly(methyl methacrylate) and poly(benzyl methacrylate) obtained via ARGET ATRP in a MOF and b) ^{13}C NMR spectra of poly(methyl methacrylate) and poly(benzyl methacrylate) obtained via ARGET ATRP in a MOF and the corresponding reference from bulk polymerization ***[4].***

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THEORY & BIO-SYSTEMS

Research in the Department of Theory & Bio-Systems

"The good thing about science is that it's true whether or not you believe in it."
Neil deGrasse Tyson

The main objective of our research activities is to understand the hidden dimensions of self-organization and pattern formation in biomimetic and biological systems. The molecular building blocks of these systems join "by themselves" and form a variety of supermolecular assemblies, which then interact to produce even larger structures and networks.

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Thesis: Critical behavior of interfaces: Wetting, surface melting and related phenomena
1989-1990: Associate Professorship (University of Munich)
1990-1993: Full Professorship (University of Cologne), Director of the Division "Theory II" (FZ Jülich)
Since Nov 1993: Director (Max Planck Institute of Colloids and Interfaces, Potsdam)

The associates of the department form several research groups. At present, the research group leaders and topics are (in alphabetic order):

- Rumiana Dimova: Biophysics Lab;
- Andrea Grafmüller: Multiscale Simulations;
- Roland Knorr: Dynamics of Biomembranes (since 2016);
- Hans Riegler: Solid-Air Interfaces;
- Tom Robinson: Biomicrofluidic Systems (since 2016);
- Sophia Rudorf: Biomolecular Processes;
- Mark Santer: Carbohydrates and Polysaccharides;
- Angelo Valleriani: Stochastic Processes;
- Ana Vila Verde: Soft Matter Simulations;
- Thomas Weikl: Proteins and Membranes.

The experimental group of Tom Robinson is an independent junior group, funded by the Max Planck Research Network in Synthetic Biology (MaxSynBio).

The main results of these research groups are described in separate reports on the following pages. These reports are ordered in a bottom-up manner, i.e., from small to large length scales, and related to four research areas: Biopolymers, Biomolecular Processes, Membranes and Vesicles as well as Interfacial Phenomena. In this introductory overview, the reports of these research groups will be briefly summarized and a few additional aspects will be highlighted.

Biopolymers

The three research groups of Andrea Grafmüller, Mark Santer, and Ana Vila Verde study the behavior of biopolymers using atomistic and coarsegrained molecular dynamics simulations. The Vila Verde group investigated the water dynamics in electrolyte solutions as well as the interactions of ions with proteins and dendrimers. Other projects of the Vila Verde group address the mechanical response of single helices and coiled coils under tension. The Santer group has worked on force field modularization for carbohydrate compounds (glycans). The modular force fields were applied to the recognition of lipopolysaccharides by proteins, to the compaction of DNA by azo-containing peptidomimetic molecules, and to GPI-anchors in lipid membranes. The Grafmüller group studied the solubility of different mono- and oligosaccharides and introduced an improved force field that describes the concentration dependence of the osmotic pressure in a reliable manner. Based on the improved force field, a coarse-grained model was developed and used to show that the water-uptake of linear and branched polysaccharides is rather different.

Biomolecular Processes

The two research groups of Sophia Rudorf and Angelo Valleriani use stochastic modelling to study protein synthesis and post-translational gene expression. The Rudorf group determined the dependence of protein translation on EF-Tu concentration and developed a new algorithm for codon optimization. Two doctoral projects of the Rudorf group address the entry of the nascent peptide chain into the ribosomal exit tunnel and the co-translational assembly of dimeric proteins. The Valleriani group studied the influence of degradation of mRNA, ribosomal drop-off, as well as protein ageing and degradation on gene expression.

One topic that is not covered in the following reports is the cargo transport by molecular motors. Some years ago, we introduced a stochastic model for the bidirectional cargo transport by two antagonistic motor teams such as kinesin and dynein. [M. I. J. Müller et al, PNAS, 2008] This theoretical model, which has received a fair amount of attention, is based on a simplified description for the force balance underlying the tug-of-war between the two motor teams. In order to improve this theory, we have recently considered two antagonistic motor teams that are elastically coupled to the cargo. We first studied the simplest case of one kinesin against one dynein, see **Fig. 1,** and found that the elastic interactions forces between the two motors depend rather strongly (i) on the unbinding rate for the single motors and (ii) on the strength of the elastic coupling between the motors. We now extended our theory to more than 1+1 motors, which revealed how the elastic interaction forces are shared among all motors from the same team.

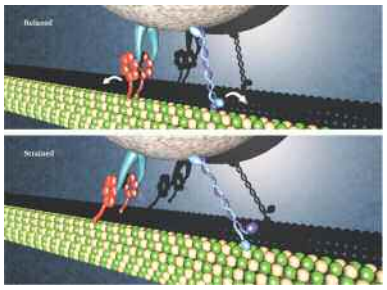

Fig. 1: Tug-of-war between one dynein motor (left, blue-red) and one kinesin motor (right, blue-purple) that step along a microtubule (green-yellow) and pull a cargo (grey) into opposite directions: In the upper panel, the two elastic linkers between the motors and the cargo are relaxed and the motors do not exert elastic forces onto each other. When one of the motors performs a discrete forward step (white arrows), the stalks become stretched and the motor proteins become strained as shown in the lower panel. [M. Ucar and R. Lipowsky, Soft Matter 13, 328 (2017)]

Membranes and Vesicles

The behavior of biomembranes and giant vesicles has been addressed by the three experimental research groups of Rumiana Dimova, Roland Knorr, and Tom Robinson as well as by the theoretical research group of Thomas Weikl. The Weikl group has elucidated the binding of membrane-anchored proteins and the conformational changes during protein binding. This group also continued its studies on the wrapping of nanoparticles by membranes.

One project that involved the concerted efforts of theory, simulation, and experiment addressed the intimate relation between the asymmetry of bilayer membranes and the spontaneous tubulation of giant vesicles. We have now developed three different methods to deduce the spontaneous curvature of membranes from the morphology of giant vesicles with nanotubes. These quantitative methods are based on the detailed image analysis of spontaneously tubulated vesicles, on the application of local forces that pull additional tubes from these vesicles, and on the initial aspiration of such vesicles by micropipettes. Giant vesicles with membrane nanotubes have unusual mechanical properties because the tubes provide a large area reservoir for the mother vesicles. Therefore, these vesicles can adapt to strong mechanical perturbations by exchanging membrane area with the tubes. As a consequence, tubulated vesicles behave, to a large extent, like liquid droplets with constant volume and variable surface area.

Jaime Agudo-Canaleijo and myself have developed a rather detailed analytical theory for the interactions of nanoparticles with membranes and vesicles. We have shown that the spontaneous curvature of the membranes provides a key parameter for the engulfment process which leads to four different engulfment regimes for a single nanoparticle. When exposed to a finite concentration of dispersed nanoparticles, a vesicle membrane exhibits distinct engulfment patterns consisting of up to three different membrane segments. Partially engulfed nanoparticles experience curvature-induced forces that bias the diffusion of these particles along the membrane. As a consequence, the probability to find such a particle at a certain membrane position depends on the local mean curvarture of the membrane. The corresponding distributions are shown in **Fig. 2** for Janus particles with one adhesive and one non-adhesive surface domain. As illustrated in this figure, any shape transformation of the vesicle implies a concomitant transformation of the particle distribution and, thus, a strong change in the associated color pattern.

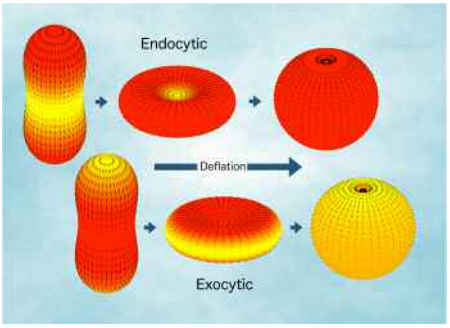

Fig. 2: When osmotically deflated, the prolate vesicle on the left is first transformed into a discocyte and subsequently into a stomatocyte (the inner segment of the stomatocyte is masked by its outer segment). When Janus particles are partially engulfed by the membranes of these vesicles, the probability to find such a particle is high for the yellow membrane segments and low for the red ones, reflecting the curvature-induced forces acting on the particles. When the particles are attached to the outer and inner membrane leaflet, corresponding to endocytic and exocytic engulfment, the particles prefer to stay at membrane positions with large negative and large positive curvature, respectively. [J. Agudo-Canalejo and R. Lipowsky, Soft Matter (2017), in press]

The Dimova group studied the effects of bilayer asymmetry and tension on lipid phase separation, the polymorphism and adhesion of giant vesicles, the spontaneous and force-induced formation of membrane nanotubes, and the shaping of vesicles by electric fields, light and proteins. The ongoing projects include curvature generation by ions, STED microscopy of nanotubes, light-controlled shape transformations, and the behavior of giant plasma membrane vesicles, so-called blebs. The Robinson group developed assays to localize membrane fusion to intramembrane domains formed by liquid-disordered or liquid-ordered lipid phases as well as new microfluidic tools for the handling and trapping of vesicles. These tools will now be used to construct multi-compartment vesicles systems ("vesicles in vesicles") and to encapsulate enzymatic reactions. The Knorr group studied shape transformations of double-membrane vesicles, which are relevant for autophagy, the reconstitution of protein cascades at membranes, and the interaction of membrane-enclosed organelles with membrane-less organelles. The latter organelles behave like liquid droplets and undergo wetting transitions at membranes and vesicles. We have identified several control parameters for these transitions which lead to a complete redistribution of the molecules that are enriched in the droplet-like organelles. Furthermore, because a membrane segment in contact with such an organelle acquires a spontaneous curvature, the wetting transitions can be used to locally control this curvature.

Interfacial Phenomena

The group of Hans Riegler continued their investigations of phase transitions and transport phenomena at solid-air interfaces. Of particular interest were drop-drop coalescence, interfacial flow and drop evaporation, melting and solidification of nano-structures as well as patterned growth induced by heterogeneous nucleation.

Biannual Series of Symposia

We continued our biannual series of topical symposia and organized a symposium on 'Multiscale Motility of Biomolecular Machines' in 2015 as well as another 'Biomembrane Days' in 2016.

International Max Planck Research School

The department of Theory & Bio-Systems was in charge of the International Max Planck Research School on "Multiscale Biosystems", which started in July 2013 and will operate at least until 2019. We recently organized an on-site evalutaion of our School, with a very positive outcome.

For additional information about research at the Department of Theory & Bio-Systems, see the subsequent reports and www.mpikg.mpg.de/th/.

Reinhard Lipowsky
Head, Department of Theory & Bio-Systems

From Ionic Solutions to Interacting Proteins

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We use molecular simulations and classical, atomistic models to investigate various systems relevant for biology. The systems chosen – ranging from simple solutions to full size proteins – reflect a general approach: we first focus on simple systems, and then apply the knowledge obtained with them to the study of more complex ones.

Our studies of *electrolyte solutions* demonstrated the strong connection between the ion-pair structure of the solution and the emergence of non-additive effects in the stiffness of the water hydrogen bond network. This connection is likely important for protein function. To enable the study of biological systems in the presence of ions, *we developed optimized parameters (force fields) for monoatomic and polyatomic* ions in water. We go beyond state-of-the-art parameterization approaches, which prove insufficient for these systems.

Experimental studies of fluorinated proteins have demonstrated the potential of fluorination to tune protein properties, but the mechanisms underlying the observed changes remain unknown. Our initial studies showed the need to follow a non-standard approach to parameterize fluorinated amino acids. Using the force field we created, we have clarified the molecular mechanisms behind changes in hydration free energies upon fluorination. This property is key to understand how proteins respond to fluorination.

Our studies of *dimeric and trimeric coiled coils* under tension are revealing how their mechanical response emerges from that of α-helices. We investigate these systems at low pulling speeds, which requires particularly long simulation times. Our results show that previous effects mentioned in the literature are not biologically relevant because they arise at high pulling speeds only.

Interactions between Water and Ions

The effects of ions on the properties of water (e.g., the strength of the hydrogen bond network), or the properties of other solutes in water (e.g., solubility of proteins) are commonly thought to be additive: the impact of a given salt on a given property is interpreted as the sum of the impact of the anions and cations.

Experiments probing water rotational dynamics – which indirectly reports on the stiffness of the water hydrogen bond network – however, have challenged this view. To gain insight into this issue, we use polarizable models to investigate the dynamics of rotation of water in aqueous solutions containing $MgSO_4$, for which the largest supra-additive effect was observed in experiment **[1]**. We parameterize these models to reproduce both the free energy of hydration of single ions and the solution activity derivative at high concentration. The models are thus appropriate to gain insight into water dynamics in a wide range of concentrations, necessary for comparison with experiment. We find that $MgSO_4$ greatly slows down water dynamics, in agreement with experiment. To understand the mechanisms behind this slow down, we investigate water dynamics for different water subpopulations near static ion pairs. We find that large, supra-additive slowdown occurs only for water molecules directly bridging the $Mg^{2+}\cdots SO_4^{2-}$ ions. Non-intuitively, supra-additive slowdown is not a purely electrostatic effect, as **Fig. 1** illustrates: water reorientation times larger than 8 ps – for which supra-additive slowdown exists – are uncorrelated with more intense local electric fields. Instead, supra-additive slowdown seems to result from a change in the free energy landscape associated with hydrogen bond breakage and formation events, for water molecules that are hydrogen-bonded to SO_4^{2-} and which simultaneously belong to the first hydration layer of Mg^{2+}.

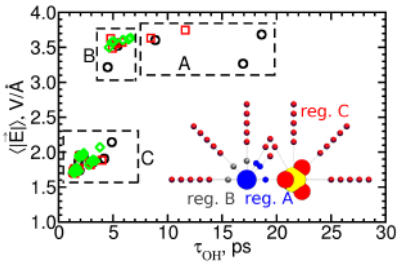

*Figure 1: Local electric field vs. water reorientation time for water molecules in each subpopulation (indicated by the small spheres in the inset) around $Mg^{2+}\cdots SO_4^{2-}$ ion pairs. Supra-additive slowdown is only observed for water subpopulations in region A **[1]**.*

The coupling between solution structure – the proportion of different types of ion pairs – and the stiffness of the water hydrogen bond network, demonstrated by the above-mentioned results, highlights the general importance of both ion-ion and ion-water coupling to understand ion-specific effects in biology. To allow the investigation of these effects, we have recently developed an *optimized force field for the alkali, alkali earth and halide ions and the TIP5P water model, based on experimental data* **[2]**. This force field is desirable for simulations of saccharides. Our results show that the state-of-the-art approach often used to parameterize anion-cation interactions is insufficient, and that existing force-fields often over-estimate the number of ions in direct contact in solution.

Interactions between Ions and Proteins

Molecular scale studies of ion-specific effects which arise from interactions between mono- or polyatomic ions and proteins, have been hindered by the absence of classical force fields that are compatible with existing force fields for proteins. To address this need, we have developed a set of parameters for the SO_4^{2-}, SO_3^{2-}, HPO_4^{2-}, $H_2PO_4^-$ ions, the methylated versions of these anions, and for CH_3COO^- **[3]**. Their interactions with positively charged amino acids and with the physiologically relevant Na^+ cation are explicitly parameterized. Our results show that existing force fields greatly overestimate interactions between negative amino acids and Na^+, as well as the strength of salt bridges in proteins. Our newly developed force field will be applied to study interactions between selectins – cationic proteins involved in cancer metastasis and in inflammatory response – and anionic polymeric inhibitors, which are being experimentally studied in the Haag group at the Free University of Berlin together with Peter Fratzl at this institute.

Fluorinated Amino Acids and Proteins

Fluorination – replacing C-H bonds by C-F bonds – of the side chains of hydrophobic residues in proteins often improves the protein's thermal stability. Despite the fact that the intrinsic physicochemical properties of fluorine are well understood, understanding and predicting how fluorination affects protein properties is not yet possible. Experimental reports on fluorinated proteins led to a number of questions regarding the *mechanisms* by which fluorination alters, e.g., the hydrophobicity of amino acids. To investigate these issues we developed a force field for fluorinated amino acids. The force field is fully compatible with the widely used AMBER force fields for proteins, but relied on a non-standard parameterization of the amino acid charges because the standard procedure proved insufficient. Our initial work focused on understanding how CH_3-to-CF_3 substitutions affect the hydration free energy of amino acids **[4]**. We find that CH_3-to-CF_3 substitutions increase the amino acid hydrophobicity, i.e., they result in less negative hydration free energies. This result is consistent with experiment. Surprisingly, however, even for a system as simple as a single amino acid, the *magnitude of the change* in hydration free energy upon a single CH_3-to-CF_3 substitution can vary between 0.5 and 1.5 kcal/mol, depending on the identity of the amino acid and the position in which fluorination occurs. These differences cannot be completely explained in terms of differences in the solvent-accessible apolar surface area between the various amino acids, as is commonly believed. Our results demonstrate that fluorination changes the free energy of hydration largely by altering the number of backbone-water hydrogen bonds, an effect that was not previously demonstrated. These results suggest that different fluorinated amino acid isomers may lead to different changes in protein structural stability, an effect which will be explored by the Koksch group at the Free University of Berlin.

Mechanical Response of Single Helices and Coiled Coils under Tension

Coiled-coils (CC; **Fig. 2**) are ubiquitous structural motifs in many proteins: e.g., they are present in the cytoskeleton and the extracellular matrix of cells.

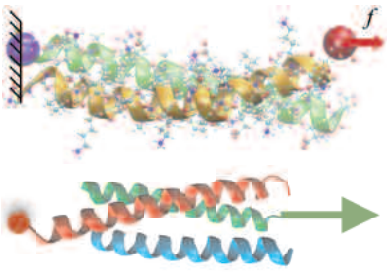

Fig. 2: Dimeric and trimeric coiled coil under a pulling force f.

Coiled-coils are thought to be necessary for chemical functions as well as for mechanical or chemomechanical ones. Our aim is to understand the *mechanical* response of coiled coils: how this response emerges from the properties of the single α-helices that compose them and how it is affected by the multimerization state (dimeric or trimeric) of the coiled coil. Clarifying these issues is critical to understand the role of coiled coils with different multimerization states in biology. We perform pulling simulations where one end of an α-helix is kept fixed, and another one is pulled (**Fig. 2**). These simulations are analogous to atomic force microscopy (AFM) experiments. We find that single α-helices and dimeric coiled coils have a very different force-velocity dependence, with α-helices being equally stiff at all speeds whereas the coiled-coil clearly becomes stiffer as the pulling speed increases (**Fig. 3**). Despite having a different force-velocity dependence, both systems behave as constant-force springs and have similar force plateaus (circa 50 pN) at the lowest pulling speed. This low velocity regime is the closest that simulations can currently get to physiologically relevant conditions and also to AFM experiments.

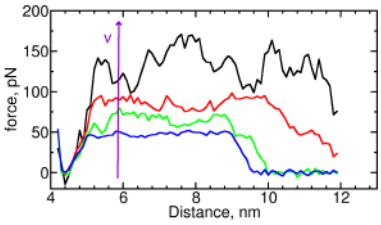

*Fig. 3: Force vs. extension for a dimeric coiled coil. The different colors indicate different pulling speeds (v), ranging from 10^6 nm/ps to 10^3 nm/ps **[6]**.*

The similarity in the force plateaus of single α-helices and of dimeric coiled coils is puzzling, because the plateau in the single α-helix is clearly related with the unfolding of that helix, but pulling of the dimeric coiled coil results only in sliding of one helix relative to the other, without net unfolding. A deeper look into our results offers a possible explanation for the similarity of the force plateaus: sliding occurs via transient opening and closing of the α-helices composing the coiled coil **[5, 6]**. Future work will include AFM experiments (in the Blank group at this institute) and simulations with mutated sequences to determine which of these trends are general and which are system-specific.

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As Glycans Grow Rich

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Since 2010: Group leader Carbohydrates and Polysaccharides in the department of Theory and Biosystems.

In virtually all organisms carbohydrate compounds *(glycans)* are involved to modify or enhance the function of other biomolecules. The glycosylation of proteins and lipids in the extracellular matrix is important for initiating cell recognition, fine tuning inter-cell communication or establishing protective barriers. These different functionalities reflect the underlying diversity in glycan composition and conformational flexibility. Developing reliable force fields for computer simulations of these biomolecules is the main theme of our work. The current research activities are centered around the question how modeling is to be pursued when glycan containing biomolecules consist of an increasing number of components. How can we improve modularity of the force fields? How then do we interpret diverging predictions of different force fields?

Recognition of Lipopolysaccharides by Proteins.
The latter problem emerged in the context of the question how phages can infect Gram-negative bacteria, which protect themselves from invasion with a dense lipopolysaccharide (LPS) coat.

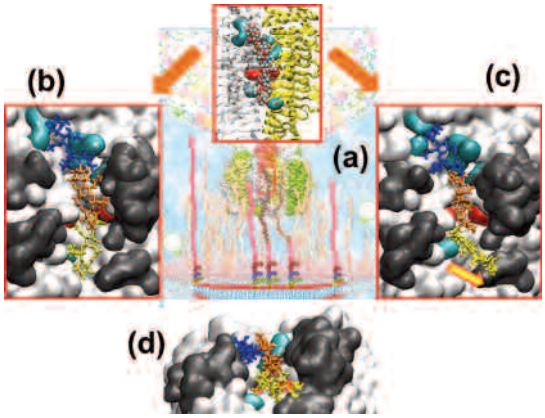

Fig. 1. (a) Schematic view of a phage approaching the LPS coat of the bacterium Shigella flexneri. The successive enhancements show how the phage grasps a fragment of the long LPS side chain. These polysaccharides consist of repeating units of tetrasaccharides, and are docked to the groove between two of the three monomers forming a tail spike protein below the capsid. Binding (b,c) is mediated mostly by hydrogen bonding residues (cyan) interacting with the first repeat unit (RU1: blue), while the trailing units (RU2: orange and RU3: yellow) sterically adapt to the side walls formed by unstructured loops (gray), see view along groove (d). Red: catalytically active sites E366/D399. (b) shows a stable pose in the GLYCAM case; (c) indicates the frequent excursions (arrow) found for CHARMM.

It is well known that recognition of certain epitopes followed by enzymatic cleavage of the polysaccharide O-Antigens is the key to this process **[1]**, see **Fig. 1**. Supporting an extensive body of experimental evidence, we were able to comprehensively characterize the recognition of a two-repeat unit epitope of Serotype Y polysaccharide to the tail spike proteins (TSP) of phage Sf6 **[2]**. Both force fields employed, GLYCAM and CHARMM, agreed in the description of the binding mode as a concerted action of hydrogen bonding, loop flexibility and conformational selection. They are at variance in predicting the placement of longer fragments, such as the 3RU dodecamer shown in (b,c). This divergence is quite useful. It directly points to the questions of how infection proceeds on time scales far longer than the atomistic, and the unspecific interaction of LPS with TPS beyond the epitope. Are LPS degraded processively, with strong anchoring within the LPS coat, or does the phage only randomly attempt to break through?

Force Field Modularization.
The great diversity of carbohydrate compounds requires a modular organization of the force fields, where complex molecules can be built up from smaller, invariant building blocks.

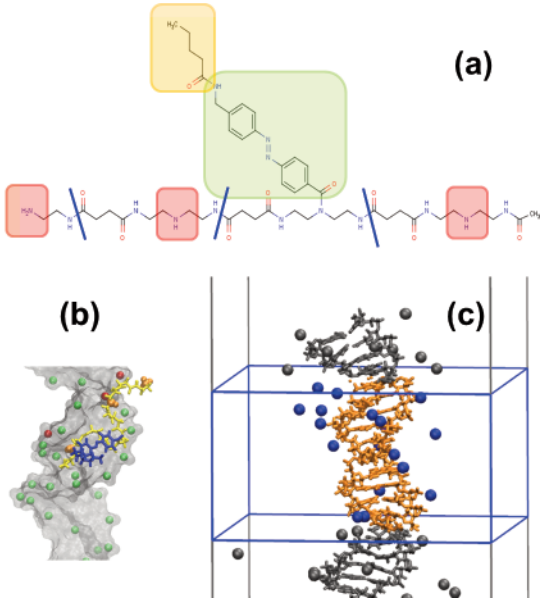

Fig. 2. (a) structure of the azo-containing peptidomimetic (Azo-PM) compacting agent. Red: protonated amine groups; green: azobenzene containing side chain; yellow: trailing hydrophopic moiety. (b) interaction of trans Azo-PM with a 22bp segment of B-DNA; green: phosphates; orange: protonated amines; read: proximal phosphates. (c) Snapshot of Na+ atmosphere around the segment, with the simulation box as indicated.

In modeling the interaction of LPS core oligosaccharides with lung surfactant proteins **[3]**, we have tested a procedure by which a carbohydrate building block is created with respect to how it is embedded into the neighboring molecular environment. It turned out that this approach can conveniently be applied to other complex biopolymers as well, such as the light sensitive, DNA compacting agent Azo-PM shown in **Fig. 2**. The blue solid lines indicate the decomposition of the molecule into different building blocks. Partial atomic charges are determined by considering combinations of building blocks and defining suitable overlap regions. The resulting model for Azo-PM was successfully used to study its interaction with a DNA strand **[4]**. The *cis*- isomer of azo moiety leads to an overall weaker interaction of the protonated amine groups with the negatively charged phosphates. In the experiment, this difference triggers decompaction/compaction of single DNA molecules under photo(UV-)induced *cis-trans* isomerization.

Conclusions and Current Developments.

How to deal with force field dependent outcomes of a computer simulation will certainly become an interesting aspect of our future work, in particular if available experimental evidence cannot favor one over the other. In this respect, complementary simulation techniques can prove valuable. In the example of dodecamer accomodation at the TSP binding groove one might obtain further information from estimating how efficiently the polysaccharide can be cleaved depending on its conformation in the binding site. Currently, we are exploring hybrid quantum mechanical/molecular mechanical (QM/MM) techniques in order to model the corresponding process of enzymatic hydrolysis explicitly. As a starting point, however, we have first returned to azobenzene derivatives. Their isomerization process is genuinely quantum mechanical, the kinetics of which is greatly influenced by an environment that can be kept at the classical molecular mechanical level. This also facilitates the use of path sampling techniques, by which we can access the dynamics of reaction mechanisms **[5]**.

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Modelling Aqueous Saccharides: How Sticky are these Sugars?

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Carbohydrates are abundant in nature and natural materials. Their function ranges from structural stability and energy storage to functions in the glycocalyx, the extracellular matrix, cell signaling and the molecular recognition of pathogens. In order to understand these diverse functions, increased efforts have been made recently to model these carbohydrates in order to elucidate their molecular properties.

All-atom molecular dynamics (MD) simulations are a useful method to study biomolecular systems **[1–5],** and several force fields have been developed specifically for carbohydrates. A comparison of several such force-fields have shown that the best agreement with the sparse experimental data, both for solution properties and hydration free energies, could be obtained using the GLYCAM06 force-field with the TIP5P water model **[6]**.

While models with atomistic resolution give a detailed picture, they often cannot reach the length and time scales required to sample larger polysaccharides. Strategies to overcome these difficulties involve the use of simplified coarse-grained models, with fewer degrees of freedom **[7–10]**. Here we describe the application these modelling strategies to hemicellulose polysaccharide systems. The simulations described below were motivated by an attempt to explain the molecular origin of the actuated motion performed by plant cell wall materials in response to hydration, e.g. in the opening of pine cones and many other processes.

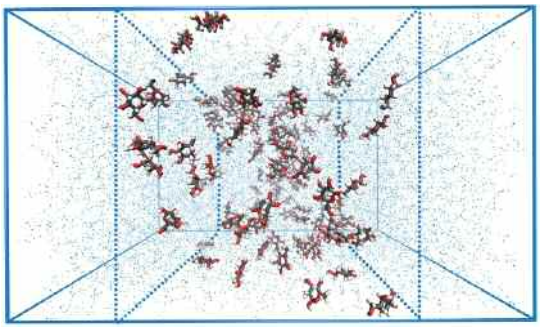

*Fig. 1: Simulation setup to measure the Osmotic Pressure **[11].***

Osmotic Pressure in Carbohydrate Solutions

A key property to quantify the aggregation of solutes is the osmotic pressure π of a solution. An intuitive method to obtain π directly in MD simulations is the use of virtual, semi-permeable membranes, which confine the solute molecules to a central region in the simulation box, as shown in **Fig. 1**. The pressure π can then be calculated from the wall force acting on the solute atoms **[11]**.

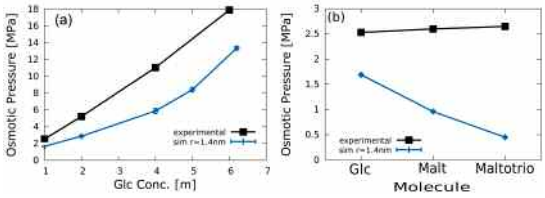

*Fig. 2: Osmotic pressure calculated as a function of concentration (a) and degree of polymerization (b) **[11].***

Fig. 2a shows π as a function of concentration for β-D-Glucose solutions, in comparison to experimental data. Clearly, the simulated results systematically underestimate π by approximately a factor of two. The low osmotic pressure indicates that, although no aggregation is directly observed in the simulated systems, the sugar-sugar interactions are overrepresented by the force-field. As expected from the previous force field comparison, other common force fields perform even worse.

Even more severe is the observation **(Fig. 2b)** that π decreases for larger molecules, i.e. a Maltose dimer and a Malto-triose, whereas experimental data shows a slight increase of π with the degree of polymerization.

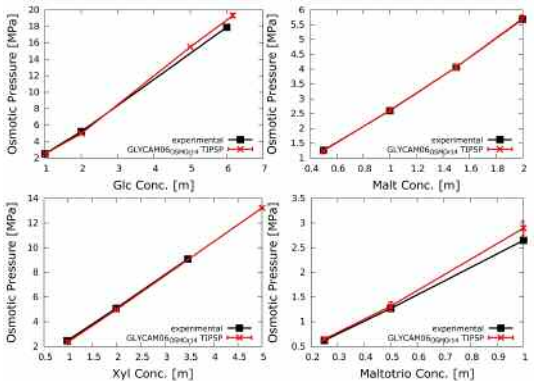

*Fig. 3: Osmotic pressure calculated using the new force field parameters $GLYCAM_{06SMOr14}$.TIP5P **[11].***

Considering these shortcomings, improved force field parameters are required to obtain any predictive power about the factors affecting the water sorption capacities. Since aggregation was found to be driven by the Lennard Jones interactions, and as the charges of the force field have been optimized specifically for carbohydrate conformations, we focus on adjusting the Lennard Jones parameters ε. The data shown in **Fig. 3**, illustrates, that the optimized parameters lead to excellent agreement with experimental data, both for molecules used in the reparametrization process (Glucose, Maltose), and for test molecules (Xylose, Maltotriose).

Factors affecting the Osmotic Pressure

We can now apply the optimized force field to gain some insight into the factors which affect π, and thus the water sorption capability of carbohydrate molecules. First, we compare the influence of the chemical structure of the monomer building blocks. While changes in the geometric configura-

tion of the atoms have no appreciable effect – Glucose, Mannose and Galactose give indistinguishable results – the removal of an OH group (e.g. Xylose) or substitution of an apolar group (e.g. 06-acetyl-β-D-galactose) both decreases the osmotic coefficient of the solution.

Then, we consider the effect of xyloglucan structure on π. To that effect, short structures with monomeric and dimeric branches are compared to linear saccharides made from the same monomers. In all cases, π is higher for the branched structure. The magnitude of the difference increased with the number of side chains, reaching ~40% for three monomer side chains. The location of the side chains has a comparatively small influence. The branching point has no appreciable effect for monomer side chains, whereas for a longer (dimeric) sidechain a small influence of the side chain location on π emerges.

A Coarse- Grained Sugar Model

The osmotic pressure calculations for linear saccharides are limited to 7 monomers. Equilibration of longer polymers could not be achieved, which illustrates the limitations of all-atom MD simulations. As many natural polysaccharides are much longer, a reliable coarse-grained representation is required to study such systems.

Therefore, we develop a procedure to generate a coarse-grained model based on the sampling at the atomistic scale, which employs Boltzmann Inversion, to obtain parameters for the bonded interactions within one molecule, and the Force-Matching method for non-bonded interactions between different molecules (and all sites not interacting by bonded interactions). This hybrid model reproduces the structural data from the atomistic system quite well, provided the solute-solute interactions and the interactions involving solvent are treated separately **[10]**.

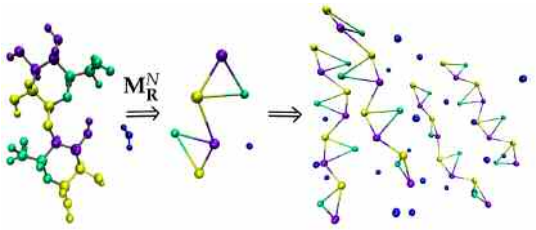

*Fig. 4: Mapping between the atomistic and coarse-grained Model **[10]**.*

To be useful for the simulation of polymer systems, it is crucial, that the developed model is transferable to different polymer lengths or concentrations. Tests have shown that the models can be transferred to different lengths and to higher concentrations, and perform with a similar accuracy as the models derived specifically at that concentration/polymer length. However, care has to be taken when the method is applied at low concentrations, where first the native, and then the transferred model fail to capture the correct aggregation behavior of the molecules. This is related to small perturbations in the long range interactions, which gain more importance at lower concentrations.

The aggregation at low concentration can be corrected by applying a small cut-off to the long range interactions. This cut-off has no appreciable effect on the system at higher concentrations. Finally, the same procedure can be used to generate implicit solvent models, which have the highest efficiency, where specific water interactions are not important.

Application

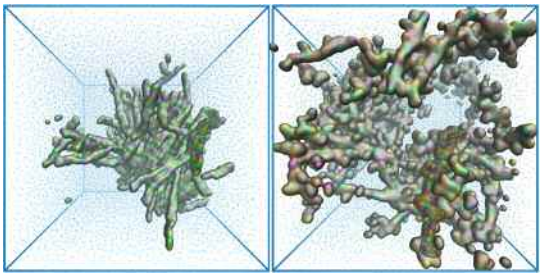

*Fig. 5: Representative snapshots from the coarse-grained system of linear (left) and branched (right) polysaccharides **[10].***

As a first application of the coarse-grained model, the water-uptake by clusters of linear or branched polysaccharide was studied and compared. The linear polysaccharides remain in tight aggregates, while the branched molecules absorb water, until their network spans the entire simulation box, as shown by the representative snapshots in **Fig. 5.**

Because the coarse-graining procedure applied to develop the model relies on reproducing the forces present in the atomistic system, and because the osmotic pressure π is calculated from the wall force acting on the sugar molecules, it is also possible, to measure π of the coarse-grained system, and excellent agreement between π measured in the atomistic and the coarse-grained systems is achieved. The computational speedup of this procedure will allow to measure π of much larger molecules and longer branches, to gain a concise understanding of the factors tuning the water sorption of polysaccharide gels, such as the hemicellulose matrix.

What about Interactions with other Molecules?

In most biological systems, carbohydrates do not act by themselves, but are in contact with other biomolecules such as lipids and proteins.

Even the simple addition of salt to the system turned out to be problematic, as no optimized ion parameters exist to be used with the TIP5P water model. Tests show, that parameters optimized for other water models do not give satisfactory results, so that a new set of LJ parameters for alkali and halide ions has been developed to reproduce the hydration free energy as well as the activity derivative, a_{cc}, and coordination numbers of chosen salts. In the process, we have shown that matching a_{cc} alone is not sufficient, because a_{cc} as a function of the interaction strength often reaches a plateau. This means that parameters leading to equally good agreement with experiment can yield very different solution structures **[12].**

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Protein Synthesis in the Cell

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The synthesis of proteins is a fundamental task of all living cells because almost every cellular process is governed by proteins. Every protein consists of at least one chain of amino acids. The concatenation of individual amino acids into peptide chains is achieved by molecular machines called ribosomes. To synthesize a protein, a ribosome uses the genetic information stored in the corresponding messenger RNA (mRNA). A mRNA consists of a sequence of codons, each of which codes for a specific tRNA and, thus, for a specific amino acid. Each amino acid is carried by a transfer RNA (tRNA) molecule. An aminoacylated tRNA and an elongation factor EF-Tu form a ternary complex that reaches the ribosome by diffusive motion. The ribosome reads the mRNA codon by codon and takes up the corresponding ternary complexes. This process is called translation. Our group studies translation at different levels from individual biochemical kinetic rates to cell-wide protein synthesis.

Ultrasensitive Dependence of Protein Synthesis on EF-Tu Concentration

The bacterial doc-phd toxin-antitoxin system has a strong influence on the rate of cell growth. The toxic protein Doc suppresses the growth rate by inhibiting the elongation factor EF-Tu, which is crucial for bacterial translation, see **Fig. 1**. Given that EF-Tu is one of the most abundant proteins in bacteria, it is astonishing that Doc is such an effective toxin. To find the origin of the high Doc efficiency, we study the effect of EF-Tu inhibition on protein synthesis within a recently established theoretical framework for bacterial translation **[1, 2].** Surprisingly, we find a very sensitive dependence of the overall translation rate on EF-Tu abundance: a small decrease in EF-Tu concentration leads to a strong suppression of overall protein synthesis, despite the extremely high cellular abundance of the elongation factor **[3].** We show that this ultrasensitivity is caused by imbalances in the interplay of different codons and tRNAs and can be observed for complex *in-vivo* protein synthesis as well as in simple artificial translation systems based on only two codons and their cognate tRNAs. Thus, the abundance of EF-Tu is a highly effective control variable for bacterial protein synthesis whereby the growth-inhibiting effect of Doc is strongly amplified.

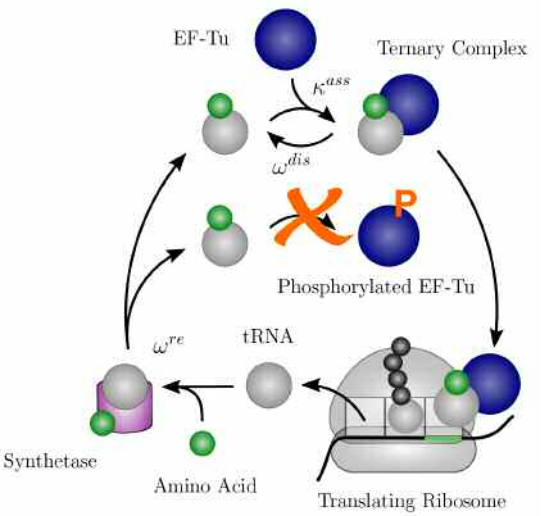

Fig. 1: Ternary Complex Formation. After a tRNA is released from a ribosome, it binds to an aminoacyl tRNA synthetase that recharges the tRNA with its cognate amino acid. The recharged tRNA binds to elongation factor EF-Tu to form a ternary complex that delivers its amino acid to a translating ribosome (upper pathway). If an EF-Tu molecule gets phosphorylated by the toxin Doc, it is no longer able to bind aminoacylated tRNAs (lower pathway).

Optimizing the Dynamics of Protein Translation

Optimizing protein translation for synthetic gene expression is a complex task. Conventionally, improvement of protein synthesis was approached by replacing rarely used codons by the target organism's preferred codons. However, this strategy does not always yield the best results. In contrast to these conventional approaches, we predict optimal codon usage based on translation speed and accuracy combined with further relevant covariates and confirm our optimization approach with proteome data from widely used prokaryotic, eukaryotic, and human expression systems **[4].** We optimized and tested heterologous expression of two genes, *manA* and *ova* in *Salmonella Enterica serovar Typhimurium,* which showed a threefold increase in protein yield compared both to wild type and commercially optimized sequences. Our multi-parameter algorithm cannot only be used for protein yield optimization but also encompasses fine-tuning protein expression, including deoptimization, e.g. for synthetic attenuated virus engineering.

Studying the Nascent Peptide Chain in the Ribosomal Exit Tunnel

Our collaborators Prof. Dr. Marina Rodnina and Dr. Wolf Holtkamp from the Max Planck Institute for Biophysical Chemistry use a stopped-flow instrument to study translation as shown in **Fig. 2**: One syringe of the instrument is filled with a solution containing the ribosomes and mRNAs, whereas the other holds the corresponding tRNAs. Translation starts

as soon as the two solutions are mixed together. During translation, the elongating nascent peptide chains traverse the ribosomes' exit tunnels. We monitor this co-translational movement via fluorescent probes attached to the N-termini of the nascent chains. Due to fluorophore quenching, the time-dependent fluorescence signal emitted by an individual peptide is determined by co-translational events, such as secondary structure formation and peptide-tunnel interactions. To obtain information on these individual events, the measured total fluorescence signal has to be decomposed into position-dependent intensities. To this end, we describe mRNA translation as a Markov process and assign a specific fluorescence intensity to each ribosomal state. **Fig. 3** shows the measured time-dependent total fluorescence intensity for poly-phenylalanine peptides and numerical results obtained by the evaluation of our model. Our theoretical description provides a good representation of the biological process. We find that the N-terminus of poly-phenylalanine experiences major environmental changes, which occur primarily during translation of the first eight amino acids.

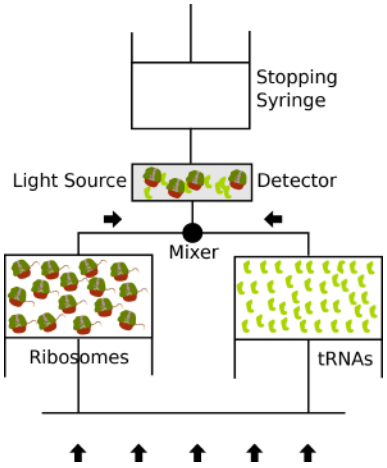

Fig. 2: Schematic drawing of a stopped-flow instrument to study translation by fluorescent probes. The syringe on the left is filled with a mixture of ribosomes and mRNAs, whereas the right syringe contains the tRNAs. Translation begins when both solutions are mixed. Progression of translation is monitored by a fluorescent signal emitted by fluorophores attached to the N-termini of the elongating peptides.

Co-Translational Assembly of Protein Subunits

Protein assembly from multiple subunits inside the crowded cell environment is subject of ongoing research. In contrast to the general thinking of protein assembly as a post-translational process, recent experiments show that protein complexes can also assemble co-translationally, i.e., subunits may assemble *before* translation has finished (Yu-Wei Shieh et al., Science 2015). Our collaborator Roy Bar-Ziv and his group from the Weizmann Institute of Science in Israel performed *in-vitro* translation experiments to assess the role of

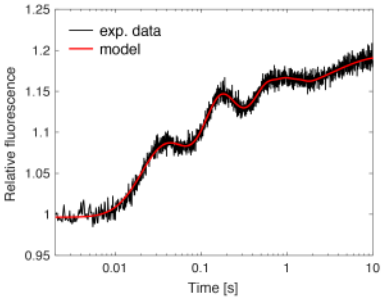

Fig. 3: Fluorescence signal of poly-phenylalanine translation (black line) obtained by a stopped-flow experiment and signal as predicted from our translation model (red line).

the spatial distance between the translation sites of different protein subunits. As a first step, we modeled the synthesis and spread-out of one type of proteins in one dimension as a Markov process (**Fig. 4**) in good agreement with the experimental data (**Fig. 5**). As a next step, we will study post- and co-translational interactions of multiple protein subunits by Gillespie simulations to understand the dynamics of protein assembly processes.

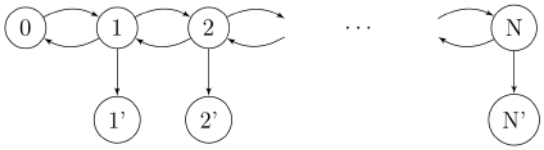

Fig. 4: Markov model for the spread-out of one type of protein in one dimension.

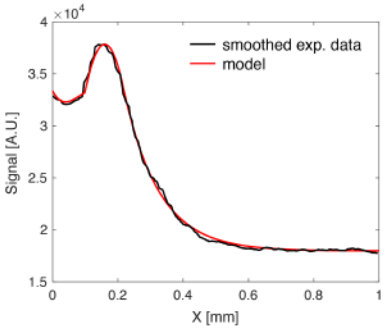

Fig. 5: Fluorescence signal of a protein from an in-vitro translation experiment (black line) and signal as predicted from the Markov model (red line).

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Post-transcriptional Regulation of Gene Expression

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Research in this group is concerned with stochastic processes in complex and biological systems. Our study includes both formal and mathematical aspects of such processes **[1],** some formulations applied to models of molecular motors **[2],** and to the understanding of stochastic processes with application to data analysis **[3],** to cell cycle dynamics **[4],** to computational neuroscience **[5],** and to population genetics **[6].**

The main research focus of the group in the years covered by this report is concerned with various processes related to the post-transcriptional regulation of gene expression. Gene expression is a generic term that is commonly related to what is known as the central dogma of molecular biology. Accordingly, genes found in the DNA are first transcribed into RNA molecules. The majority of the total RNA molecules present in each cell plays a key role in the production of proteins. Some species of RNA molecules become part of ribosomes. Some RNAs become transfer RNA, called also tRNA. Some RNAs are found in the form of small or micro RNA and finally a prominent role in gene expression is played by messenger RNA molecules (mRNA). Protein synthesis is the final product of gene expression: in this process, the ribosomes read the information encoded in the mRNA and synthesize the proteins using the amino-acid delivered by the tRNAs. This process is called translation. The particular way in which the ribosome reads the mRNA is the basis of what we know as the genetic code. The ribosome reads the nucleotide sequence of the mRNA one triplet per step. To each triplet, called codon, corresponds one amino-acid that will be incorporated to the nascent protein. The amount of proteins corresponding to a given gene present in the cell will thus depend on several factors. The first factor is the amount of mRNAs of that gene: this is determined by the balance between the synthesis rate of the mRNA (transcription rate) and the degradation rate of the mRNA. The second factor is the amount of ribosomes translating each mRNA molecules, which eventually determines the protein synthesis rate. The final factor is the degradation rate of the proteins.

Stability of mRNA

The RNA molecules that become part of the ribosome are called rRNA. Both rRNA and tRNA are very stable. Their function is to provide the machinery of the process of translation, independently of what has to be translated. The mRNA molecules instead are typically not so stable and their lifetime is regulated by some internal cellular mechanisms. Indeed, when the cell needs to change the kind of proteins to be synthesized, due for instance to some stressful condition, it can do so by changing the composition of the cell mRNA population **[7].** Beside the important role played by the regulation of transcription, one way to tune the amount of mRNA is to activate or deactivate specific degradation mechanisms. In eukaryotic organisms, one such degradation mechanism is driven by short and specific RNA sequences called miRNA. From the molecular biology viewpoint, it is often very important to know which factors and in which temporal sequence they affect a specific biochemical process. In the case of miRNA it was known that this RNA first forms a complex called miRISC and then it acts by recruiting the target mRNA and other protein complexes called NOT1 and PAN3. Despite very insightful experiments, it was not clear if miRISC first recruits the mRNA and then the proteins or *vice versa*. In a recent study **[8],** we have analysed the experimental data and shown that they are only compatible with miRISC first binding to NOT1 and/or PAN3 and then recruiting the mRNA (**Fig 1**). In the analysis of the data we have employed a hierarchical approach and modelled the single-molecule degradation as a continuous time Markov chain. As a side product, we have found that there must be another degradation mechanism for the targeted mRNA that accounts for about 20% of the degradation events.

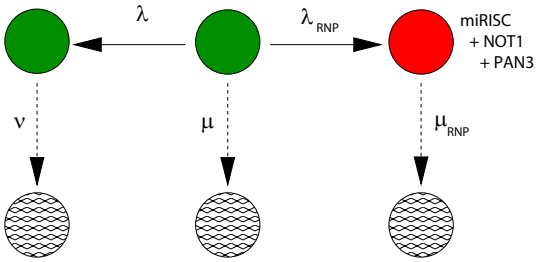

Fig. 1.The experimental data for the degradation of a specific mRNA in drosophila can be explained by means of this most parsimonious model in which the miRISC factor first recruits NOT1 and/or PAN3 and then binds to the target mRNA (red state). As a by-product, we find that another alternative pathway (left green state) is also necessary ***[8].***

Drop-off of Ribosomes

Another way to modulate the amount of proteins synthesized per mRNA is through what is known as translational control. One of the ways to see if translational control is at work is by monitoring the change in the amount of ribosomes per mRNA for all genes in the cell **[7].** The experimental technique mostly used in recent times for this analysis is called riboseq, which consists in blocking the ribosomes during the process of translation and analysing the short strings of mRNA found inside the ribosome body. After aligning those short strings (called "reads") with the DNA, it is possible to infer the spatial distribution of ribosomes along each mRNA species and the increase or decrease of the ribosome density per mRNA after certain stress conditions **[7].** Another process known to happen during translation is when ribosomes abort the synthesis of proteins and abandon the mRNA. This process is called ribosome drop-off (**Fig 2**).

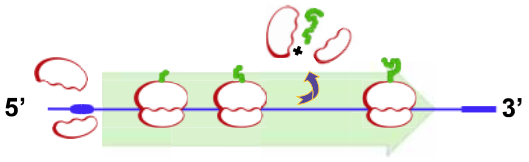

Fig. 2. In the process of translation, the ribosome starts at the 5' (left) end of the mRNA and proceed towards the 3' (right) end thereby synthesizing the protein. When drop-off occurs, the ribosome has a certain probability to stop translation at any point and thus leave the mRNA and release the nascent protein. Under the condition of very small initiation rate, the drop-off leads to decreasing ribosome density along the mRNA ***[9].***

Although some specific RNA sequences may be responsible for drop-off at certain mRNA species, it has also been postulated that ribosomes drop-off as a consequence of unspecific processivity errors. While in the late 70's experimental research found evidence of ribosome drop-off in *Escherichia coli*, recent research based on riboseq data found no trace of ribosome drop-off in this organism. This lack of evidence seemed to us quite strange because this organism possesses a set of enzymes and special RNA molecules specifically devoted to take care of the toxic effects of ribosome drop-off. We thus decided to analyse a large set of riboseq data from different labs by developing and applying more advanced and sensible data analysis techniques **[9].** Finally, we found out that across all data collected under normal growth conditions there is clear quantitative evidence of ribosome drop-off at a rate consistent with the rate found experimentally in the late 70's. Furthermore, we could see that several acute stress conditions have the effect of increasing the rate of ribosome drop-off, thus indicating that ribosome drop-off may be one of the first reaction modes of *E. coli* under acute stress.

Protein Ageing and Degradation

Further down in the chain of processes that regulate gene expression we have protein degradation. In prokaryotic cells, proteins have an average lifetime typically longer than the cell division time. This makes the detection of their degradation difficult because its rate is much smaller than the dilution rate due to cell division. In eukaryotic cells, instead, there are many proteins whose lifetime is shorter than the cell cycle, thus rendering the measurement of their decay experimentally accessible. One key technique to detect protein decay is to first pulse the cells with labelled amino acids and then chase the labelled proteins and measure their decaying amount over time. The data resulting from these pulse-chase experiments are traditionally analysed by assuming an exponential decay. However, if proteins age during their lifetime then a more complex data analysis approach is necessary and was developed in our group **[10].**

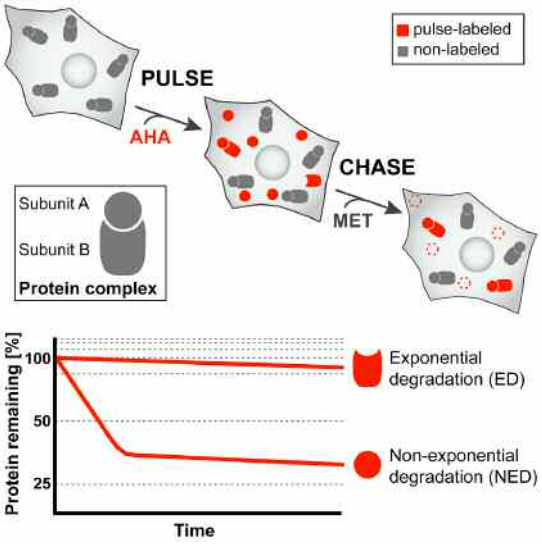

Fig. 3. Pulse and chase experimental technique combined with mass spec analysis allows to monitor the decaying amount of proteins over time with a minimal disturbance of the normal cell functioning. When proteins decay exponentially, their decay pattern is a straight line in a log-linear plot ***[10].*** *It is likely that isolated single subunits of protein complexes decay exponentially but become more stable once the complex is formed* ***[11].***

In fact, this advanced approach (**Fig 3**) is a tool to detect ageing from decay data. In a collaborative project with the group of Matthias Selbach at the MDC in Buch, protein decay from mice cells was measured by means of mass spec data. We found that at least 15% of all proteins have a non-exponential decay, which means that these proteins age during their lifetime **[11].** Ageing, in fact, means that the probability to be degraded per unit of time changes with the age of the molecule. In the specific case of the measured decay patterns, we found that for those ageing proteins their degradation rate decreased with age. Although the ultimate reason for this increase in stability with age is not clear for each single protein species, control experiments showed that some proteins normally found in complexes have a first phase in their life in which they are still not incorporated in the complex and thus very unstable. The increase in stability occurs when they are finally incorporated into the protein complex.

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Protein Binding and Membrane Adhesion

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Binding of Membrane-anchored Proteins

Cell adhesion processes and the adhesion of vesicles to the membranes of cells or organelles depend sensitively on the binding constant and binding kinetics of the membrane-anchored receptor and ligand molecules that mediate adhesion. Since the binding equilibrium constant K_{2D} and the on- and off-rate con-stants of these receptor and ligand molecules are difficult to measure in their natural two-dimensional (2D) membrane environment, a central question is how they are related to the binding equilibrium constant K_{3D} and the on- and off-rate constants of soluble variants of the receptors and ligands that lack the membrane anchors and are free to diffuse in three dimensions (3D). The binding constant K_{3D} and on- and off-rate constants of these soluble receptors and ligands can be quantified with standard experimental methods **[1, 2, 3].**

A membrane-anchored receptor can only bind to an apposing membrane-anchored ligand if the local membrane separation l at the site of the receptor and ligand is within an appropriate range. This local separation l of the membranes varies – along the membranes, and in time – because of thermally excited membrane shape fluctuations. Experiments that probe the binding equilibrium constant K_{2D} imply averages in space and time over membrane adhesion regions and measurement durations. Our recent simulations and theories indicate that these averages can be expressed as **[1]**

$$K_{2D} = \int K_{2D}(l) P(l)\, dl$$

where $K_{2D}(l)$ is the binding equilibrium constant as a function of the local membrane separation l, and P(l) is the distribution of local membrane separations that reflects the spatial and temporal variations of l. The function $K_{2D}(l)$ is maximal at a preferred local separation of the receptors and ligands, and asymmetric around this maximum because the complexes can tilt at smaller separations but need to stretch at larger separations (**see Fig. 1c**). Our simulations show that the distribution P(l) of the local separation is well approximated by a Gaussian function in situations in which the adhesion is mediated by a single type of receptors and ligands. The two key membrane properties that emerge from this general theory are the average separation and relative roughness of the membranes, which are the mean and standard deviation of P(l).

The binding constants K_{2D} and K_{3D} of membrane-anchored and soluble receptors and ligands can be calculated from the translational and rotational entropy loss upon binding **[1, 3]**. As a function of the local membrane separation l, the binding constant K_{2D} has the general form **[1]**

$$K_{2D}(l) = \sqrt{8\pi} K_{3D} \frac{A_b}{V_b} \frac{\Omega_{RL}(l)}{\Omega_R \Omega_L}$$

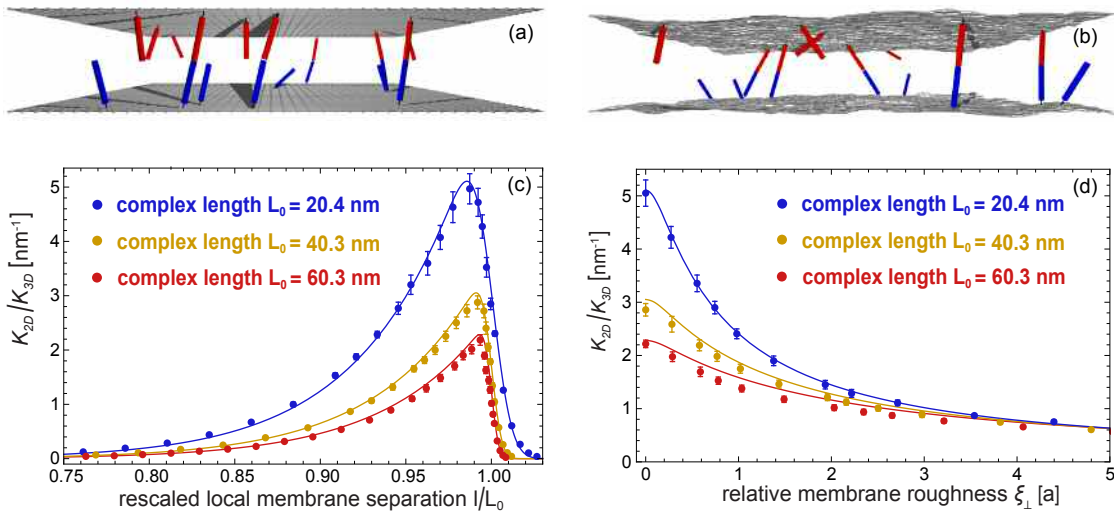

*Fig. 1: (a) Snapshot from a Monte Carlo (MC) simulation with receptors and ligands anchored to parallel and planar membranes. The receptors and ligands diffuse along the membranes and rotate around their anchoring points. (b) Snap-shot from a MC simulation with flexible membranes that exhibit thermally excited shape fluctuations. (c) Ratio K_{2D}/K_{3D} of the binding constants of membrane-anchored and soluble receptors and ligands versus local membrane separation l for different lengths L_0 of the receptor-ligand complexes. The binding constant K_{3D} of soluble variants of the receptors and ligand is determined by the binding potential of the receptors and ligands and does not depend on the complex length L_0. (d) Ratio K_{2D}/K_{3D} of binding constants versus relative membrane roughness of two thermally fluctuating membranes at their preferred average separation. The binding constant K_{2D} strongly decreases with the relative membrane roughness. The data points in (c) and (d) represent MC data, and the lines theoretical results without data fitting (from Ref. **[1]**).*

where Ω_R, Ω_L, and $\Omega_{RL}(l)$ are the rotational phase space volumes of the unbound receptor R, unbound ligand L, and bound receptor-ligand complex RL relative to the membranes, and A_b and V_b are the translational phase space area and translational phase space volume of the bound ligand relative to the receptor in 2D and 3D. Our theory for the ratio of K_{2D} and K_{3D} agrees with data from Monte Carlo simulations without fit parameters (**see Fig. 1**), and can be extended to the on- and off-rate constants of the receptors and ligands **[2]**.

Conformational Changes during Protein Binding

The function of proteins is affected by their conformational dynamics, i.e. by transitions between lower-energy ground-state conformations and higher-energy excited-state confirmations of the proteins. Advanced nuclear magnetic resonance and single-molecule experiments indicate that higher-energy conformations in the unbound state of proteins can be similar to ground-state conformations in the bound state, and vice versa. These experiments illustrate that the conformational change of a protein during binding may occur before a binding event, rather than being induced by this binding event. However, determining the temporal order of conformational transitions and binding events typically requires additional information from chemical relaxation experiments that probe the relaxation kinetics of a mixture of proteins and ligands into binding equilibrium. These chemical relaxation experiments are usually performed and analysed at ligand concentrations that are much larger than the protein concentrations. At such high ligand concentrations, the temporal order of conformational transitions and binding events can only be inferred in special cases.

We have derived general equations that describe the dominant chemical relaxation kinetics at all protein and ligand concentrations **[4]**. Our general equations allow to clearly infer from relaxation data whether a conformational transition occurs prior to a binding event ('conformational selection'), or after the binding event ('induced fit'), see **Fig. 2**.

Wrapping of Nanoparticles by Membranes

Nanoparticles are wrapped spontaneously by biomembranes if the adhesive interactions between the particles and membranes compensate for the cost of membrane bending **[5, 6, 7].** In previous simulations and elasticity calculations, we have observed the cooperative wrapping of spherical nanoparticles in membrane tubules. For spherical nanoparticles, the stability of the particle-filled membrane tubules strongly depends on the range of the adhesive particle-membrane interactions. Our recent elasticity calculations show that elongated and patchy particles are wrapped cooperatively in membrane tubules that are highly stable for all ranges of the particle-membrane interactions, compared to the individual wrapping of the particles **[6]**. The cooperative wrapping of linear chains of elongated or patchy particles in membrane tubules may thus provide an efficient route to induce membrane tubulation, or to store such particles in membranes. In addition, we have investigated how the wrapping process of spherical nanoparticles depends on the initial curvature of the membrane **[7]**.

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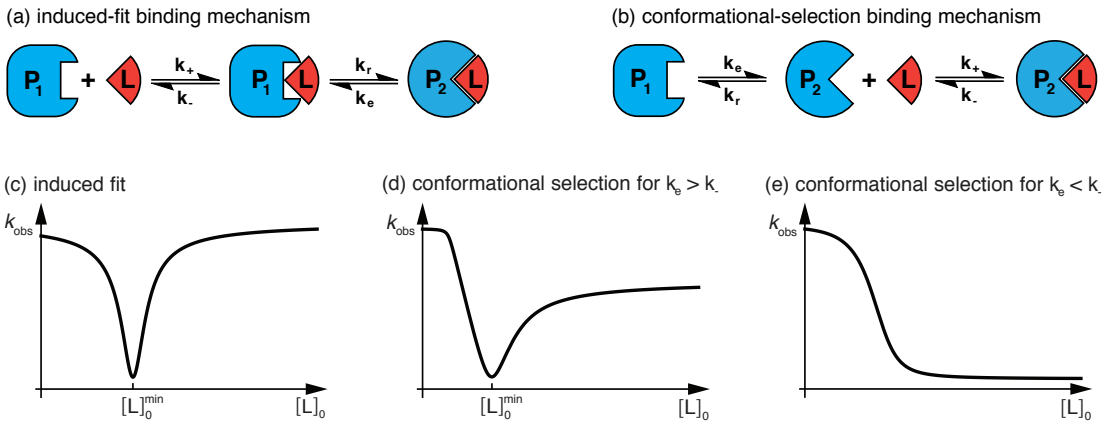

*Fig. 2: Characteristic chemical relaxation of induced-fit and conformational-selection binding (from Ref. **[4]**). (a) In induced-fit binding, the change between the conformations P_1 and P_2 of a protein occurs after binding of the ligand L. (b) In conformational-selection binding, the conformational change of the protein occurs prior to ligand binding. (c) As a function of the total ligand concentration $[L]_0$, the dominant, smallest chemical relaxation rate k_{obs} of induced-fit binding is symmetric with respect to a minimum located at $[L]_0^{min} = [P]_0 - K_d$ where $[P]_0$ is the total protein concentration and K_d the overall dissociation constant. (d) The dominant relaxation rate k_{obs} of conformational-selection binding has a characteristic minimum for $k_e > k_-$, but is not symmetric with respect to this minimum. (e) For $k_e < k_-$, the dominant rate k_{obs} of conformational-selection binding decreases monotonically with $[L]_0$.*

Bilayer Asymmetry and Spontaneous Tubulation

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Biological and biomimetic membranes consist of molecular bilayers with two monolayers or leaflets. These leaflets can differ in their composition or be exposed to different aqueous solutions. Because of these bilayer asymmetries, the membranes prefer to attain a certain curvature. In the past, this preferred or spontaneous curvature, which can be positive or negative, was typically treated as a phenomenological parameter, and very few attempts have been made to estimate its magnitude.

What we have achieved within the last couple of years is to develop new and general methods by which one can determine the spontaneous curvature in a quantitative manner. Our results show that the magnitude of this curvature can vary over several orders of magnitude, from 1/(20 nm) to 1/(50 μm).

On the molecular scale, one can distinguish a variety of mechanisms for the local generation of membrane curvature. As described below, these mechanisms include the adsorption and depletion of small solutes, the binding of flexible polymers, and the insertion of glycolipids with large head groups. All of these mechanisms can generate large spontaneous curvatures to which the vesicle membranes adapt by the formation of small buds and thin nanotubes.**[1]** These membrane protrusions involve thin membrane necks, which play an essential role in many biological processes such as endocytosis and cytokinesis.

Mechanisms of Local Curvature Generation

Adsorption and desorption of small solutes. The two leaflets of a bilayer membrane are typically exposed to two aqueous solutions that differ in their solute composition. Let us first consider solutes such as ions or monosaccharides that are smaller than the membrane thickness, which has a typical value between 4 and 5 nm. Attractive interactions between the solutes and the membrane lead to adsorption layers adjacent to the two leaflets **[2]**, repulsive interactions to depletion layers **[3]**. Both types of layers are illustrated in **Fig. 1**. If the aqueous solutions have different solute compositions, the two leaflets of the bilayer experience different molecular interactions and the asymmetric membrane acquires a certain preferred or spontaneous curvature. It is important to realize that both attractive and repulsive membrane-solute interactions generate a preferred curvature. Furthermore, the curvature generated by depletion layers has the opposite sign and a different magnitude compared to the one generated by adsorption layers, see **Fig. 1**.

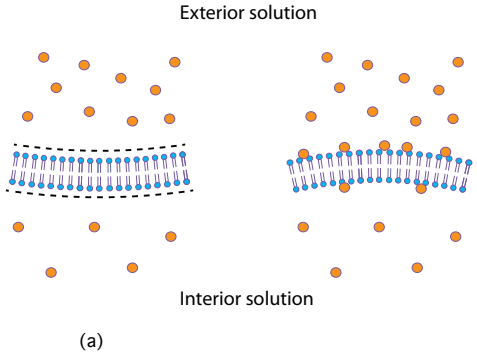

Fig. 1: Segments of lipid bilayers (blue) exposed to small solutes or 'particles' (orange): (a) The particles experience repulsive interactions with the membrane and form two depletion layers (broken lines) adjacent to the two bilayer leaflets. The bilayer then prefers to bulge towards the interior solution and acquires a negative spontaneous curvature; and (b) The particles experience attractive interactions with the membrane and form two adsorption layers adjacent to the two membrane leaflets. The bilayer now prefers to bulge towards the exterior solution and acquires a positive spontaneous curvature.

The spontaneous curvature generated by the adsorption or depletion of small solutes has been recently elucidated by analytical theory and molecular simulations. **[2, 3]** Both for adsorption and for depletion, the spontaneous curvature is found to vary linearly with the concentration difference between the exterior and interior solution. For adsorption, spontaneous curvature values up to 1/(24 nm) were observed in the molecular simulations. These large values can be used to control the budding of relatively small vesicles (project of Rikhia Ghosh).

Binding of flexible polymers. Local membrane curvature can also be generated by the binding of flexible polymers. In general, one should distinguish between hetero-polymers with a few specific anchor groups that bind to the membrane and homo-polymers for which all monomers are attracted by the membrane. One example for the latter case is provided by the adsorption of polyethylene glycol (PEG) chains onto ternary lipid bilayers with different compositions corresponding to liquid-disordered and liquid-ordered phases. This process has been elucidated by atomistic molecular dynamics simulations as illustrated in **Fig. 2. [4]** The PEG molecules are only weakly bound to the membranes, with relatively short contact segments (or 'trains'), and relatively long loops in between. The two terminal OH groups of the PEG molecule were observed to be frequently bound to the membrane via hydrogen bonds. The curvature generated by these adsorbed polymers was not determined in the simulations but was deduced from the spontaneous tubulation of giant vesicles. The m-value obtained by three different methods of image analysis was -1/(125 nm) for the liquid-disordered and -1/(590 nm) for the liquid-ordered membranes. **[4]**

Insertion of glycolipids with large head groups. Cellular membranes often contain glycolipids with large head groups. Because of the mutual exclusion of these head groups, the membranes should prefer to bulge towards the leaflet with the higher ganglioside concentration. This expectation has been confirmed for membranes with a few mole percent of

the ganglioside GM1, as studied by two different experimental methods based on tubulation **[5]** and on initial micropipette aspiration **[6]** as well as by atomistic and coarse-grained molecular simulations (projects of Markus Miettinen and Aparna Sreekumari). In the two experimental studies, the spontaneous curvature was found to vary between -1/(130nm) and -1/(260nm) depending on the overall GM1 concentration.

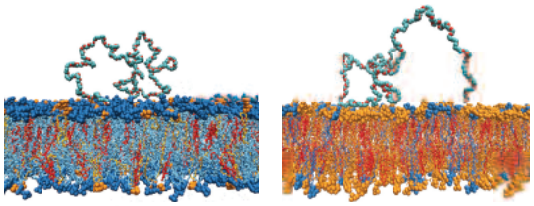

*Fig. 2: Polyethylen glycol (PEG) chains adsorbed onto (a) a liquid-disordered and (b) a liquid-ordered bilayer as observed in atomistic molecular dynamics simulations with explicit water. **[4]** The PEG chains consist of 180 monomers. The bilayers are composed of DOPC (blue), DPPC (orange), and cholesterol (red).*

Spontaneous Tubulation of Giant Vesicles

Giant vesicles often attain a spherical shape even if their membranes have a large spontaneous curvature. When such a vesicle is deflated osmotically, an increasing fraction of the vesicle membrane can adapt to the spontaneous curvature by forming small buds and nanotubes. The nucleation and growth of these membrane protrusions proceeds as follows. **[4]** Initial deflation leads to the formation of a small spherical bud that is connected to the mother vesicle by a thin membrane neck. For negative spontaneous curvature, the bud protrudes into the vesicle interior as shown in **Fig. 3**. Upon further deflation, the vesicle can follow two kinetic pathways which lead (i) to the extension of existing buds into necklace-like tubes and (ii) to the formation of new buds, see red and black arrows in Fig. 3. These competing pathways generate many different morphologies as experimentally observed for PEG adsorption **[4],** see **Fig. 4**, and for asymmetric ganglioside bilayers **[5, 6]**.

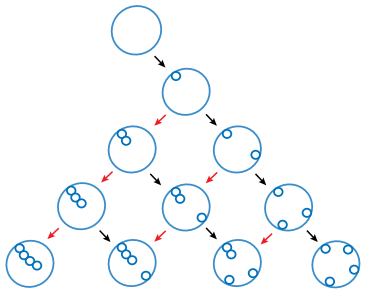

Fig. 3: Polymorphism arising from the osmotic deflation of a GUV in the presence of a large negative spontaneous curvature: Initial deflation of the spherical vesicle at the top leads to the formation of a small spherical in-bud. Further deflation steps can lead to the formation of additional in-buds (black arrows) or to the extension of existing in-buds into extended necklace-like in-tubes (red arrows). As a result of these two kinetic pathways, the vesicle can attain a large variety of shapes as illustrated here for four successive deflation steps.

When the length of a necklace-like tube reaches a certain critical value, the tube changes its morphology and transforms into a cylindrical one. **[4]** This necklace-to-cylinder transformation is disfavored by the end-caps of the cylinder but favored by the reduced volume of the cylindrical tube. The volume reduction implies a free energy contribution that is proportional to the tube length whereas the bending energy of the end- caps is independent of this length. Therefore, if a vesicle membrane forms several tubes, the shorter ones will be necklace-like whereas the longer ones will be cylindrical as observed experimentally, see the example in **Fig. 4(b)**.

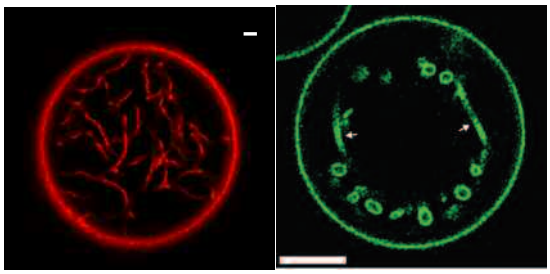

*Fig. 4: Giant vesicles with many nanotubes protruding into the vesicle interior: (a) Nanotubes formed by a liquid-disordered membrane (red) with a spontaneous curvature of -1/(125nm); and (b) Necklace-like tubes coexisting with two cylindrical tubes (white arrows) formed by a liquid-ordered membrane (green) with a spontaneous curvature of -1/(590 nm). **[4]** The scale bar is 2 μm in (a) and 10 μm in (b). The spontaneous curvature is generated by the adsorption of PEG chains as in **Fig. 2**.*

Mechanical Robustness of Tubulated Vesicles

Giant vesicles with membrane nanotubes have unusual mechanical properties because the tubes provide a large area reservoir for the mother vesicles. Therefore, these vesicles can adapt to strong mechanical perturbations by exchanging membrane area with the tubes. The vesicle membranes then experience a small mechanical tension that remains essentially constant until all nanotubes have been retracted. **[1]**

In order to elucidate this behavior, we used giant vesicles composed of POPC and a few mole percent of the ganglioside GM1. These vesicle form stable nanotubes protruding into the vesicle interior **[5, 6]** Micropipette aspiration can then be used to expose the vesicles to adjustable mechanical stresses and to retract the tubes in a controlled and reversible manner. **[6]** The mechanical robustness of the tubulated vesicles is demonstrated by their complete and reversible aspiration into the micropipettes, thereby mimicking the passage of such vesicles through small blood vessels (capillaries).

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Nanoparticles Interacting with Membranes and Vesicles

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In order to enter a cell, a nanoparticle must first cross the outer cell membrane. This entry process, known as endocytosis, begins with the adhesion of the nanoparticle to the cell membrane, followed by the engulfment of the particle by the membrane. The adhesion and engulfment steps of endocytosis can be mimicked in model systems consisting of nanoparticles in contact with lipid or polymer vesicles. Therefore, these steps are governed by an interplay between membrane-nanoparticle adhesion and membrane bending and do not require the coupling to chemical reactions such as nucleotide hydrolysis. Previous theoretical studies focused on the simplest case of nanoparticles interacting with planar and symmetric bilayer membranes. However, biological membranes are neither planar nor symmetric. In fact, they often display complex shapes with non-uniform curvature, and compositional asymmetry between the two leaflets of the bilayer is a hallmark of all cellular membranes. Extending the theoretical framework of curvature elasticity, we have recently shown that both spontaneous curvature, which provides a quantitative measure for the bilayer asymmetry, and membrane curvature have a rather strong effect on the engulfment process.

Engulfment Regimes for a Single Nanoparticle

Depending on the coverage of the particle surface by the membrane, we can distinguish three particle states (**Fig. 1**): (i) free (F) states in which the membrane does not spread over the particle surface at all, in spite of the attractive membrane-particle interactions; (ii) partially engulfed (P) states with a partial coverage of the particle surface by the membrane; and (iii) completely engulfed (C) states with full coverage of the particle by the membrane. In the latter case, the membrane forms a narrow neck that connects the particle-bound membrane to the unbound mother membrane. Combining numerical calculations with theoretical considerations, we have discovered exact analytical conditions for the energetic stability of free and completely engulfed states. **[1]** The completely engulfed state is stable provided the radius of the particle R_{pa} exceeds a certain critical radius R_{ce}, which depends on the particle-membrane adhesiveness, the bending rigidity and the spontaneous curvature of the membrane, and the local mean curvature of the mother membrane at the position of the narrow neck. On the other hand, the free state is stable only if the radius of the particle is smaller than a second critical radius R_{fr}, which again depends on the particle-membrane adhesiveness, the bending rigidity of the membrane and the local mean curvature of the membrane at the point of contact with the particle, but turns out to be independent of the spontaneous curvature. Combining these two stability conditions, we obtain four distinct engulfment regimes according to the stability of the free and completely engulfed states: the free regime (F stable, C unstable), the completely engulfed regime (F unstable, C stable), the bistable regime (both F and C stable, separated by an energy barrier) and the partially engulfed regime (both F and C unstable).

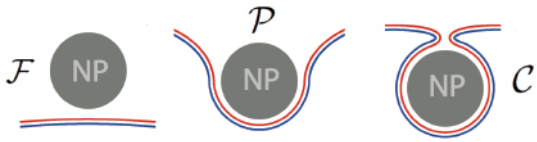

Fig. 1: A nanoparticle (NP, grey) in contact with a membrane with bilayer asymmetry (red and blue leaflets) can attain a free (F), partially engulfed (P) or completely engulfed (C) state. In the latter state, the membrane forms a narrow neck between the particle-bound and unbound membrane segments.

Engulfment Patterns of Nonspherical Vesicles Exposed to Many Nanoparticles

The two stability conditions that define the four engulfment regimes depend on the local curvature of the membrane. Therefore, when a nonspherical vesicle with nonuniform curvature is exposed to many nanoparticles, the vesicle membrane consists, in general, of several membrane segments that belong to different engulfment regimes. As a consequence, nonspherical vesicles can exhibit distinct engulfment patterns. **[2]** Examples for such patterns are displayed in **Fig. 2,** for the particular case of a prolate vesicle. It is important to note that not all combinations of engulfment regimes can be present on the surface of a single vesicle. In fact, our theory predicts that only 10 distinct engulfment patterns are possible.

Curvature-Induced Forces Acting on Uniform and Janus-like Nanoparticles

Going beyond the stability analysis of F and C states, we have developed an analytical theory for the case in which the particle size is small compared to the vesicle size. This theory provides the full energy landscapes of the membrane-particle systems, including the height of the energy barriers for the bistable regimes and the binding energies of partially engulfed particles. **[3]** Our theory predicts that the energy of partially engulfed particles depends on the local mean curvature of the vesicle membrane. As a consequence, partially engulfed nanoparticles experience curvature-induced forces that act to displace the particles towards membrane segments of lower or higher mean curvature, depending on whether the particles originate from the outside or inside of the vesicle, respectively. The partial engulfment of nanoparticles with a chemically uniform surface requires fine tuning of particle size and adhesiveness with respect to the properties of the membrane. In contrast, Janus particles with one strongly adhesive and one non-adhesive surface domain are always partially engulfed. Therefore, the curvature-induced forces are directly accessible to experimental studies when the vesicles are exposed to such Janus particles **(Fig. 3).**

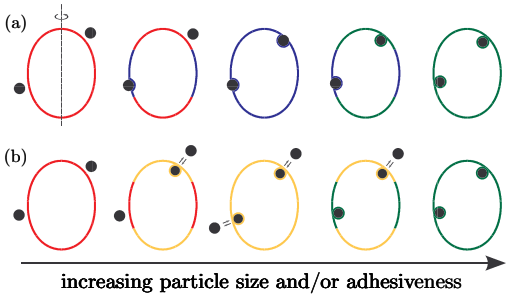

Fig. 2: Engulfment patterns of nanoparticles (black) on a prolate vesicle. The spontaneous curvature of the membrane is positive in (a) and negative in (b). The patterns involve four types of membrane segments: free segments with no engulfment (red) and bistable segments with energy barriers (orange) as well as segments decorated by partially engulfed (blue) and completely engulfed (green) particles. A change in particle size or adhesiveness leads to continuous morphological transitions between these patterns.

Endocytosis via Adhesion-Induced Segregation of Membrane-Anchored Receptor Molecules

So far, we have considered membranes with a uniform lateral composition. In order to model the more complex process of endocytosis in real cells, we have investigated the possibility of adhesion-induced segregation of membrane components, resulting in particle-bound and unbound membrane segments that differ in their bending rigidities and spontaneous curvatures. **[1]** In this way, we could explain experimental data for clathrin-mediated endocytosis of gold nanoparticles by HeLa cells. These data show a non-monotonic dependence of the particle uptake on the particle size with a maximum at a particle diameter of about 50 nm.

Stabilization of Narrow Membrane Necks by Adhesive Surfaces and Constriction Forces

As mentioned before, a completely engulfed particle implies a narrow membrane neck, see **Fig. 1.** It is important to note that such narrow necks arise in many other membrane processes. Important examples are the budding and tubulation of supported lipid bilayers, the formation of extracellular and outer membrane vesicles by eukaryotic and prokaryotic cells, cytokinesis during cell division, or the collective engulfment of many particles into necklace-like tubes, see **Fig. 4.** Furthermore, in cells, the formation of narrow necks is often assisted by constriction forces directly applied to the membrane neck by proteins such as dynamin in endocytosis, or actomyosin in cytokinesis. In order to account for these different situations, we have extended our stability analysis of narrow necks to different geometries and included constriction forces acting at the neck. **[4]** As a result, we obtained relatively simple stability conditions that are directly applicable to many systems of experimental interest and provide bounds on the material parameters of the systems.

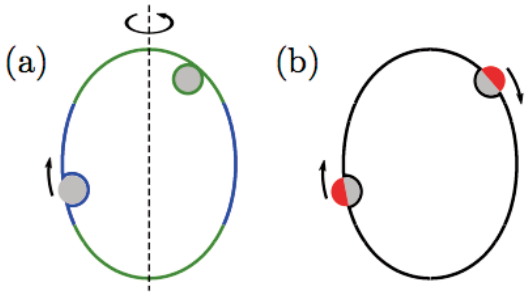

Fig. 3: (a) Prolate vesicle (green-blue) in contact with uniform adhesive nanoparticles (grey). In this example, particles are completely engulfed at the strongly curved poles (green) and partially engulfed at the weakly curved equatorial region (blue). In the endocytic case shown here, partially engulfed particles experience a curvature-induced force towards regions of lower membrane curvature, whereas completely engulfed particles experience no such force. (b) For the same vesicle, Janus particles with one strongly adhesive (grey) and one non-adhesive (red) surface domain are partially engulfed everywhere on the membrane, and therefore always experience curvature-induced forces towards regions of lower membrane curvature.

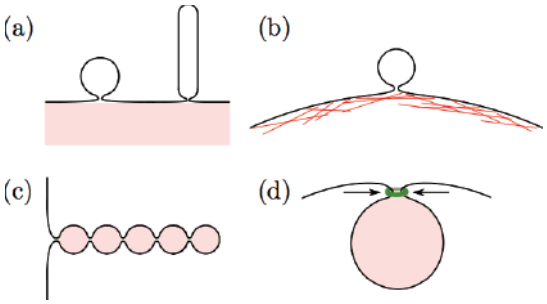

Fig. 4: Different systems in which narrow membrane necks form in the presence of adhesive surfaces (pink) or constriction forces. (a) Budding or tubulation of a supported lipid bilayer; (b) Formation of giant plasma membrane vesicles originating from the outer cell membrane in the presence of the adhesive actin cortex; (c) Engulfment of many nanoparticles into necklace-like tubes; and (d) Engulfment assisted by a contractile ring (green), representing endocytosis-associated protein machinery.

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The Colors and Shapes of Vesicles

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Giant unilamellar vesicles (GUVs) are tiny membrane compartments filled with aqueous solution. One needs a microscope to see them, but the view is often spectacular and reveals many important aspects of membrane behavior. For example, by employing suitable fluorescent labels, the vesicles appear colored and one can resolve membrane heterogeneities inherent to biological membranes (**see Fig. 1c**). External perturbations, such as the presence of added molecules, applied flows or electric fields, will set the picture under the microscope in motion as they lead to dynamic behavior that can be monitored from microseconds to hours. The resulting changes of the vesicle shape can tell us much about the membrane mechanical properties. This report will discuss phase separation in membranes as can be observed from vesicle images obtained with fluorescence microscopy and membrane shapes and morphological changes induced by external factors.

Imaging of GUVs is not always simple. Because of convection, they can be displaced, thus hampering long-term observations. We recently developed a method to immobilize the vesicles. The approach is based on building a cage of agarose around the GUVs **[1],** without compromising the mechanical properties of their membrane as is the case of vesicles encapsulating this polysaccharide **[2].** Our immobilization strategy allows us to trap and hold the vesicle for high-resolution pictures and long-term observations, see **Fig. 1.**

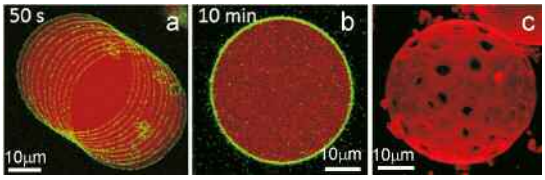

*Fig. 1: Immobilizing GUVs in agarose allows for long-term observations **[1]**. (a) Superimposed time scans over 50 seconds of the equatorial section of one GUV exhibiting a small drift; measurements requiring long acquisition times will be compromised. The vesicle membrane is labeled in green and the encapsulated solution in red. (b) Superimposed time scans over 10 min of a vesicle immobilized in agarose. The vesicle is trapped by the agarose cage around it and does not drift. (c) High-resolution image of a multicomponent GUV with domains. The vesicle is immobilized in agarose.*

Phase Separation in Membranes

For many years, the prevailing view of the cell membrane structure has been the fluid mosaic model proposed by Singer and Nicolson. More recently, it has been proposed that cell membranes may contain lipid domains of liquid-ordered (Lo) and liquid-disordered (Ld) phases and that the functionality of proteins can be influenced by the phase state of the lipids around them. GUVs can be employed to visualize phase separation in membranes made of only a few components. At constant temperature, the phase diagram of a ternary lipid mixture is given by the Gibbs triangle as in **Fig. 2.** In this example, the mixture consists of DOPG, a charged unsaturated lipid, egg sphingomyelin (eSM), and cholesterol (Chol). Each point in the Gibbs triangle represents a certain membrane composition. The membrane can exhibit Lo, Ld or solid (S) phases as well as phase coexistence (e.g. the vesicle in **Fig. 1c** exhibits Ld/Lo phase coexistence). The phase state of the membrane can be assessed from the domain shapes and mobility. Domains are visualized by incorporating a small fraction (<0.5 mol%) of fluorophores, which preferentially partition into a certain phase.

Two-component membranes can also exhibit coexistence of fluid and solid (or gel) phases. We recently found out that, when added to the lipid POPC, even small fractions of the glycolipid GM1 (a few mol %) are sufficient to induce micron-sized gel-like domains attributing facets to GUVs **[3, 4].** Being enriched in neuronal membranes, GM1 concentration fluctuations will easily shape the membrane morphology, fluidity and stiffness in cells.

Inspired by the asymmetric environment of the plasma membrane, we investigated vesicles with asymmetry of the solutions across their membrane. The solution exchange around the vesicles was performed with microfluidic devices, see report by Tom Robinson. We found that the bilayer phase state is affected by solution asymmetry and presence of salt **[5]** as illustrated with the example in **Fig. 2.** These results have direct implications for protein adsorption onto these membranes and for the repartitioning of proteins within membrane domains.

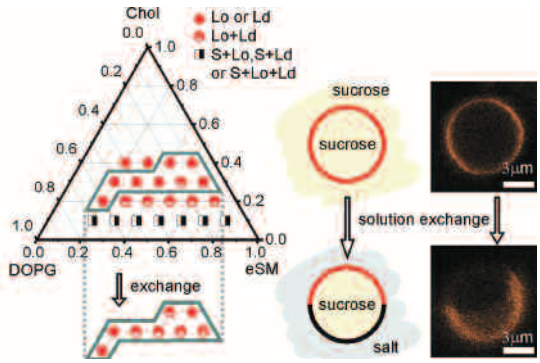

*Fig. 2: Effect of trans-membrane solution asymmetry on the phase behavior of DOPG/eSM/Chol membranes at room temperature: filled circles correspond to homogeneous membranes; half-filled symbols to vesicles with domains. The phase diagram for GUVs with symmetric sucrose/sucrose (in/out) conditions changes after imposing asymmetric sucrose/salt conditions via exchange of the vesicle external solution with high-salinity buffer (see changes in the region delineated by the polygon showing the vesicle compositions which we have examined experimentally). The cartoons and confocal images on the right illustrate the solution conditions and the dominant domain pattern within the delineated section **[5].***

Are Vesicles Always Spheres?

Researchers new to vesicles, whether giant or not, intuitively expect them to be spherical. This is not necessarily so. If a vesicle membrane is fluid and under low tension, it will undulate when exposed to the Brownian motion of water. Membrane flexibility is characterized by their bending rigidity, which depends not only on membrane composition and the presence of inclusions **[3],** but also on molecules and ions in the bathing media **[6].** Typically, the bending rigidity is of the order of 10 k_BT, which is why the membrane of vesicles under low tension can exhibit thermal fluctuations. Upon deflation, vesicles may adopt a variety of shapes depending, among others, on their area-to-volume ratio. Furthermore, GUVs are easy to deform when exposed to perturbations such as electric fields or adhesion as discussed below.

Membrane Nanotubes

When exposed to bilayer asymmetry, the membrane will develop spontaneous curvature (see report of Reinhard Lipowsky) which can be directly seen in GUVs. For example, even the weak adsorption of poly(ethylene glycol) (PEG), a molecule that is generally considered not to interact with membranes, can generate spontaneous curvature sufficient to drive the formation of cylindrical or pearl-like membrane nanotubes in GUVs **[7, 8],** see **Fig. 3a.** Asymmetrically anchored GM1 can also drive tubulation (**Fig. 3b**) as a result of the generated spontaneous curvature **[4].** This membrane property can be measured by pulling inward or outward tubes from GUVs using optical tweezers **[9],** see **Fig. 3c, d.**

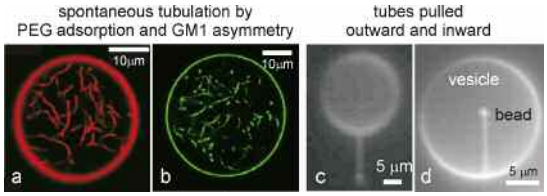

*Fig. 3: Membrane nanotubes in vesicles. Tubes can be spontaneously generated by (a) asymmetric PEG adsorption **[7, 8]** or (b) GM1 asymmetrically anchored in the membrane **[4].** One can also mechanically pull (c) outward or (d) inward tubes via manipulating a membrane-attached bead with optical tweezers **[9].***

Shaping Vesicles with Electric Fields, Light and Proteins

The overall vesicle shape is also easy to modulate. Application of electric fields offers one way of shaping vesicles. Strong DC pulses can induce short-lived prolate deformations **[10, 11],** while weak DC fields can be employed to reversibly adhere and press charged vesicles onto an electrode, **Fig. 4a [12, 13],** a process similar to electrowetting. Another approach, employed in our group, for changing the vesicles morphology relies on the light-induced isomerization of a tetrafluorazobenzene derivative (F-azo). Inserted into the membrane, F-azo increases the vesicle area upon *trans-cis* isomerization under UV light and the vesicles can expel outward buds **[14].** The process is completely reversed under blue light, **Fig. 4b.**

Buds generated in GUVs can also point towards the vesicle interior. ESCRT proteins can induce inward buds in GUVs and even detach these buds inside the mother vesicle via scission. Membrane scission or fission is a step which also occurs after the closure of the phagophore cup and the formation of the autophagosome during the process of autophagy **[15, 16],** see report of Roland Knorr.

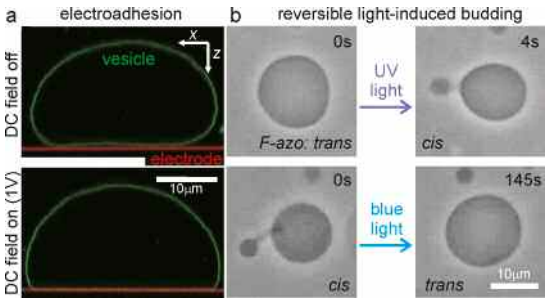

*Fig. 4: Modulating the vesicle morphology. (a) The application of a DC field to a deflated vesicle (green) resting on the electrode surface (red) induces reversible adhesion to the electrode while deforming the vesicle into a truncated sphere **[12, 13].** (b) Under UV or blue light, the reversible isomerization of the light-responsive molecule F-azo incorporated in the membrane can induce reversible vesicle budding **[14]**.*

All in all, giant vesicles are susceptible to all kinds of reshaping, whether induced by adsorbed or anchored molecules, protein scaffolds, (electro)adhesion, or wetting. A beautiful spectrum of responses can be observed under the optical microscope helping us to elucidate underlying mechanisms of membrane behavior and interactions. And this, only by following the shape and color of vesicles.

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Dynamics of Bio-Membranes

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2010/11: DFG Post-doc Fellow
2011-2016: Postdoctoral Scientist (Morphological transitions of biomembranes during autophagy; Dept. of Theory and Biosystems, MPI of Colloids and Interfaces)
Since 10/2016: Research Group Leader, Dept. of Theory and Biosystems, MPI of Colloids and Interfaces

How lipid vesicles and organelles regulate their changes in morphology and topology is of fundamental importance in cell biology. Topological transformations of membranes (membrane fusion and scission), for example, take part in all vesicular transport pathways, as well as during autophagy, viral infection, and cell division as well as in the dynamics of organelles such as mitochondria. Moreover, applications such as liposomal drug delivery or production of monoclonal antibodies (cell-cell fusion) depend on changes in membrane topology.

Autophagy is a complex membrane process within eukaryotic cells and used to digest cytosolic components including organelles. This process involves an extraordinary large number of membrane shape transformations as illustrated in **Fig. 1 [1, 2].** The process is regulated by a large number of proteins which were identified by Yoshinori Ohsumi and coworkers.

In this group, which was established in 2016, we investigate the dynamics of bio-membranes by focusing on four different topics: 1) Morphological transitions of autophagic membranes, 2) Membrane scission during autophagy, 3) Interaction of membrane-bound organelles with non-membrane-bound organelles; and 4) Reconstitution of membrane proteins. All themes deal with understanding the changes of membrane shapes by applying a different set of experimental methods at the interface between biochemistry and biophysics, typically in combination with theoretical approaches as developed in the department. Experimentally, we collaborate with various groups at the MPIKG, very closely with those of R. Dimova and T. Robinson.

Shape Transitions of Autophagic Membranes

Autophagy is regulated by a conserved set of autophagy related proteins (Atgs), many of them seem to be essential for the various steps in **Fig.1.** Atg8 was known to regulate the size of the autophagosomes. By a combination of theory and experiment, we clarified the underlying mechanism of the size regulation, see step 3 in **Fig. 1 [1, 3].** We currently focus on the question how closed autophagosomes can manage to reopen into cup-shaped organelles (dotted arrows and step 6 in **Fig. 1**). Such events can be observed when topological transformations during autophagy do not occur in the correct order (step 5 without step 4, **Fig. 1**) leading to abortion of the process. Such incidents might lead to severe physiological consequences and thus, are important to understand. Some recent insight is shown in **Fig. 2.**

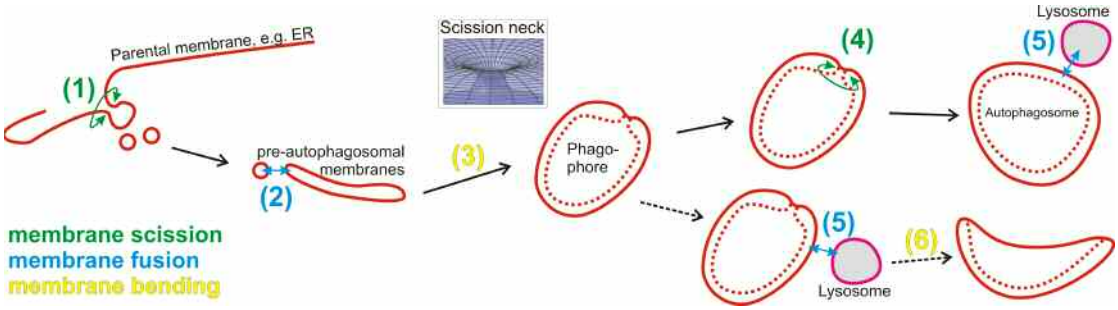

Fig. 1: Shape transformation of membranes during autophagy. Five main steps can be distinguished (continuous arrows): two early and two late topological transitions (membrane fusion and membrane scission) with one major change of membrane morphology in between (membrane bending and autophagosome closure). The case that topological transformations do not occur in the correct order (dotted arrows), for example fusion with the lysosome (step 5) without prior membrane scission (step 4), can impair autophagy severely. Phagophores can reopen (step 6) and thus, the cargo cannot be degraded.

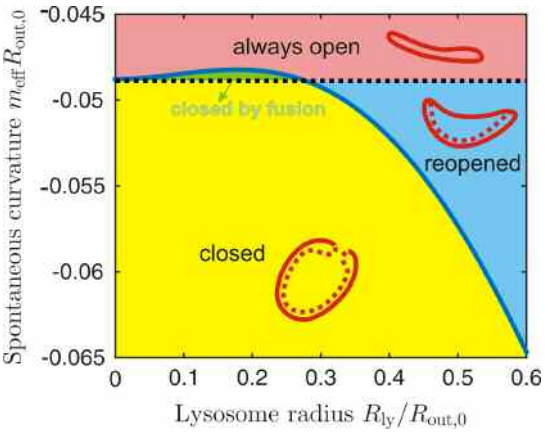

*Fig. 2: Phase diagram for the bending of phagophores. We show that the shape stability of the autophagosomes is critically influenced by alterations of two organelle properties: reduced volume and membrane spontaneous curvature. The membrane spontaneous curvature determines if phagophores were open or close initially (dotted line). The radius of the fusing lysosome (relative to the radius of the autophagosome) and associated changes in spontaneous curvature determine, if autophagosomes were closed or reopen after their fusion with the lysosome **[4]** Under very specific conditions (green area), open phagophores can close by fusion with lysosomes.*

The second membrane scission event during autophagy is still not understood (step 4, **Fig. 1**) **[4].** The timing of this event is critical for successful autophagy (**Fig 2.**). The membrane morphology of the second autophagic scission neck is similar to membrane structures which are cleaved by ESCRT proteins, **Fig. 1,** inset. Therefore, ESCRTs might be involved during autophagy as well, but, so far, there is no experimental evidence for this involvement. One reason is that the correct morphology of the neck is difficult to observe *in vitro*.

Future work will be dedicated to develop reliable protocols to obtain biomimetic models of such scission necks. These model systems will be employed to functionally reconstitute protein cascades which lead to autophagic membrane scission.

Reconstitution of Protein Cascades at Membranes

The importance of membrane proteins is highlighted by the fact that about 30 % of all proteins are membrane proteins and that every second pharmaceutical drug is supposed to target membrane proteins.

An important focus of the group is towards gaining a more fundamental understanding of membrane proteins. Reconstitutions of single proteins or reaction cascades in synthetic model membranes enable us to decipher protein function *in vitro* by studying them in well-defined environments such as giant unilamellar vesicles. Previously, we reconstituted a minimal, ubiquitin-like conjugation machinery and showed that this cascade changes the properties of membranes as predicted theoretically by us **[1, 3].**

Recent work includes contributions to the development of a new method to immobilize model membranes **[5]** (see R. Dimova, Biophysics lab) and to the reconstitution of the copper ATPase CopA. Copper ATPases are vital for activation of essential copper-dependent enzymes and for removal of excess copper from cells. CopA is an integral membrane protein with eight transmembrane domains. We demonstrated a quantitative correlation between ATPase activity and metal transport with a turnover ratio Cu : ATP of one **[6]**.

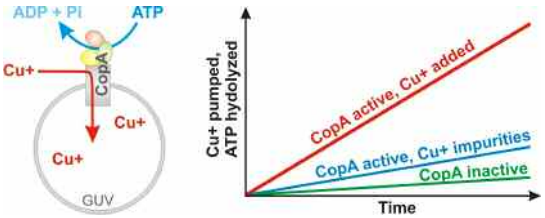

Fig. 3: Fig. 3: Copper (I) transport across membranes of GUVs mediated by the ATPase CopA.

Interaction of Membrane-bound Organelles with Non-membrane-bound Organelles

In living cells, many subcellular structures behave like liquid droplets, examples are stress granules or nucleoli. These non-membrane-bound compartments concentrate certain reactants, which can mediate specific reactions in turn. An active regulation of the interfacial contact area between membrane-bound and non-membrane-bound organelles would have tremendous implication for all signalling pathways transporting information from the outside to the inside of cells, i.e. linking the plasma membrane and the cytoplasm. Our goal therefore is to gain fundamental understanding of the interactions between liquid droplets and bio-membranes. Initial data suggest that liquid droplets can switch between three different states depending on environmental conditions: 1) without contact to membranes (dewetting), 2) spatially restricted interaction with membranes (partial wetting); and 3) full coverage of the membrane by the droplet (complete wetting). These main morphologies are highlighted in **Fig. 4.** By simply altering the salinity of the environment it was possible to reversibly change the size of the interface between reconstituted ribonucleoprotein droplets and bio-membranes.

In the future, our work will shed light on details of the two wetting transitions, will reveal additional factors influencing wetting and thus, enables us to fine-tune wetting states. The fundamental understanding of intracellular wetting processes has important implications for cell biology since it will allow to specifically manipulate signalling pathways linking cyto-/nucleo-plasms, non-membrane-bound organelles and cellular membranes.

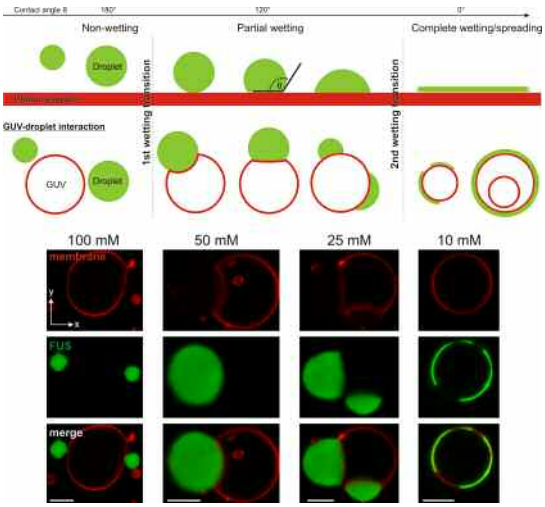

*Fig. 4: Wetting transitions of ribonucleoprotein granules on bio-membranes **[7].** The sketches illustrate wetting transitions which can be observed on planar surfaces and the corresponding shapes which can be expected to occur between droplets and vesicles. The images show confocal cross sections for various ionic strengths. Scale bar, 10 µm.*

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From Membrane Fusion to Multi-compartment Biomimetic Systems

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Compartmentalisation is one of the key features to emerge from the evolution of eukaryotic cells. Their multi-compartment structure, consisting of membrane-bound organelles, ensures vital spatial separation of different cellular functions and metabolic processes. Transport of molecules between these compartments is mediated by membrane proteins but can also proceed via the fusion of two separate membranes. To study these and other cellular processes, an increasingly common technique is to use artificial cells. Our group produces synthetic lipid vesicles and uses them as biomimetic systems. This engineering approach allows us to tune certain components, such as the membrane composition, in a highly controlled manner. We achieve a further level of control by using microfluidic devices to handle these delicate cell-sized objects. Currently, we use this combination of synthetic lipid vesicles and microfluidic technology to study two membrane fusion systems. In the future we will also create biomimetic organelles assembled from multi-compartment lipid vesicles, with the goal of initiating enzymatic reactions within them.

The first section of this report presents results on membrane fusion conducted within Dr. Rumiana Dimova's group. The second section discusses the progress and future aims of the Robinson lab.

Membrane Fusion Systems

The fusion of two biological membranes is essential to processes such as neurotransmission, egg fertilization, exocytosis, and viral infection. Studying this process *in vivo* presents many challenges due to the complexity of cells and the difficulty in controlling environmental factors. Here we use lipid vesicles to control the membrane composition in order to better understand the mechanisms and components necessary for membrane fusion.

Domain-specific Membrane Fusion

Because a variety of different cellular processes rely on membrane fusion, it is vital that cells are able to spatially confine fusion events to specific organelles or sites in the plasma membrane. For this reason we are interested in demonstrating domain-specific fusion in a model cell system using lipid vesicles. Our inspiration comes directly from nature which uses the SNARE protein complex to fuse biological membranes in eukaryotic cells. Membrane fusion is energetically unfavourable as a hydration barrier must first be overcome. To achieve this, different protein domains insert themselves into the two opposing membranes which are then brought together when a zipper-like complex is formed. Once they are in close contact, fusion can proceed, although the precise mechanism is still unknown. Here, we use two SNARE-mimetic systems where the ligand and receptor pairs are based on DNA hybridisation, or coiled-coil peptides (in collaboration with Prof. Janshoff, University of Göttingen). In both cases they are linked to lipids within large unilamellar vesicles (LUVs) or giant unilamellar vesicles (GUVs). GUVs with liquid-liquid phase-separation are grown in a physiologically relevant buffer **[1]** and the lipidated receptor is confined to either the liquid ordered or liquid disordered phase. Domain- or phase-specific fusion is achieved when LUVs with the ligand are introduced and fuse only to the GUV phase with the corresponding receptor (**Fig.1a**) **[2].** Domain-specific docking (**Fig. 1b**), and lipid mixing (**Fig. 1c**) have been proven. Preliminary data using a content mixing assay and microfluidics indicates full fusion events (**Fig. 1c**). Future work will involve combining spatially specific fusion with spatially specific fission in the same GUV system.

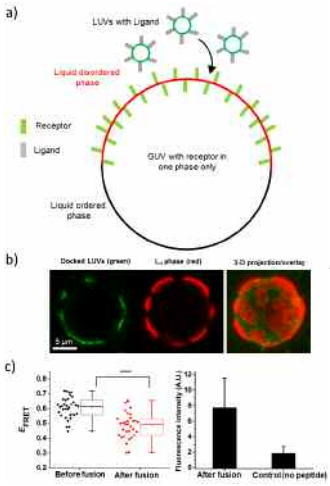

Fig. 1: a) Cartoon of location-specific fusion assay. b) Demonstrating that the LUVs (green) dock to the liquid-ordered phase and not to the liquid-disordered phase (red) on the GUV. c) Left: FRET-based lipid mixing assays proves at least hemi-fusion. Right: content mixing assay indicates full fusion.

Charge-based Membrane Fusion

Although proteins are ultimately responsible for fusion of biomembranes, little is known about the role of the lipids themselves. Considering that biological membranes are charged and SNARE proteins are usually reconstituted in liposomes containing charged lipids, it is not clear whether charge is important for the protein environment itself or as the fusion trigger. Here, we developed a charge based fusion assay using model membranes consisting purely of synthetic lipids (**Fig. 2a**) (in collaboration with the Riske group, Federal University of São Paulo). We show that positively charged LUVs containing the cationic lipid DOTAP and a fluorescent lipid analogue spontaneously fuse to negatively charged GUVs **[3].** The electrostatic interaction initially brings the membranes into close contact and the aromatic rings of the fluorophore are believed to cause membrane destabilisation and subsequent fusion. A FRET-based lipid mixing assay was implemented within a microfluidic device to monitor the fusion dynamics (**Fig. 2b**) and the fusion efficiency was shown to be strongly dependent on the percentage of negatively charged lipids in the GUVs. These results could also be interesting for cell labelling or drug delivery applications.

Biomimetic Vesicles in Microfluidic Systems

Traditional vs. Microfluidic Handling of Vesicles

A core technology in the group is microfluidics. These are small devices with micron-sized fluidic channels containing picolitre volume chambers. The use of microfluidic systems has exploded in the past 10 years with applications ranging

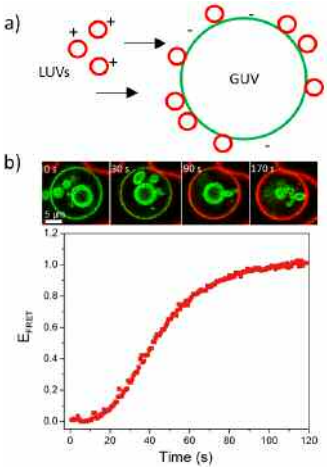

Fig. 2: a) Cartoon of charge-based fusion assay. b) Top: time series of fusion as the outer membrane of a multi-vesicular GUV (green) becomes increasingly saturated with LUVs (red). Bottom: FRET efficiency increase as the lipids of the two membranes mix.

of single-cell analysis to so called 'Lab-on-chip' in the field applications. Here we use the technology for the handling and creation of lipid vesicles. Imaging and studying GUVs is traditionally performed in simple millilitre volume observation chambers. While easy to use, this setup does not allow the rapid and homogeneous delivery of analytes to the GUVs. Moreover, tracking of single GUVs over time is non-trivial. Microfluidic technology, on the other hand, can overcome these challenges. One of our devices contains micrometre sized posts that are engineered to trap and isolate single GUVs (**Fig. 3a**) **[4].** Once captured, the vesicles are stable for hours or days, which allows single vesicle tracking and analysis over time **[1].** Moreover, the fluidic flow control offers the opportunity to rapidly and homogenous exchange the surrounding solution and therefore add or remove solutes which interact with the vesicle's membrane (**Fig. 3b**).

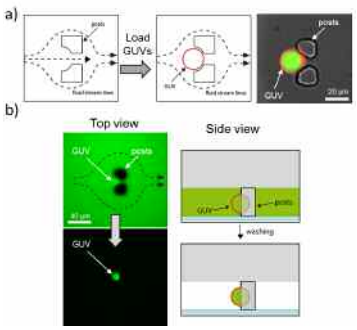

Fig. 3: a) A microfluidic device with micrometre-sized posts to capture a single GUV for analysis. b) Fluidic control allows washing steps to exchange the solution surrounding the GUV ***[4].***

Multi-compartment Vesicle Systems

A key requirement of eukaryotic cells is their ability to compartmentalise different functions within different organelles. The aim of the work here is to study the role of compartmentalisation by creating a multi-compartment vesicle system to mimic cellular organelles (see **Fig. 4**). The challenge here lies in reliably encapsulating smaller vesicles within larger GUVs. Therefore more sophisticated vesicle production methods will need to be explored. One such approach will be to use a microfluidic device to generate water-in-oil droplets that will serve as templates for GUV formation. The advantage here is that the size of the vesicles can be controlled allowing us to inject small GUVs inside larger droplets. Once

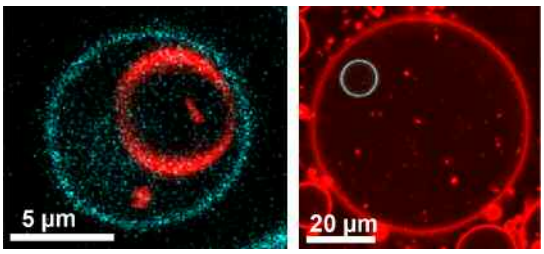

Fig. 4: Confocal images of multi-compartment GUV systems mimicking cell organelles.

these multi-compartment vesicles are created, we will use phase-separated membranes and adhesive moieties for self-organisation and triggering of morphological changes.

Encapsulating Enzymatic Reactions

Many enzymatic pathways are confined to specific organelles or proceed between different organelles. This project aims to dissect the role of compartmentalization of biosynthetic pathways in eukaryotes by studying the first steps of the biosynthesis of the molybdenum cofactor (Moco). While in prokaryotes all steps for Moco biosynthesis are localized in the cytosol, in eukaryotes the first step is localized in the mitochondria and a stable intermediate is transported to the cytosol where all further steps proceed. We are planning to separate the steps using the bacterial proteins for Moco biosynthesis (in collaboration with Prof. Leimkühler, University of Potsdam) and will encapsulate them into vesicles. This will enable studies of the transported intermediate in detail and will give insights into the role of mitochondria for Moco biosynthesis in humans.

Novel Microfluidic Vesicle Trapping Systems

Although the current microfluidic systems have been successfully implemented in a number of different applications involving GUVs **[4–6],** we are continually improving the platform to enable more advanced handling and manipulation of vesicles. To this end, we have developed a device that is able to trap large collections of GUVs to allow better statistics (**Fig. 5**). Moreover, a dense assembly of vesicles could be used to model cells in their natural environment within multicellular organisms.

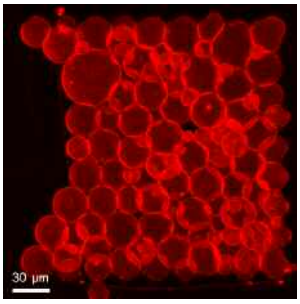

Fig. 5: 3-D confocal microscopy image of tissue-like assemblies of GUVs captured in a novel microfluidic device

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Phase Transitions and Transport Phenomena at Interfaces

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We focus on the impact of interfacial contributions on volume flows (via surface Marangoni flows) and on interfacial energy contributions on the phase behaviour of nano-size systems.

These phenomena are of practical relevance. Phase transition processes of small/confined systems are ubiquitous. Liquid flows induced by surface tension gradients are also widespread in nature and in technology (e.g., ink jet printing).

Our research is strongly motivated by application but clearly focuses on a better fundamental understanding of the phenomena.

Drop-Drop Coalescence, Interfacial Flow and Drop Evaporation.

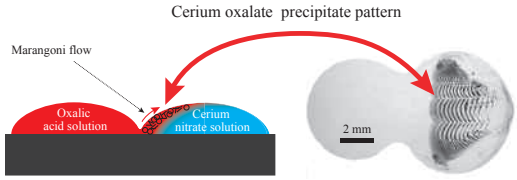

Fig. 1: Patterned precipitation of Cerium-Oxalate appearing during the coalescence of sessile drops with reacting liquids. The stripes consist of different aggregate sizes causing different light scattering ***[1].***

We investigate the coalescence behavior of two sessile drops that contain different chemical reactants (cerium nitrate and oxalic acid) and its impact on the formation of the solid precipitate (cerium oxalate). With different liquids, the surface tension difference in the moment of drop–drop contact can induce a Marangoni flow. This flow can strongly influence the drop–drop coalescence behavior and thus, with reacting liquids, also the reaction and its products (through the liquid mixing). We find three distinctly different coalescence behaviors ("barrier", "intermediate", "noncoalescence"), in contrast to only two behaviors that were observed in the case of nonreacting liquids. The amount of liquid mixing and thus the precipitation rate are very different for the three cases. The "intermediate" case, which exhibits the strongest mixing, has been studied in more detail. For high oxalic acid concentrations, mainly needle-like aggregates, and for low concentrations, mainly flower-like precipitate morphologies are obtained. In a transition range of the oxalic acid concentration, both morphologies can be produced. With the applied coalescence conditions, the different aggregate particles are arranged and fixed in a precipitate raft in a regular, periodic line pattern (**Fig. 1**). The drop-drop coalescence configuration is a convection-reaction-diffusion system, which can have stationary as well as oscillatory behavior depending on the system parameters.

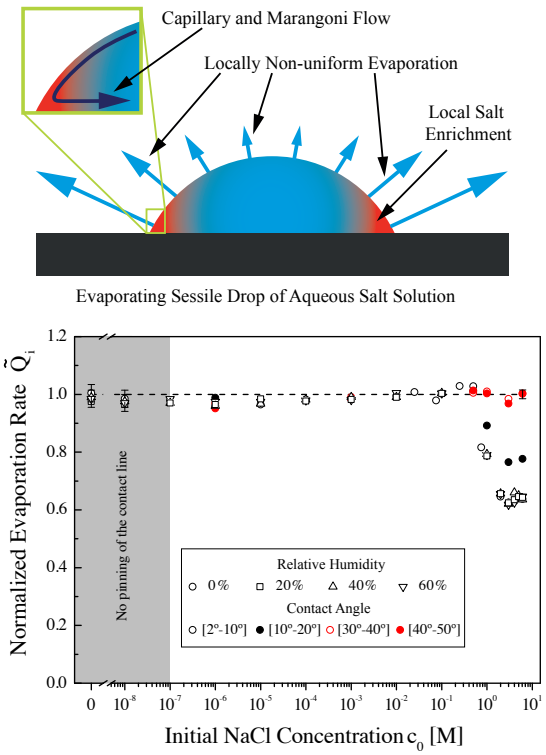

Fig. 2: The evaporation behaviour of sessile drops of salt solutions is governed by the interplay between the locally non-uniform evaporation behaviour inherent to sessile drops and the resulting non-uniform local liquid composition. This can induce a combination of capillary and Marangoni flow near the drop periphery (top). As a result the evaporation behavior of salty sessile drops can be significantly different to sessile drop with uniform composition (lower graph, deviation from dashed line) ***[4].***

In a related project we investigate the evaporation behaviour of sessile drops from mixtures of liquids with nonvolatile components (NaCl, **Fig. 2**). Experiments were performed with seven decades of initial NaCl concentrations, with various droplet sizes and with different contact angles. The investigations reveal that the evaporation depends in a complicated way on the salt concentration and droplet shape. Even if the change of the vapor pressure due to the salt is taken into account the evaporation rate is significantly lower for high salt concentrations and small contact angles than what is expected from the well-accepted diffusion-controlled evaporation scenario for sessile droplets. Particle tracking velocimetry reveals that this modification of the evaporation behavior is caused by Marangoni flows that are induced by surface tension gradients originating from the local evaporative peripheral salt enrichment. In addition it is found that droplets with NaCl concentrations as low as 10^{-6} M are rapidly pinned as soon as evaporation starts, whereas droplets with lower salt concentration do evaporate in a constant contact angle mode. Supposedly, this pinning is caused by deposits of solid salt grains. Such deposits can occur even at

very low salt concentrations due to the peculiar evaporation and flow conditions at the drop periphery. These findings are relevant for a better understanding of the widespread phenomenon of corrosion initiated by sessile droplets.

Melting/Solidification of Nano Size Structures

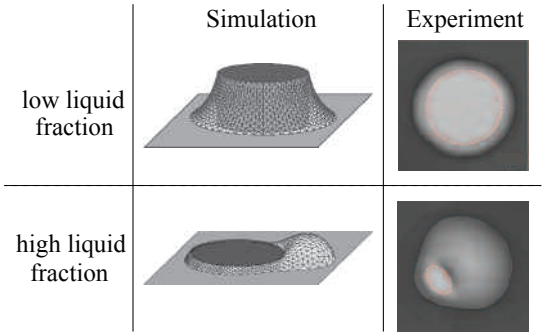

Fig. 3: Melting behaviour of nano size cylinders. Within a certain temeprature range solid and liquid can coexist. Depending on the relative amount of liquid the liquid/vapor interface may form either an axisymmetric rouloid morphology (low liquid fraction) or a bulged morphology (high liquid fraction). Results from simulations are in agreement with experimental data from optical reflection microscopy ***[6].***

Most studies on melting under confinement focus only on contributions from the solid and liquid melt phases and the solid/melt interface. Capillary effects from a second interface (liquid/vapor) are typically neglected. We analyze the melting behavior of small cylindrical aggregates in vapor environment attached to planar surfaces. For the assumed boundary conditions (cylindrical solid with a nonwetting top plane and a wettable side wall), the solid and the liquid phases can coexist within a certain temperature range. Due to capillary instability, the liquid phase can form either an axisymmetric rouloid morphology or, above a certain threshold liquid volume fraction, a bulge that coexists with a rouloid-like section (**Fig. 3**). The melting points of the two morphologies are different. Our theoretical analysis describes the melting behavior of a real system of small aggregates of long chain alkanes on planar substrates as observed by optical microscopy. It also gives qualitative insights into the melting behavior of small aggregates with anisotropic wetting behaviors in general. It reveals in particular how melting points and melting pathways depend on the pathways leading to complete melting.

Patterned Growth Induced by Heterogeneous Nucleation

We investigate experimentally heterogeneous nucleation processes that occur repeatedly/reproducibly at the same location under the same conditions. We investigate in particular the nucleation and growth of aggregates induced by and located at nano size, local „active" sites. Active sites are interfacial locations, where the energetic barrier for heterogeneous nucleation is different (lower) than for heterogeneous nucleation in the neighboring (homogeneous) interfacial environment. Conical pores are for instance active sites for capillary condensation.

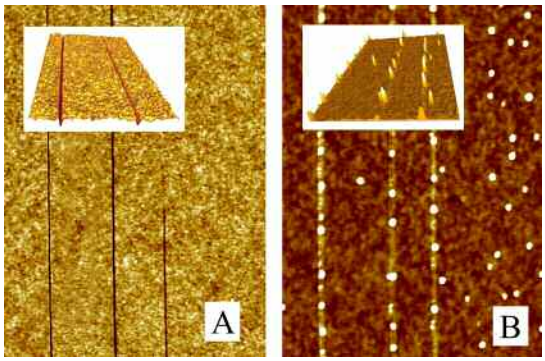

Fig. 4: AFM-image of nano size scratches prior (A) and after deposition of C60 (B). The scratches are about 20nm wide, 1nm deep, and more than µm long ***[7].***

Our active sites are very small „nanoscratches" (dents or groves) in a planar, smooth surface. The nucleation/growth of solute aggregates is induced by exceeding the solute solubility limit in a solute/solvent system as the concentration of a nonvolatile solute increases due to the continuously evaporating solvent. It is found that solute aggregates (C60) grow preferentially at the active sites. We investigate:
1.) How the nanoscratch geometry influences its nucleation „activity" (lowers the nucleation barrier);
2.) How adjacent active sites influence each other (we use arrays of active sites);
3.) How reproducible/repeatable the nucleation sites act (ergodicity); and
4.) How random/stochastic the seemingly smooth environment really is regarding heterogeneous nucleation;

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A great deal of the Marangoni-flow activities are done in collaboration with French research groups (CEA, Saclay and ICSM, Marcoule). Some of the nucleation studies are performed within an international graduate school (funded by DFG) in collaboration with universities in the Berlin area and partners in the US (NC State).

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MAX PLANCK RESEARCH GROUP

Mechanoresponsive Molecules as Building Blocks for Smart Materials

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Smart materials are designed to display an intrinsically programmed, pre-defined response when exposed to an external stimulus (**Fig. 1**). This unique property makes them attractive for a large range of different applications, ranging from aerospace engineering to regenerative medicine. Our focus is on the development of tuneable materials, which possess a specific response to an externally applied shear or stretching force. In particular, we are interested in materials that change their optical properties or release chemically reactive groups in response to the applied force.

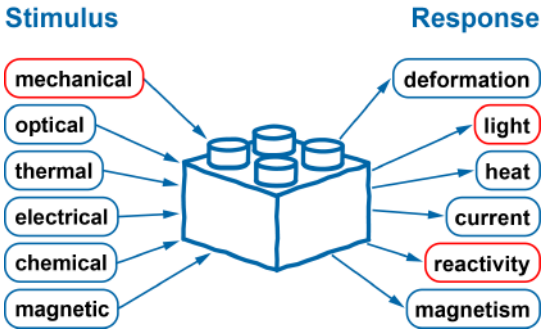

Fig. 1: Smart materials contain specific molecular building blocks that convert an external stimulus into a pre-defined response. For example, a mechanical stimulus may trigger the emission of light or release chemically reactive groups.

Mechanoresponsive materials allow for answering many questions of fundamental interest to the Materials Science community. At the same time, they form the basis for developing highly innovative materials for a range of different applications. Topics of interest for our group are:

- observation of (local) defect formation and propagation inside a material,
- development of soft biomimetic materials that are able to report on the early stages of mechanical damage and/or to self-heal this damage,
- investigation of the molecular mechanisms involved in mechanical cell-material interactions,
- development of synthetic materials that mimic the natural environment of cells or are able to interfere with cellular mechanotransduction pathways.

Towards these goals, we are developing materials as well as methods that allow for a detailed characterization of our newly synthesized materials and their molecular constituents **[1, 2]**.

Mechanoresponsive Molecular Building Blocks

The key components required for the synthesis of functional materials with these applications are self-reporting and/or self-healing mechanoresponsive molecular building blocks (**Fig. 2**). We are specifically interested in the development of self-reporting building blocks that allow for the optical detection of their molecular mechanical state (i.e. molecular force sensors **[1, 2]**). Of further interest are self-healing building blocks. These building blocks undergo a mechanically reversible reaction that involves either covalent or supramolecular bonds, which act as pre-defined mechanical breaking points.

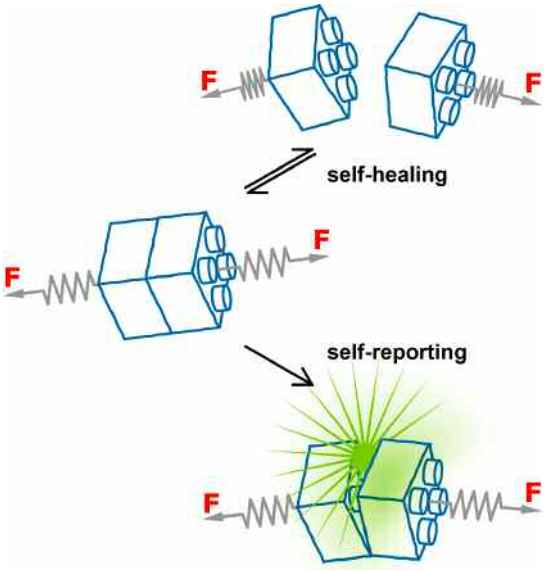

Fig. 2: Mechanoresponsive molecular building blocks possess an intrinsically programmed response to an externally applied force. Self-healing building blocks break into fragments that may subsequently reassemble. Self-reporting building blocks generate an optically detectable signal as soon as the applied force exceeds a threshold value.

Many different molecular structures can serve as mechanoresponsive building blocks. Chemists have developed a number of small molecule mechanophores and integrated them into polymeric materials for the detection of mechanical deformation and damage **[1].** But also biomolecules are used **[2, 3],** e.g. for the synthesis of mechanoresponsive hydrogels for cell culture applications. One drawback of current designs is that only a small number of these structures is calibrated, i.e. it is not known which force is required to obtain the desired molecular response. Our primary goal is, therefore, to develop new mechanically calibrated molecular building blocks that are suitable for both biological and non-biological applications. In the following we will introduce one small molecule mechanophore (example 1) as well as one biomolecular building block (example 2).

Example 1 – Triazole Building Blocks

The number of building blocks that combine self-healing with self-reporting properties is very limited. Triazole rings, formed in so-called 'click chemistry' reactions, are possible candidates, which may integrate both functions in one and the same molecule. Triazoles form in the cycloaddition reac-

tion between alkynes and azides (N_3). If this reaction would be mechanically reversible (cycloreversion), the azide and alkyne starting materials would be released and become available for subsequent reactions (**Fig. 3**). They may either reform material crosslinks (self-healing) or react with fluorogenic reporter molecules, such as azido-coumarin (self-reporting).

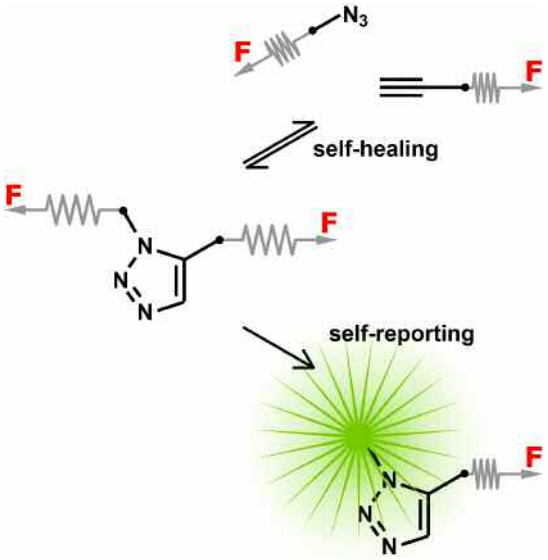

Fig. 3: Possible applications of triazole rings as mechanoresponsive building blocks with self-healing and self-reporting properties.

The envisioned mechanically induced cycloreversion was investigated using density functional theory calculations (in collaboration with Günter Schneider, Oregon State University, Corvallis (OR), USA). To obtain a detailed mechanistic picture, different triazole molecules were investigated and the force was applied to different atoms **[4].** The 1,5 regiosomer, shown in **Fig. 3**, is the product of the ruthenium-catalysed reaction of an azide with a terminal alkyne. For this example, the desired cycloreversion was observed, suggesting that triazoles are indeed highly interesting mechanophores. From an application point-of-view, however, the ruthenium catalyst would have to be added to the material to utilize these properties.

To overcome this limitation, cyclooctynes can be used as an alternative. These ring-shaped alkynes react with azides in the absence of a catalyst and are, therefore, ideally suited as material building blocks. Density functional theory calculations of the triazole formed in the reaction with aza-dibenzocyclooctyne (DIBAC) show that also this molecule undergoes cycloreversion **[4].** DIBAC is currently investigated with single-molecule force spectroscopy to experimentally verify the computer-based predictions.

Example 2 – Peptide-based Building Blocks

The mechanically induced cycloreversion of triazoles requires forces larger than 500 pN, as covalent bonds need to be broken in this reaction. For biological applications, building blocks are needed that react in a force range between 10-200 pN. For this purpose, a library of peptide-based building blocks is currently being developed. The design of these building blocks is inspired by naturally occurring coiled coil structures, which fulfil mechanical function in biological tissues.

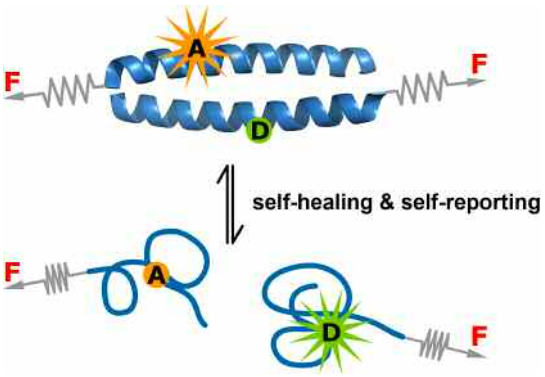

Fig. 4: Possible applications of coiled coil-forming peptides as mechanoresponsive building blocks with self-healing and self-reporting properties.

Coiled coils (CCs) are superhelical structures that are stabilized by hydrophobic and ionic interactions (**Fig. 4**). Using short synthetic CCs, we are currently performing single-molecule force spectroscopy to determine the mechanical stability of different CC structures. Our results show that the force required to break a CC dimer depends on the CC length **[5]** and amino acid sequence, in particular the helix propensity. Molecular dynamics simulations (Ana Vila Verde and Reinhard Lipowsky; Theory & Bio-Systems) as well as metal-stabilized helical structures (Matthew Harrington; Biomaterials) will shed further light on the underlying mechanisms in the future.

Using the obtained knowledge, we have generated a set of CC sequences that break in the range between 20-60 pN. These mechanically calibrated CC building blocks are now being used as crosslinkers for hydrogels. Equipped with a fluorescence-based reporter system (donor and acceptor for Förster resonance energy transfer; FRET), it will become possible to optically read out the mechanical state of every individual CC (**Fig. 4**). This self-reporting hydrogel allows for correlating the mechanical properties of the building blocks with the properties of the bulk material. We anticipate that this new material will serve as a powerful platform for investigating and influencing cellular mechanotransduction mechanisms.

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EMERITUS GROUP

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Nanostructured Interfaces and Composites General

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The Emeritus group was working until 31.01.2016, and after that time I have been as guest in the institute without responsibility for people and laboratories. The main aim has been to finish work started in the department interfaces and to transfer projects to other institutions and help scientists advance their career. Hence I have continued mentoring various young scientists in the MPICI or worldwide, mostly but not exclusively former co-workers. This involved discussions and advices on a personal as well as scientific level, and concerning the latter the interaction has often been so close, that it yielded joint publications. Some of the joint work will be listed below.

Experimental Work in the MPICI

The group had a long-lasting effort to transfer knowledge gained on self-repairing coatings into applications. It is based on corrosion inhibitor filled containers releasing their content upon an environmental change in pH or redox potential, typical for a corrosion pit. The technical feasibility had been demonstrated and patented by the Max Planck Society. The economic and ecologic advantages had also been elaborated. Scientifically appealing remained the development of new containers by different methods, and one approach is emulsion polymerization. In this case one can prepare core/shell particles by polymerization in an emulsion droplet, if the polymer is insoluble in the oil and precipitates to the droplet surface. We already in 2012 introduced an approach established in other fields, where the oils as well as the polymers are characterized by the so-called three Hansen parameters. These describe polar, dispersion and hydrogen bonding interactions. By systematic studies of polymer swelling in different solvents we could then show for different polymers, how different the parameters of oil and polymer can be still to enable solubility. Thus we derived solvent conditions to obtain compact, core/shell or multicompartment capsules **[1].** (**Fig. 1**)

This project has been transferred to a cooperation partner (Enviral), and discussions are ongoing, if they would license and produce coatings in the company or if a start-up would be founded with participation of the Max Planck Society.

Work on sonochemical modification of solids and light induced pH changes to manipulate responsive hydrogels by the groups of E. V. Skorb (now Harvard Univ., Boston) and D. V. Andreeva (Uni Bayreuth, now Institute for Basic Research, Ulsan, Korea) will be reported in the chapter of the Biomaterials department, where these experiments have been perfomed with my participation.

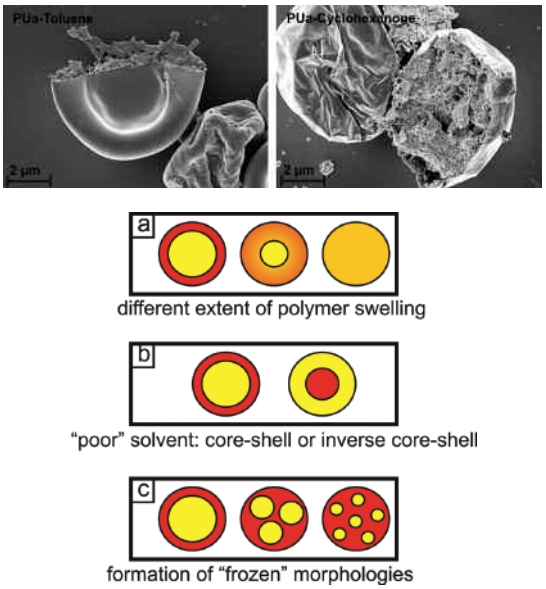

Fig. 1: Left: Electron microscopic images of capsules with core/shell (top) or with compact morphology (bottom) depending on the solvent toluene or cyclohexanone, respectively. Right: Scenarios of different morphologies depending on the solvent quality. ***[1]***

Experimental Work Outside the MPICI

Nanoplasmonic Surfaces

The most intense cooperation has been with the group of G. Zhang at Jilin University **[2].** There the technique of colloidal lithography in connection with angle dependent reactive ion etching has been extensively refined to obtain extremely regular nanostructured Ag surfaces. As an example **Fig. 2A** shows Ag nanocone arrays, which in this case serve to trap light at specific wavelengths, depending on the structure, that can be manipulated by the preparation conditions. Consequently the intensity of the surface enhanced Raman spectrum (SERS) strongly depends on the excitation wavelength (**Fig. 2B**). The trapping of light near the cone foot can be also simulated by finite difference time domain (FDTD) simulations for different cone heights as shown **in Fig. 2 C-F.**

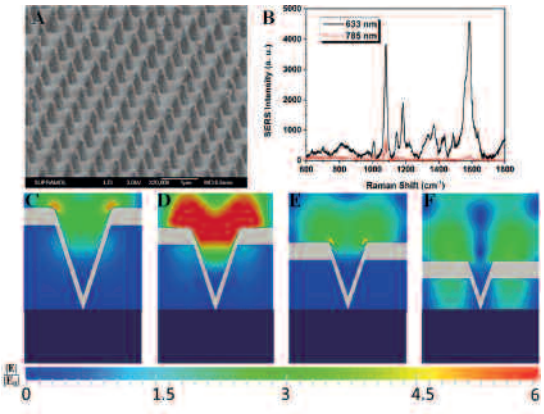

Fig. 2: A: Electron micrograph of an inverse Ag nanocone array, B:SERS spectra of p-aminothiophenol in these arrays for two different wavelegths, C-E: simulated electric field intensities for cone heights of 500, 400, 300 and 200 nm, respectively at the maximum absorption wavelength ***[2]***

As a very new and exciting way of surface structuring we have managed to prepare slits with width controlled to better than 1 nm (**Fig. 3**) by a technique called nanoskyving. Such a structure is sketched in **Fig. 3a,** and the dark lines in the center in b-f indicate, that the gap width can be varied with nm precision. This is important, as the FDTD simulations in **Fig. 3g** reveal, that the highest field strengths are achieved for an intermediate gap width of 5 nm. This can be verified by the SERS spectra of a probe, that exhibit maximum intensity for a 5nm gap width. One also realizes, that there is a periodic field variation along the normal to the macroscopic surface, indicating a three dimensional standing wave in the gap. Hence also the height of the structure, in this case 150nm, is important. **[3]**

These structures are interesting on one hand because of plasmonic effects, on the other hand they enable the study of molecules in well-defined, confined geometry, e.g. polymers with motional constraints. These studies will be continued in cooperation with the department of A. Fery at the Institute of Polymer Research, Dresden.

As another offspring from this research we have started to study photochemistry in the plasmonic field, which indeed shows , that one can deposit a photoproduct, in this case Ag nanoparticles, at positions of maximum plasmonic fields (unpublished).

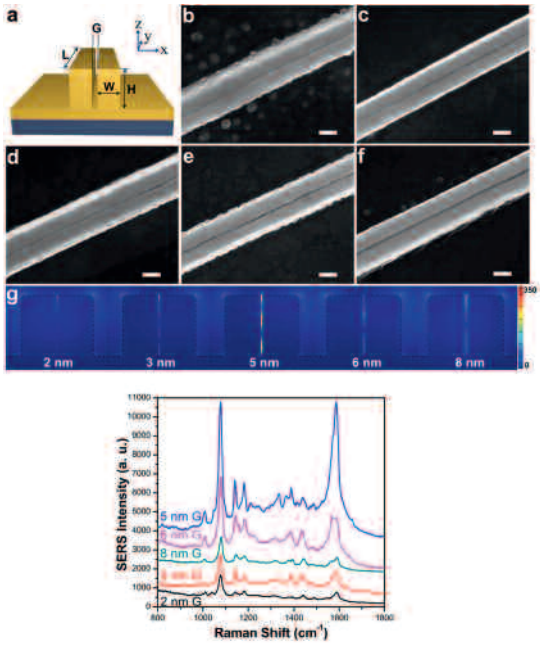

Fig. 3: a) Sketch of a 1D nanogap structure with selectable parameters. b-f) SEM images of Au nanogaps with widths 2, 3, 5, 6 and 8 nm. g) FDTD simulations of the plasmon field intensities in the nanogaps with scale colors representing field intensities (from ref. 3). Bottom: SERS spectra of a dye probe for different gap widths. ***[3]***

Capsules from Peptide Assemblies

In cooperation with the group of Xuehai Yan at the Institute of Process Engineering in Beijing peptide assemblies were studied into different directions:

- They can be responsive and biocompatible drug delivery vehicles.
- They may serve as biomimetic structures directing light to reactive centers, where a product is desired.

In an optimum way light could generate a photocatalyst, that uses the light path previously optimized or self-organized for optimum light capture. For the first case **Fig. 4** presents a scheme of the assembly of a peptide/ porphyrin particle that is intended to serve for photodynamic therapy. The success is also demonstrated in an animal experiment, where the particle administration and light activation demonstrate a decay of the tumor with time **[4].**

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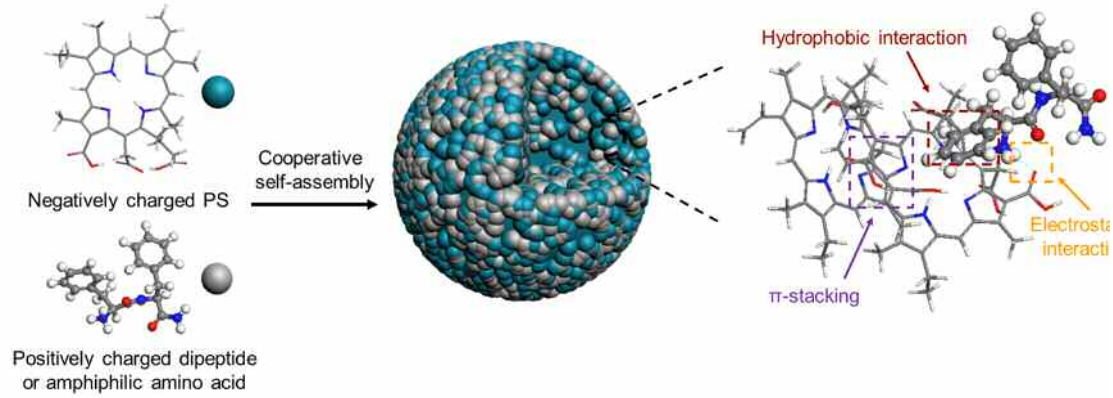

Fig 4: Scheme of the assembly of a nanoparticle from a cationic dipeptide and a porphyrin that serves as sensitizer for photodynamic therapy, d) development of an animal tumor with time after treatment with the free drug (red), with drug/peptide particles (blue) compared to the control (black). ***[4]***

On the second topic, we have shown that self-assembling a porphyrin and a peptide may lead to a tubular structure with strong $\Pi - \Pi$ interactions. This then leads to efficient excitonic energy transfer along the tubes. In the presence of titania and Pt one thus photoproduces TiO_2 and Pt particles, and these may serve for water splitting and hydrogen production, respectively (**Fig. 5**) **[5].** This could be a model of simple prebiotic H_2 producing bacteria resulting from self-organization of molecules and minerals.

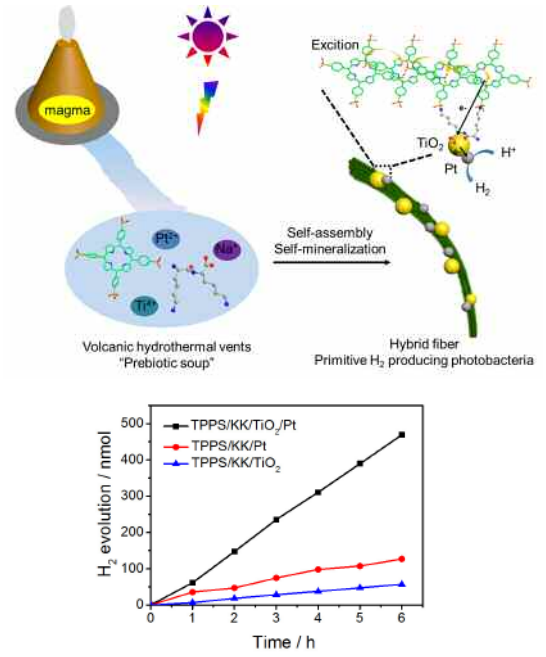

Fig. 5: Left - Scheme of the tubular assembly of a dipeptide and a porphyrin leading to enhanced exciton transport. In the presence of metal ions one then can synthesize nanoparticles, that can catalytically split water (TiO_2) and convert this into hydrogen (Pt). Right: Photoproduced hydrogen for tubules only coated by titania (blue), by Pt (red) and by both nanoparticles (black). ***[5]***

Ultrasonic Enhancement of Phase Transfer

In cooperation with the Institute for Separation Chemistry at Marcoule (T. Zemb) and Univ. Montpellier (A. Stocco) we studied the possibility of enhancement of phase transfer by ultrasound to improve oil/water separation. One effect could be to reduce the clotting of filters /6/, another to roughen the interface by ultrasonic excitation. The latter has been measured by optical reflection and ellipsometry under excitation with MHz ultrasound. **Fig. 6** shows, that roughnesses around 100 nm can be achieved for the oil/water as well as for the air/water interface. **[7]** This is a promising result, but experiments, if this really enhances phase transfer, are still missing.

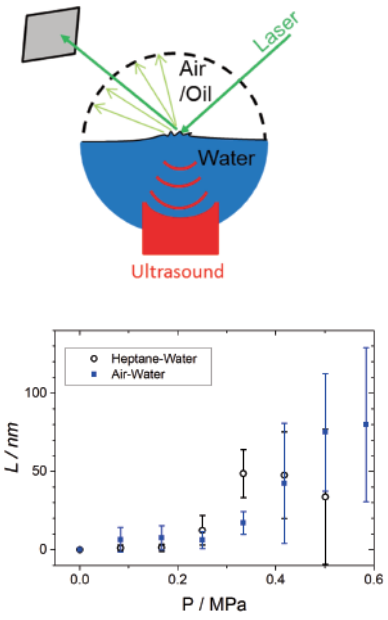

Fig. 6: Left: Scheme of the set-up to measure optically the surface roughness under ultrasonic excitation. Right: Surface Roughness L for different ultrasonic intensities for the air/ water (blue) and for the oil/ water interface (black). ***[7]***

Cooperations with other Groups

As space is limited I would like to mention briefly only a few groups, where the interaction has been most intense and fruitful. In a cooperation over years with the groups of A. G. Skirtach (Univ. Gent) and D. V. Gorin (Univ. Saratov) we studied the penetration of nanoparticles into cells. Together with the groups of A. Yashchenok and B. Parahonskiy we now showed that elongated nanoparticles are easier uptaken, probably because of the stronger adhesion and membrane distortion **[8].**

The group of H. M. Xiong at Fudan Univ. in Shanghai has long-lasting experience in preparing ZnO nanoparticles These are biocompatible, can be made porous and photoluminescent. Therefore we could show that they are very suitable carriers for theranostic applications **[9].**

The group of X. Zhang at the Royal Melbourne Institute of Technology has developed powerful methods to control oil/ water separation in a microfluidic channel, and the precipitation can lead to defined nanodroplets on surfaces. On patterned substrates one can form unique droplet shapes, and their evolution is determined by minimization of the surface energy. These shapes have been simulated in cooperation with B. E. Pinchasik at the MPI of Polymer Research in very good agreement with experiments **[10].**

The group of C.H. Lu at Tianjin Univ. had developed here the technique of periodically wrinkling of a surface by stretching and compression, that can be made very regular on large areas. Now we have extended this in combination with controlled dewetting to obtain regular colloid arrangements on large areas **[11].**

With the group of N. Khachab at the King Abdullah University the anisotropic and chiral interactions of Fe2O3 nanoparticles have been used to achieve unusual assemblies. In special we have achieved toroidal arrangements **[12].**

Outlook

This will be my last contribution to the biannual report of the MPICI, as most of my future work will not be performed in the institute. Besides the activities as associate editor for ACS Nano and consultant for CEA and for Jilin University I will continue mentoring young scientists irrespective if I am co-author of their publications, and some of the related groups have been mentioned in this report. It has been fun working with these, and it has also been fun to work with many highly motivated scientists as well as non-scientists in the institute, and I want to thank them and my colleagues for the friendly and cooperative atmosphere. Above all I would like to thank my former secretary Stefanie Riedel for the many efforts she spent for the department and me. She was the manager of the department as well as of the Emeritus group. She as well as the other co-workers, once given enough freedom, will equally well perform in other environments, and I wish them good luck.

H. Möhwald, D. Akcakayiran, D. V. Grigoriev, D. Radziuk, M. Schenderlein, E. Scherke
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APPENDIX

Organigramm
Organization Chart

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- Advanced Raman Spectroscopic Imaging of Biological Tissues/Dr. Admir Masic
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  (Since September 2017 Full Professor at the Laboratory of Solution Chemistry of Advanced Materials and Technologies (SCAMT), University St. Petersburg)
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BMBF-PTJ	WoodWisdom-Net: WOP-Wood Supply TP Mechanische und nanostrukturelle Charakterisierung von Pappeln	Dr. Eder BM	01.02.2012–31.01.2015	Universitty Helsinki, Helsinki Swedish University of Agricultural Sciences, Umea
BMBF-PTJ	EXIST-Forschungstransfer: Smart Pigments für nachhaltige umweldfreundliche Antikorrosionsbeschichtungen "SigmA"	Dr. Grigoriev GF	01.06.2014–30.11.2015	
BMBF	KMU – innovative-8: ProgRate Prognostische Marker in der Rheumatoiden Arthritis zur Verwendung als Therapieentscheider	Dr. Konthur BS	01.03.2013–31.12.2015	in.vent Diagnostica GmbH, Hennigsdorf Charité Universitätsmedizin Berlin
BMBF-AiF	Entwicklung und Herstellung der Nanopartikel und Nanocontainer zur Einbindung in elektrolytische und mechanische Zink-Schichten im Labormaßstab	Prof. Möhwald Dr. Grigoriev GF		
BMBF	Biotechnologie2020+ Strukturvorhaben: MaxSynBio – Max Planck Forschungsnetzwerk Synthetische Biologie Teilprojekte A - I	Prof. Lipowsky TH	01.08.2014–31.07.2017	MPI für Dynamik komplexer technischer Systeme, Magdeburg MPI für Biochemie, Martinsried MPI für molekulare Physiologie, Dortmund Friedrich-Alexander-Universität, Erlangen MPI für molekulare Zellbiologie und Genetik, Dresden MPI für Polymerforschung, Mainz MPI für Intelligente Systeme, Stuttgart MPI für terrestrische Mikrobiologie, Marburg MPI für Dynamik und Selbstorganisation, Göttingen
BMBF	Kortikale Porosität und Osteozytennetzwerke bei Osteoporose	Prof. Fratzl Dr. Wagermaier BM	01.02.2015–31.07.2018	Zentrum für Muskel- und Knochenforschung, Berlin Julius Wolf Institut, Berlin Universitätsklinikum Hamburg Universität Würzburg Institute of Medical Genetics and Human Genetics, Berlin
BMBF	Verbundprojekt 05K2016 – 3PhaseNR: Entwicklung einer planaren Drei-Phasen Wechselwirkungs-umgebung für die Neutronenreflektometrie	Dr. Schneck BM	01.01.2016–31.12.2018	Institut Laue-Langevin, Grenoble

BM – Abteilung Biomaterialien/Department of Biomaterials
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GF – Abteilung Grenzflächen/Department of Interfaces
KC – Abteilung Kolloidchemie/Department of Colloid Chemistry
TH – Abteilung Theorie & Bio-Systeme/Department of Theory & Bio-Systems

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BMWi	CDN-theRA-Dx; Biomarker-Proteine für die rheumatoide Arthritis in verschiedenen Expressions-systemen	Dr. Konthur BS	01.01.2016–30.09.2017	in.vent DIOGNOSTICA GmbH, Hennigsdorf Charité Universitätsmedizin Berlin
BMBF	Manteltier mimetische Unterwasser-Klebstoffe basierend auf Zellulose und Polyphenolen	Dr. Harrington BM	01.09.2016–31.08.2018	Pohang University fo Science and Technology, Südkorea University of Mons, Belgien

EU

EU/ERC Adv. Grant	Molecular Biomimetics and Magnets Biomineralization: Towards Swimming Nanorobots	Dr. Faivre BM	01.01.2011–31.12.2015	
EU	Quantitative Glycomics and Glycoproteomics for Biomarker Discovery	Dr. Kolarich BS	01.08.2011–31.07.2015	
EU	Diagnostic and prognostic biomarkers for inflamma-tory bowel disease	Dr. Kolarich BS	01.10.2012–30.09.2016	The University of Edinburgh, UK Genos Doo Za Vjestacenje I Analiz, Osijek, Coratia Ludger Ltd, Abingdon, UK IP research Consulting Sasu, Noisy le Grand, france Azienda Ospedaliero-Universitaria Careggi, Firenze, Italy Academisch Ziekenhuis Leiden - Leids Universitair Medisch Centrum, Leiden, Netherlands Faculty of Science University of Zagreb, Zagreb, Coratia Cedars-Sinai medical Center, Los Angeles, US
EU		Prof. Antonietti KC	01.10.2012–30.09.2016	Advanced European lithium sulphur cells for automotive applications Kemijski Institut, Ljubljana, Slovenia Centre National de la Recherche Scientifique, Paris, France Chalmers University of Technology, Goeteborg, Sweden Sincrotrone Trieste S.C.p.A., Basovizza Trieste Italy Centre of Excellence for Low-Carbon Technologies, Ljubljana, Slovenia Renault SAS, Boulogne Billancourt, France Solvionic SA, Toulouse, France Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Münschen Saft SAS, Bagnolet, France Volvo Technology AB, Goeteborg, Sweden

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EU	Training network in innovative polyelectrolytes for energy and environment	Prof. Antonietti KC	01.05.2012–30.04.2016	University of the Basque Country, Leioa, Spain Centre National de la Recherche Scientifique, Paris, France Linkopings Universitet, Linkoping, Sweden Universite de Liege, Liege, Belgium Fundaction IMDEA Energia, Mostoles, Spain Kitozyme SA, Herstal, Belgium Procter&Gamble Italia SPA, Santa Palomba-Pomezia, Italy
EU	Nanomedicine for target-specific imaging and treatment of atherothrombosis: development and initial clinical feasibility	Dr. Faivre BM	01.02.2013–31.01.2018	Institut National de la Sante et de la Recherche Medicale, Paris, France Assistance Publique - Hopizaux de Paris, Paris, France Inserm-Transfert SA, Paris, France Academic Medical Center, Amsterdam, The Netherlands Medical University of Graz, Clinical Institute for Medical and Chemical Laboratory Diagnosis, Graz, Austria Syddansk Universitet, Odense, Denamrk Universitätsklinikum Erlangen, Erlangen University of Twente, Enschede, Netherlands CEA-LETI, Commissariat à l'énergie atomiques et aux énergies alternatives, Paris, France CLINAM - European Foundation for Clinical Nanomedicine, Basel, Switzerland WizSoft, Tel Aviv, Israel nanoPET Pharma GmbH, Berlin Semmelweis University, Budapest, Hungary Bracco Imaging S.p.A., Milan, Italy Edinethics Ltd., Edinburgh, UK

EU

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
EU	Systems Glycobiology of Gastric Cancer	Dr. Kolarich BS	01.05.2013–30.04.2017	University of Gothenburg, Goeteborg, Sweden National Institute for Bioprocessing Research & Training, Dublin, Ireland Institute of Molecular Pathology and Immunology of the University of Porto, Porto, Portugal Swiss Institute of Bioinformatics, Geneva, Switzerland Umeå University, Umeå, Sweden University of Copenhagen, Copenhagen, Denmark OLINK AB, Uppsala, Sweden University of Siena, Siena, Italy Uppsala University, Uppsala, Sweden Syddansk Universitet, Odense, Denmark Ariana Pharma SA, Paris, France
EU	Complex wetting phenomena	Dr. Miller GF	01.01.2014–31.12.2017	Technische Universität Darmstadt "Aristotle University of Thessaloniki, Greece Aristotle University of Thessaloniki, Greece Hebrew University of Jerusalem, Israel Loughborough University, UK Universidad Complutense de Madrid, Spain Maria Curie-Sklodovska University, Lublin, Poland University of Twente, Enschede, Netherlands Evonik AG, Essen Unilever UK Central Resources Limited, London, UK
EU	1D magnetic nanostructures using mineralizing peptides	Prof. Fratzl BM	01.03.2014–29.02.2015	
EU	Network for Integrated Cellular Homeostasis	Prof. Lipowsky Dr. Valleriani TH	01.01.2012–31.12.2015	University of Groningen, Groningen, Netherlands University of Potsdam University of Aberdeen, UK Consejo Superior de Investigaciones Científicas, Madrid, Spain University of Oxford, UK DSM Biotechnology Center, Delft, Netherlands AstraZeneca, London, UK RiNA GmbH, Berlin

EU

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
EU	Nanoporous Poly(Ionic Liquid) Membrane – NAPOLI	Dr. Yuan KC	01.03.2015–29.02.2020	
EU	Development of Selective Carbohydrate Immunomodulators Targeting C-type Lectin Receptors on Antigen Presenting Cells	Prof. Seeberger BS	01.01.2015–31.12.2018	Asociacion Centro de Investigacion Cooperativa en Biomateilales - CIC biomaGUNE, Spanien Glycodiag, Chevilly, Frankreich Universita Degli Studi Di Milano, Italien Universite Joseph Fouruer Grenoble, Frankreich Agencia Estatel Consejo Superior de Investigaciones Cientificas, Madrid Stichting VU.VUMC, Amsterdam Deutsches Krebsforschungsinstitut, Heidelberg Universiteit Leiden, Niederlande Glycouniverse GmbH & Co. KGAA, Berlin The University of Manchester, UK DC4U, Bussum, Niederlande Midatech Biogune, Derio, Spanien
EU	Automated synthesis of S. pneumoniae 7F capsular polysaccharide repeating unit as candidate for conjugate vaccines	Prof. Seeberger BS	01.04.2015–31.03.2017	
EU	Rapid and Inexpensive Diagnosis of Heparin Induced Thrombocytopenia Using Glycan Arrays Containing Synthetic Glycosaminoglycans	Prof. Seeberger BS	01.04.2015–30.09.2016	
EU	High energy lithium sulphur cells and batteries	Prof. Antonietti KC	01.06.2015–31.05.2019	Kemijski Institut, Ljubljana, Slovenia Saft SAS, Bagnolet, France Centre National de la Recherche Scientifique, Paris, France Solvionic SA, Toulouse, France Chalmers University of Technology, Goeteborg, Sweden Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Münschen Picosun Oy, Espoo, Finnland Westfälische Wilhelms-Universität Münster Fundacio Institut de Recerca de L'Energia de Catalunya, Sant Adria De Besos, Spanien Accurec-Recycling GmbH, Mühlheim Tel Aviv University, Isreal Insitut National de L Environnement et des Risques Ineris, Verneuil En Halatte, Frankreich Peugeot Citroen Automobiles S.A., Velizy-Villacoublay, Frankreich

EU

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
EU	Exploiting Glycosylation of Colorectal Cancer for the development of improved diagnostics and therapeutics	Dr. Varon Silva BS	01.09.2015–31.08.2019	Academisch Ziekenhuis Leiden - Leids Universitair Medisch Centrum, Leiden, Netherlands Ludger Ltd, Abingdon, UK Genos Doo Za Vjestacenje I Analiz, Osijek, Coratia Centre National de la Recherche Scientifique, Paris, France Stichting VU.VUMC, Amsterdam Alma Mater Studiorum - Universita de Bologna, Italien Nova ID FCT - Associacao Para A Inovacao e Desenvolvimento Da DCF, Caparica, Portugal
EU	A training network for the rational design of the next generation of well-defined glycoconjugate vaccines	Prof. Seeberger BS	01.11.2015–31.10.2019	Novartis Vaccines and Diagnostics S.R.L., Siena, Italien Instituto De D Medicina Molecular, Lissabon, Portugal Universita Degli Studi Di Milano, Italien Universiteit Leiden, Niederlande Asociacion Centro de Investigacion Cooperativa en Biomateilales - CIC biomaGUNE, Spanien Centre National de la Recherche Scientifique, Paris, France The University of Manchester, UK Sveiciliste U Rijeci, Medicinski Fakultet, Rijeka, Kroatien Ludwig-Maximilians Universität, München Glycouniverse GmbH & Co. KGAA, Berlin

DFG

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
DFG	Multivalenz als chemisches Organisations- und Wirkprinzip: Neue Architekturen, Funktionen und Anwendungen	Prof. Seeberger BS	01.01.2012–31.12.2015	Humboldt-Universität, Berlin Technische Universität Berlin Freie Universität Berlin Charité - Universitätsmedizin Berlin Leibniz-Institut für Molekulare Pharmakologie (FMP) Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)
DFG	Grundlegende Untersuchungen zu strukturellen Ordnungsübergängen in Materialien im Kontext der Biomineralisation	Prof. Fratzl BM	01.01.2012–31.12.2016	Weizmann Institute of Science, Israel DIP Grant

DFG

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
DFG	Hygroskopische Eigenschaften von natürlichen Oligosacchariden; Modellentwicklung und Test für die Wechselwirkungen mit Wasser	Dr. Grafmüller TH	01.11.2012–30.10.2015	
DFG	Stochastic processing of mRNA and tRNA by ribosomes during translational elongati	Prof. Lipowsky TH	01.07.2012–11.06.2015	
DFG	Stochastic modelling of protein synthesis by ribosomes	Prof. Lipowsky TH	12.06.2015–11.06.2018	
DFG	Materials World Network: Structural design and micromechanical properties of mechanotransducing biological materials	Dr. Politi BM	01.12.2012–31.11.2015	
DFG	Mechanische Anpassung von Biomaterialien durch Protein-Metall-Komplexe	Dr. Harrington BM	01.01.2014–31.12.2016	
DFG Emmy-Noether-Programm	Targeting C-type lectins on dendritic cells using carbohydrate-analogs for the specific delivery of tumor vaccines	Dr. Rademacher BS	01.06.2012–31.10.2016	
DFG	Multiscale Smart Coatings wiht Sustained Anticorrosive Action	Dr. Shchukin Prof. Möhwald GF	01.09.2012–31.08.2015	NIMS Louisiana Tech University Kazan Federal Universtiy
DFG	New Methods for the Synthesis of glycosylphosphatidylinositol anchored proteins with therapeutic applications	Dr. Varón Silva BS	01.11.2012–30.10.2015	
DFG	Untersuchung des Einflusses und der Funktion unterschiedlicher Ceramidsubspezies auf die Nanostruktur und die Dynamik von Stratum corneum Lipidmodellsystemen	Prof. Brezesinski KC	01.03.2013–28.02.2016	Martin-Luther-Universität Halle-Wittenberg Universität Leipzig Institut für Angewandte Dermatopharmazie an der Martin-Luther-Universität Halle-Wittenberg e.V.
DFG	Graduiertenkolleg "1524"	Dr. Agudo TH	01.03.2013–29.02.2016	
DFG Transregios	Funktionelle Biomaterialien zur Steuerung von Heilungsprozessen in Knochen- und Hautgewebe - vom Material zur Klinik	Prof. Seeberger BS	01.07.2013–30.06.2017	Universitätsklinikum Leipzig Universität Leipzig Technische Universität Dresden Universitätsklinikum Dresden Helmholtz-Zentrum für Umweltforschung Leipzig-Halle Leibniz-Institut für Polymerforschung Dresden e. V. Innovent e. V., Jena

DFG

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
DFG	eScience-konforme Standards für die Morphologie	Prof. Fratzl BM	01.09.2014–30.08.2017	Zoologisches Forschungsmuseum Alexander Koenig (ZFMK) Leibniz-Zentrum für Biodiversität der Tiere (ZFMK) Museum für Naturkunde Leibniz-Institut für Evolutions- und Biodiversitätsforschung Universität Rostock Rheinische Friedrich-Wilhelms-Universität Bonn
DFG	Magneto-Aerotaxis bei magnetotaktischen Bakterien	Dr. Faivre BM	01.10.2014–30.09.2017	
DFG	Magneto-Aerotaxis bei magnetotaktischen Bakterien	Dr. Klumpp TH	01.11.2014–31.10.2017	
DFG	Selbstheilende Metallopolymere: Vom biologischen Modell bis zu synthetischen Materialien	Dr. Harrington BM	01.07.2014–30.06.2017	Max-Planck-Institut für molekulare Pflanzenphysiologie, Potsdam
DFG Transregios	Verbesserte anti-Kohlenhydrat-basierte Impfstoffe durch gezielte Aktivierung des angeborenen Immunsystems	Prof. Seeberger BS	01.07.2014–30.06.2018	Charité - Universitätsmedizin Berlin
DFG	Skalenkaskaden in komplexen Systemen	Dr. Weikl TH	01.10.2014–30.06.2018	Freie Universität Berlin
DFG	Untersuchung des Ablaufes der Kalzit-biomineralisation in Coccolithophoriden	Dr. Faivre BM	01.09.2014–30.08.2017	
DFG Emmy-Noether-Programm	Die Physik der nicht-spezifischen Wechsel-wirkungen zwischen Biomembranen	Dr. Schneck BM	01.11.2014–31.10.2017	
DFG	Greigit oder Magnetit: Umwelt und genetische Faktoren, die die Biomineralisation in magnetotakti-sche Bakterien kontrollieren	Dr. Faivre BM	01.04.2015–31.03.2018	
DFG	Biometric Materials Research: Functionality by Hierarchical Structuring of Materials	Prof. Fratzl Dr. Aichmayer Dr. Zaslansky Dr. Faivre Dr. Burgert Dr. Schlaad Dr. Cölfen BM	01.05.2010–	(MPI KOLL ist Koordinator, 7 Teilprojekte am Institut) Institut National Polytechnique; E.N.S.E.E.G./ L.T.P.C.M. Grenoble Foundry Institute of RWTH Aachen Department of Materials Engineering, Technical University Berlin Evolutionary Biomaterials Group, MPI für Metallforschung, Stuttgart Department of Materials Science and Engineering, University Erlangen-Nürnberg Dept. Of Microstructure Physics and Metal Forming, MPI Eisenforschung Düsseldorf Plant Biomechanics Group, Botanic Garden, University of Freiburg

DFG

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
DFG	Gottfried Wilhelm Leibniz-Programm	Prof. Fratzl Dr. Dunlop Dr. Wagermaier Dr. Dean BM	01.09.2010–31.08.2017	5 Subprojekte am Institut
DFG	Exzellenzcluster UniCat: Unifying Concepts in Catalysis Humboldt-Universität Berlin	Prof. Möhwald GF Prof. Antonietti KC	01.01.2008–31.12.2010 01.11.2012–31.10.2017	Technische Universität Berlin Freie Universität Berlin Universität Potsdam Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin
DFG	Synthese pflanzlicher Kohlenhydrate und ihre Anwendung in der Biologie	Dr. Pfrengle BS	15.12.2014–14.12.2017	
DFG	ERA_Chemistry_Biomimetische Bindung und Organisation von Magnetit-Nanopartikeln	Dr. Faivre BM	23.02.2015–22.02.2018	
DFG	Aufklärung der Mechanismen der Chitin-Faser-Orientierung in Athropodenkutikula	Dr. Politi BM	09.07.2015–08.07.2018	Technische Universität Dresden Hochschule Bremen
DFG	Die Funktion des Osteozytennetzwerks und dessen Einfluss auf das Knochenmaterial	Dr. Weinkamer BM	10.08.2015–09.08.2018	
DFG	Die Funktion des Osteozytennetzwerks und dessen Einfluss auf das Knochenmaterial	Dr. Wagermaier BM	10.08.2015–09.08.2018	
DFG	Empirisches Verständnis von Glykosylierungs-reaktionen	Prof. Seeberger BS	02.07.2015–01.07.2018	
DFG	Strukturelle Glykobiologie der Wechselwirkungen von Viren mit bakteriellen Polysacchariden	Dr. Neu BS	03.09.2015–02.09.2018	
DFG	Strukturelle Flexibilität des optischen Disigns der Arthropodencornea	Dr. Politi BM	12.11.2015–11.11.2018	Humboldt Universität Berlin
DFG	Multifunktionelle geschichtete Magentit Komposite	Dr. Faivre BM	16.12.2015–15.12.2017	Universität Konstanz Universität Erlangen Forschungszentrum Jülich GmbH

Supranationale Einrichtungen

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
ESA/ESTEC	Topical Team: Foam and Emulsion Technologies-Concerted Action Team (FETCAT)	Dr. Miller BM	01.01.2013–31.12.2015	CNR, Genua, Italien Universität Florence, Italien Universität Marseille, Frankreich Universität Compienge, Frankreich Murmansk State Technical University, Russland Aristotele Universität Thessaloniki, Griechenland Universität Stockholm, Schweden EniTecnologie, Milano, Italien University College Dublin, Irland Nestlé Research Center, Lausanne, Schweiz Wageningen University, Niederlande Univerity of Manchester Institute of Science and Technology, Großbritanien Institute of Food Research, Norwich, Großbritanien Norwegian Univerity of Science and Technology, Trondheim, Norwegen St. Petersburg State Univerity, Russland Université d'Orsay et CNRS, Frankreich Université de Marne La Vallée, Frankreich Unilever, Großbritanien Norsk Hydro ASA, Norwegen IPF, Dresden
ESA/ESTEC	FOR ESA-MAP Soft Matter Dynamics	Dr. Miller BM		Deutsches Zentrum für Luft- und Raumfahrt, Köln Uiversite Paris-Sud Le Centre National de la Recherche Scientifique, Paris University of Liege, Belgien Aberystwyth University, Ceredigion, UK TeclisParc de Chancolan, Frankreich Trinity College, Dubin, Irland Universität Düsseldorf University Twente, Niederlande University of Rennes 1, Frankreich Universität Erlangen Duke University, Durham, UK CNR, Padova, Italien Research Committee AUTH, Thessaloniki, Griechenland IFP Energies nouvelles, Frankreich Loufakis Chemicals S.A., Griechenland Nestlé S.A., Vevey, Schweiz University of Pennsylvania, USA Moscow State University, Russland ESPCI Paris

Supranationale Einrichtungen

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
HFSP Research Grant		Dr. Dean BM	01.09.2013–31.08.2015	Wyss Institut - Harvard University, USA Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)
Royal Society of Chemistry	Researcher Mobilty Grant	Dr. Fellinger KC	25.04.2016–06.06.2016	

Stiftungen

Körber-Stiftung	Körber-Preis 2007	Prof. Seeberger BS	01.01.09.2007–	
VW-Stiftung	Synthetic Woven Bone Development by an Unconventional Biochemical Process	Prof. Omelon BM	01.02.2014–31.07.2015	
GIF-German Israeli Foundation	Emulsion-templated Porous Carbons: Hierarchical Porosities and Surface Functionalities	Prof. Antonietti KC	01.01.2013–31.12.2015	Technion, Haifa, Israel
GIF-German Israeli Foundation	Targeting Antibiotic Resistance of Bacteria with Self-Immolative Dendritic Prodrugs	Prof. Seeberger BS	01.01.2015–31.12.2017	Tel Aviv University
Lundbeck Foundation	Improved mechanical functionaltity of chitin based biological materials by inorganic fortification	Prof. Fratzl Dr. Leemreize BM	01.03.2015–29.02.2016	
Lundbeck Foundation	Improved mechanical functionaltity of chitin based biological materials by inorganic fortification	Prof. Fratzl Dr. Leemreize BM	01.03.2016–31.01.2017	
Böhringer Ingelheim Stiftung	Fragment-based design of targeted delivery vehicles: High specificity through low affinity heteromultivalent interactions	Dr. Rademacher BS	01.11.2016–31.10.2017	
DARPA	Radial Approach to the Automated Synthesis of Small Molecules	Dr. Gilmore BS	01.09.2016–31.08.2017	

Sonstige deutsche Forschungsfinanzierer

DAAD	Projektbezogener Personenaustausch mit der China	Prof. Brezesinski GF Prof. Seeberger BS	2014–2015 2014	Shanghai Institute of Applied Physics, China Jiangnan University, Wuxi, China
DAAD	Projektbezogener Personenaustausch mit Polen	Prof. Brezesinski GF	2014–2015	Warsaw University of Technology, Poland

Sonstige deutsche Forschungsfinanzierer

Zuwendungs-geber	Thema	Projektleiter	Bewilligungszeitraum	Zusammenarbeit mit
DAAD	Projektbezogener Personenaustausch mit Hong Kong	Dr. Yuan KC	2014–2015	The Hong Kong Polytechnic University
DAAD	Projektbezogener Personenaustausch mit Portugal	Prof. Brezesinski BS	2015	Universidade do Minho, Braga, Portugal
DAAD	Projektbezogener Personenaustausch mit Portugal	Dr. Kolarich BS	2016–2017	Institute of Molecular Pathology and Imm, Portugal
DAAD	Projektbezogener Personenaustausch mit China	Dr. Yuan KC	2015–2016	Zhe Jiang University, China

Ausgewählte Veranstaltungen
Selected Events

2015

· **21.-23. April Nanobrücken**
MPI of Colloids and Interfaces

· **23. April Girls' Day**
Max Planck Campus, Potsdam Golm Science Park

· **5. June Alumni Meeting**
MPI of Colloids and Interfaces

· **6.-10. July 6th Bubble and Drop Interfaces (B&D2015)**
MPI of Colloids and Interfaces

· **21. September Dedication Extension Building**
MPI of Colloids and Interfaces

· **28.-29. September 21st Ostwald-Kolloquium**
MPI of Colloids and Interfaces

· **4. December Biomolecular Systems Day**
MPI of Colloids and Interfaces

· **7.-9. December Multiscale Motility of Biomolecular Machines**
Harnack-Haus, Berlin

· **8.-11. December ILMAT III**
Harnack-Haus, Berlin

2016

· **22.-25. February Euro Bio-inspired - International School and Conference on Biological Materials Science**
Kongresshotel Potsdam

· **28. April Girls' Day**
Max Planck Campus, Potsdam Golm Science Park

· **26. May Interfacing Interfacial Science**
MPI of Colloids and Interfaces

· **27. May Alumni Meeting**
MPI of Colloids and Interfaces

· **5.-7. September Biomembrane Days 2016**
MPI of Colloids and Interfaces

Wissenschaftliche Abschlüsse
Scientific Degrees

Bachelor Theses

Department of Biomaterials

2015

Latza, V.: Synthese eines Dioligospiroketalstabs. Universität Potsdam.

Department of Biomolecular Systems

2016

Heine, D.: Glycomic Characterisation of the von Willebrand factor. Universität Düsseldorf (2016).

Miedbrodt, J.: Evaluierung der Lektinspezifität für die selektive Glykopeptidanreicherung. Freie Universität Berlin.

Hilgert, L.F.: Evaluating the role of SPPL3 on the protein N-glycome. Freie Universität Berlin.

Killian, L.M.: Screening and identification of novel ligands for the C-type lectin receptor human Langerin. Freie Universität Berlin.

Diploma Theses

Master Theses

Department of Biomaterials

2015

Günther, E.: Probing the intracellular chemistry of magnetotactic bacteria using fluorescence microscopy. Universität Potsdam.

Huss, J.: The material design behind serotiny: A comparative study of two Banksia species along a climatic gradient in Western Australia. Universität Freiburg.

Schiro, Gabriele: Influence of redox potential on the biomineralization prozess in Magnetospirillum magneticum utilizing a bioreactor. Universität Freiburg.

2016

Tunn, I.: Characterization of metal-binding synthetic coiled coil peptides. Universität Potsdam.

Department of Biomolecular Systems

2015

De Kruijff, G.: Development of a new protecting group strategy for the automated solid-phase synthesis of plant oligosaccharides. Universität Mainz.

Molavi, N.: Fragment evolution of thiazolo pyrimidines as murine Langerin inhibitors. Freie Universität Berlin.

2016

Baukmann, H.: Potentially allosteric modulators of the C-type lectin DC-SIGN identified by Fragment-based screening. Universität zu Lübeck.

Georgieva, E.: Structural Characterization of DC-SIGN via Molecular Dynamics and Mutagenic Studies. Freie Universität Berlin.

Schmidt, H.: Biochemical and Cellular Characterization of the Human C-Type Lectin Receptor Langerin. Freie Universität Berlin.

Matic, A.: Synthesis of Glycosyl Fluorides for the Enzymatic Synthesis of Xylans. Freie Universität Berlin.

Department of Colloid Chemistry

2015

Tröger-Müller, S.: Synthesis and Application of Sustainable Ionic Liquids. Universität Potsdam.

Wissenschaftliche Abschlüsse
Scientific Degrees

PhD Theses

Department of Biomaterials

2015

Aido, M.: The influence of age and mechanical loading on bone structure and mechanical properties. TU Berlin.

Birkhold, A.: A 4D Imaging Approach to Monitor Bone Remodeling. TU Berlin.

Bortel, E.: Maturation of murine long bones: a high resolution micro-computed tomography study. TU Berlin.

Pinchasik, B.-E.: Manipulation of Microbubbles Inspired by Bubble Use in Nature. Universität Potsdam.

Razi, H.: An In Silico Study of Age-related Changes in the Mechanical Regulation of Bone Adaptation. TU Berlin.

Repp, F.: Computational Analysis of Dynamic Bone Structure and Processes - Osteocyte Networks & Healing. HU Berlin

Roschger, A.: Quantitative Analysis of Local Mineral Content and Composition During Bone Growth and Remodeling. HU Berlin.

Schmitt, C.: The Role of Protein Metal Complexes in the Mechanics of Mytilus californianus Byssal Threads. Universität Potsdam.

Schütz, R.: The Temple Scroll and the Structural Properties of Collagen. TU Berlin.

Timofeeva, N.: Effect of ions and amino-acid sequence on collagen structure – a molecular dynamics study. Universität Potsdam.

Turcaud, S.: Some Patterns of Shape Change controlled by Eigenstrain Architectures. Université Grenoble Alpes, France.

Widdrat, M.: Formation and Alteration of Magnetite Nanoparticles. Universität Potsdam.

2016

Bayerlein, B.: The Role of Organic Interfaces in the Formation and the Mechanical Performance of the Prismatic Layer of the Bivalve Shell Pinna Nobilis. TU Berlin.

Forien, J.-B.: Hierarchy of microstructural features as the origin of fracture resistance in dentine. TU Berlin.
Olszewska, A.: Forming magnetic chain with the help of biological organisms. Universität Potsdam.

Reinecke, A.: Impact of Protein Structure on the Mechanics and Assembly of Mytilus Byssal Threads. Universität Potsdam.

Schmidt, I.: Structure and Properties of Calcium Carbonate Microlens Arrays. TU Berlin.

Seidt, B.: Structural and mechanical characterization of bio-inspired hybrid materials by multi-scale analysis. TU Berlin.

Zou, Z.: Formation and Stability of Amorphous Calcium Carbonate. TU Berlin.

Department of Biomolecular Systems

2015

Hütter, J.: Carbohydrate-mediated cell targeting and the role of C-type lectin receptors in autoimmunity. Freie Universität Berlin.

Matthies, St.: Total Synthesis of Complex Biomolecules: De Novo Synthesis of Legionaminic Acids and Continuous Flow Glycosylation. Freie Universität Berlin.

Reinhardt, A.: Immunological Relevance of Conserved Lipopolysaccharide Inner Core Structures of Pathogenic Gram-Negative Bacteria. Freie Universität Berlin.

Monnanda, B. P.: Host Responses to Presentation of Particulate Virulence Factors of Bacteria and Parasites. Freie Universität Berlin.

Schumann, B.: Synthesis and Immunological Evaluation of Oligosaccharide-Antigens as Vaccine Candidates for Streptococcus pneumoniae Serotypes 1 and 8. Freie Universität Berlin.

2016

Weishaupt, M.: Automated Solid-Phase Synthesis of Carbohydrate Antigens. Freie Universität Berlin.

Johannssen, T.: Identification and characterization of C-type lectin receptors in infection and autoimmunity. Freie Universität Berlin.

Bröcker, F.: Towards vaccines and therapeutic antibodies against Clostridium difficile based on synthetic glycans. Freie Universität Berlin.

Möginger, U.: Glycomics and Glycoproteomics of Natural and Synthetic Glycoproteins. Freie Universität Berlin.

Hinneburg, H.: Development of highly sensitive and selective applications for glycoproteomics and clinical glycomics. Freie Universität Berlin.

Alagesan, K.: The Mass Spectrometry Toolkit for Glycoprotein Characterisation: Development of Novel Analytical Methods and Technologies for Glycomics and Glycoproteomics.

Hanske, J.: Investigation of the Structural Basis of Ligand Recognition of the C-Type Lectin Receptor Langerin. Freie Universität Berlin.

Aretz, J.: Fragment-based Design of Novel Lectin Ligands. Freie Universität Berlin.

Department of Colloid Chemistry

2015

Ambrogi, M.: Application of Poly(Ionic Liquid)s for Functional Carbons. Universität Potsdam.

Chen, Z.: Novel Strategies to Improve (Photo)catalytic Performance of Carbon Nitride-based Composites. Universität Potsdam.

Fettkenhauer, C.: Ionothermale Synthese funktioneller Kohlenstoffnitride. Universität Potsdam.

Grygiel, K.: Poly(Ionic Liquid) Stabilizers and New Synthetic Approaches. Universität Potsdam.

Kirchhecker, S.: Renewable Imidazolium Zwitterions as Platform Molecules for the Synthesis of Ionic Liquids and Materials. Universität Potsdam.

Molinari, V.: Ni-based materials for the catalytic conversion of lignocellulosic biomass into valuable products. Universität Potsdam.

Schwarz, D.: Nanoporous Melamine Resin Materials: Synthetic Strategies, Shape Control And Adsorption Properties. Universität Potsdam.

Secker, C.: Polypeptoid Block Copolymers: Synthesis, Modification, and Structure Formation. Universität Potsdam.

2016

Ledendecker, M.: En route towards advanced catalyst materials for the electrocatalytic water splitting reaction: Mechanistic insights into the formation of metal carbides, phospides, sulfides and nitrides. Universität Potsdam.

Pampel, J.: Ionothermal Carbon Materials: Advanced Synthesis and Electrochemical Applications. Universität Potsdam.

Täuber, K.: Porous Membranes from Imidazolium- and Pyridinium-based Poly(ionic liquid)s with Targeted Properties. Universität Potsdam.

Steeples, E.: Amino acid-derived imidazolium salts: platform molecules for N-heterocyclic carbene metal complexes and organosilica materials. Universität Potsdam.

Department of Theory & Bio-Systems

2015

Faber, M.: Folding Dynamics of RNA Secondary Structures. A structure based approach. Universität Potsdam.

Rudorf, S.: Protein Synthesis by Ribosomes. Universität Potsdam.

2016

Agudo, J.: Effects of Bilayer Asymmetry on Naotube Formation and Particle Engulfment by Biomembranes and Vesicles". TU Berlin.

Sin, C.: Post transcriptional mechanisms in gene expression control. Universität Potsdam.

Steinkühler, J.: Partitioning of membrane components in adhering vesicles. TU Berlin.

Habilitations

2015

Yuan, J.: Poly(Ionic Liquids): Innovative Polyelectrolytes for Materials Applications. Universität Potsdam.

2016

Dunlop, J. W. C.: The physics of shape changes in biology. Universität Potsdam.

Personalien
Appointments and Honors

Ehrungen/Mitgliedschaften/Honorarprofessuren
Honors/Memberships/Honorary Professorships

2015

Prof. Dr. Markus Antonietti:	Director of the Department of Colloid Chemistry was elected Foreign Member of the Royal Swedish Academy of Engineering Sciences (IVA)
Prof. Peter Fratzl:	Director of the Department of Biomaterials, became member of the Academy of Sciences and Literature, Mainz
Prof. Dr. Peter H. Seeberger:	Director of the Department of Biomolecular Systems received the Humanity in Science Award
Dr. Nina Fechler:	Group Leader in the Department of Colloid Chemistry, received the 9th Potsdam young scientist award
Dr. Jiayin Yuan:	Group Leader in the Department of Colloid Chemistry, has been awarded a Dr. Hermann Schnell Fellowship of the GDCh (Gesellschaft Deutscher Chemiker; German Chemical Society)

2016

Prof. Dr. Markus Antonietti:	Director of the Department of Colloid Chemistry received the Humboldt-Gay Lussac Award of the French Academy of Sciences
Prof. Dr. Markus Antonietti:	Director of the Department of Colloid Chemistry received the Liebig Medal of the German Chemical Society
Dr. Admir Masic:	Independent Researcher in the Department of Biomaterials, received the 2016 Gold WITec Paper Award
Dr. Christoph Rademacher:	Group Leader in the Department of Biomolecular Systems, received an ERC Starting Grant of the European Research Council
Dr. Sophia Rudorf:	Group Leader in the Department of Theory & Bio-Systems, received the Michelson Award 2016 of the University Potsdam
Dr. Jiayin Yuan:	Group Leader in the Department of Colloid Chemistry, has been awarded the Dozentenpreis from the Fund of Chemical Industry
Vaxxilon:	founded by the Max Planck Society together with the Swiss biotech company Actelion Ltd., named „Science Start-Up of the Year 2016“ (Falling Walls Venture science competition).

Ruf an eine Universität
Appointments

2015

Dr. Stefan Klumpp: Group Leader in the Department of Theory & Bio-Systems, accepted a position as W2 Professor for Theoretical Biophysics at the Georg-August-University Göttingen.

Dr. Bernd Lepenies: Group Leader in the Department of Biomolecular Systems, accepted a position as W2 Professor for Infection Immunology at the University of Veterinary Hannover, Germany.

Dr. Admir Masic: Group Leader in the Department of Biomaterials, accepted a position as Assistant Professor at the Massachusetts Institute of Technology, Department of Civil and Environmental Engineering.

2016

Dr. Daniel Kolarich: Group Leader in the Department of Biomolecular Systems, accepted a position as Associated Professor at Griffith University, Australia

Dr. Menny Shalom: Group Leader in the Department of Colloid Chemistry, accepted a position as Professor for Physical Chemistry and Nanotechnology at the Ben Gurion University, Israel

Publications

Biomaterialien 2015

Journal Article

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Bertinetti, L.; Hangen, U. D.; Eder, M.; Leibner, P.; Fratzl, P.; Zlotnikov, I.: Characterizing moisture-dependent mechanical properties of organic materials: humidity-controlled static and dynamic nanoindentation of wood cell walls. Philosophical Magazine 95 (16-18), 920544, pp. 1992 - 1998 (2015)

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