Book of Abstracts

25 GDCh JCF

HANNOVER

Communicating the Future

FJS 2022
HANNOVER

23-26 MAR MAR
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Our world is constantly changing
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In times of rapid change, companies need to look at how their work not only adapts but also actively contributes to a better world. At BASF, every team and every individual has a role to play, and everyone contributes to our global mission: to provide innovative, clean and efficient solutions for a better tomorrow. The world needs solutions. We need you.

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Wednesday, 23.03.2022

08:00 - 18:00  Registration
Lichthof, Building 1101 (Welfenschloss)
For workshop participants the registration will take place
in the entrance hall of the organic chemistry building
(building 2505, Schneiderberg 1B)

13:30 – 16:00  Excursion to ACTEGA Terra (online) - by Altana

13:30 – 15:00  Workshop: How does drug discovery work? Ask Boehringer
Ingelheim scientists anything you like! - by Boehringer
Ingelheim

13:30 – 16:00  Workshop: Professionelles Bewerben - Todsünden und
Tugenden - by MLP Finanzberatung SE

13:30 – 16:00  Workshop: Startups in chemistry - how does that work?
(Keynote & Practical Workshop) - by chemstars.nrw

13:30 – 16:00  Workshop: Let’s talk transformation: how to make
#fullycircular happen - by Covestro

16:30 – 18:00  Workshop: Career Talk: What is it like to be part of the Research
and Development team at BASF? - by BASF

16:30 – 18:30  Workshop: Synthesis – Retrosynthesis – Analytical Methods-
Patents in research - by CAS

16:30 – 18:30  Workshop: Reference Text Searching - Biosequence searching
- Searching materials - Patents in research - by CAS

16:30 – 18:30  Workshop: Gehaltsverhandlung - Wie verdiene ich mehr Geld?
- by MLP Finanzberatung SE

18:00 – 21:00  Networking Evening by Covestro
Lichthof, Building 1101 (Welfenschloss)
Welfengarten 1, 30167 Hannover
Thursday, 24.03.2022

08:45 – 09:15  Opening Ceremony
Room E415, Building 1101, 4th Floor

09:15 – 10:15  Plenary Lecture: Prof. Dr. Dr. h.c. Markus Antonietti
Max Planck Institute of Colloids and Interfaces, Potsdam, Germany
“From CO\textsubscript{2}-negative Chemical Products to Waste Plastic Recycling: A Chemistry Setting the Base of Possible Global Sustainability Cycles”

10:30 – 11:15  Awards Ceremony
Carl-Roth Award
Dres.-Volker-und-Elke-Münch Award
Room E415, Building 1101, 4th Floor

11:15 – 12:15  Oral Presentations
Room E415, Building 1101, 4th Floor

Sarina Maßmann: “Selective modification of unprotected carbohydrates for cross-linking in waterborne coatings”

Daniel Ditz: “Switching Selectivity in HMF Oxidation with CTF Photocatalysts”


André Niebur: “Untangle the Intertwined: What Happens During Colloidal MoS\textsubscript{2} Nanosheet Syntheses?”

12:15 – 13:30  Lunch Break
Lichthof, Building 1101 (Welfenschloss)
13:30 – 14:30  
**Industry Lectures**  
Room E415, Building 1101, 4th Floor  
**Boehringer Ingelheim:** “Using digital tools for drug design”  
**ISC3:** “Let’s discuss Sustainable Chemistry! - But what even is Sustainable Chemistry?”  
**BCNP Consultants:** “Supporting decision-maker in tech companies and tech-related institutions”

14:45 – 15:45  
**Plenary Lecture: Prof. Dr. Michèle Heurs**  
Max-Planck-Institute für Gravitationsphysik, Hannover; Germany  
“Gravitational wave astronomy — a new window to the universe”

16:00 – 17:00  
**Workshop: Berufseinstieg in der Chemie - by VAA Führungskräfte Chemie**

16:00 – 17:00  
**Plenary Lecture: Prof. Dr. Deborah Kays**  
University of Nottingham, Nottingham, UK  
“Small molecule activation and catalysis using highly unsaturated complexes”

17:15 – 18:00  
**BASF: Dr. Bernhard von Vacano**  
“Sustainable Materials for a Circular Economy”  
Room E415, Building 1101, 4th Floor

18:15 – 20:00  
**Poster Session**  
Entrance Hall, Building 1101 (Welfenschloss)

20:00 – open  
**Nightlife**  
Meeting point: 19:45 in front of the Welfenschloss
Program

Friday, 25.03.2022

08:45 – 09:45
Plenary Lecture: Prof. Dr. Matthias Preller
University of Applied Sciences Bonn-Rhein-Sieg, Rheinbach, Germany
“Exploring the Infinitely Small of Diseases and their Treatment”

09:45 – 11:00
Skillworkshop: Effektiv kommunizieren - by McKinsey & Company

10:00 – 11:00
Oral Presentations
Room E415, Building 1101, 4th Floor
Tim Kröber: “A mutant-selective inhibitor for inositol hexakisphosphate kinases”
Philipp Spieß: “Direct Synthesis of Enamides via Electrophilic Activation of Amides”
Ryan M. Tipker: “Configurational Lability at Tetrahedral Phosphorus: syn/anti-Isomerization of a P-Stereogenic Phosphiranium Cation via Intramolecular P-Epimerization”
Rebeca Fortes Martin: “Water-in-Oil Microemulsions as Soft-Templates for the Self-Assembly of Nanoparticle Clusters into Filament Networks”

11:15 – 12:15
Industry Lectures
Room E415, Building 1101, 4th Floor
Evonik: “Evonik Health Care - Career Talk”
Altana: “ALTANA Innovations for a Sustainable Future: Selfdiagnostic Polymers”

12:15 - 13:30
Lunch Break
Entrance Hall, Building 1101 (Welfenschloss)
13:30 – 14:30  **Plenary Lecture: Prof. Dr. Mischa Bonn**  
Max Planck Institute for Polymer Research, Mainz, Germany  
“Chemical activity of water interfaces”

14:45 – 15:15  **NFDI4Chem: FAIR4Chem Award**  
Room E415, Building 1101, 4th Floor

15:15 – 16:00  **Covestro: Rolf Albach**  
“Sustainable development through continuous improvement”  
Room E415, Building 1101, 4th Floor

16:30 – 17:00  **25 Years of JCF**  
Room E415, Building 1101, 4th Floor

17:00 – 17:30  **Plenary Lecture: Prof. Dr. Markus Kalesse**  
Leibniz University Hannover, Hannover, Germany  
“Stereoselective Sparteine-free 1,2-Metallate Rearrangements in Natural Products Syntheses”

17:30 – 18:00  **Plenary Lecture: Jun.-Prof. Dr. Anna Krawczuk**  
Georg-August University Göttingen, Göttingen, Germany  
“Structure-property correlation in a solid state via quantum crystallography tools”

18:30 – 21:00  **Conference Dinner by BASF**  
Back Entrance Building 1101 (Welfengarten)

21:00 – open  **Evening Event**  
Lichthof, Building 1101 (Welfenschloss)
**Saturday, 26.03.2022**

09:00 – 09:30  **Morning Get-Together**  
Enterprise Hall, Building 1101 (Welfenschloss)

09:30 – 10:30  **Oral Presentations**  
Enterprise Hall, Building 1101 (Welfenschloss)

**Janine Richter:** “Direct copper deposition from copper(II) oxide in ionic liquid”

**Jakob Reichstein:** “Communicating Particles: Identification Taggart and Temperature Recorder in One Single Supraparticle”

**Klaudja Caushi:** “Investigating An Asset-Based Approach to Teaching Undergraduate General Chemistry”

**Pascal Engelhardt:** “Synthesis of a proline-derived module and its application in the development of α-helical peptides as potential SARS CoV-2 inhibitors”

10:45 – 12:15  **Panel Discussion: Communicating the Future**

**Albert Osterhaus,** Research Center for Emerging Infections and Zoonoses at the University of Veterinary Medicine Hannover

**Charlotte Wermser,** Press and Communication Department at Helholtz Centre for Infection Research Braunschweig

**Sebastian Seiffert,** Johannes-Gutenberg University Mainz

Entrance Hall, Building 1101 (Welfenschloss)

12:15 – 12:30  **Group Photo**  
Enterprise Hall, Building 1101 (Welfenschloss)

12:30 – 13:00  **Closing Ceremony**  
Enterprise Hall, Building 1101 (Welfenschloss)

14:30 – 17:45  **Social Activities**

**Royal Garden Ensemble** (Meeting Point: Main entrance to the museum and Great Garden)

**Hannover-walkabout** (Meeting Point: Hannover Tourist Information Center at Ernst-August-Platz)

**Sprengel-Museum** (Meeting Point: main entrance of the Sprengel museum)

**Hannover Zoo** (Meeting Point: main entrance of Hannover Zoo)
CREATING IDEAS THAT SHAPE THE FUTURE. WHY NOT?

We believe science needs curiosity, courage, and people who explore new paths.

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Greetings

Greetings of Janina Carolin Höner, Maxim Gindele and
Karen Hindricks
Heads of Conference FJS 2022 Hannover

Dear participants,

Welcome to FJS 2022 - Communicating the future!
This motto came up during our initial planning of the
FJS in the beginning of last year. Back then, still in a small team, we thought of focusing the
conference on the topic of science communication. This topic will not only be covered in
special program events but will also be represented by interdisciplinary science beyond the
border of chemistry.

The pandemic has taught us that science communication is a necessary “aspect” for
scientists. In addition, cooperation and communication between the different disciplines of
natural science is essential. To facilitate interdisciplinary exchange, we cooperated with
different young organizations of natural sciences for organizing the FJS: the young society of
biochemistry and microbiology (jGBM), the young German physics society (jDPG) and the
young physico chemists (yPC). Furthermore, one of the conference highlights will be the panel
discussion at the last day of the conference. Herein, different views and aspects of science
communication will be discussed.

Due to the pandemic it was not possible to meet in person for more than 2 years, and the last
Spring Symposium in presence took place already three years ago. Nevertheless, in the last
year, a great digital symposium was organized by the JCF Boards from Berlin, Dresden, Halle
and Leipzig. When we started our planning of the conference in early 2021, we worked towards
a Spring Symposium in presence, hoping that we can meet, discuss and celebrate science
together. But on the road to FJS 2022 we needed to pass several obstacles. Not only were we
constantly unsure whether our conference will be allowed to take place. We adapted our
conference plans, sometimes by week, following new restrictions and limitations. With our
organizing meetings mainly in a digital format, some of our team members have never met in
presence until the conference, which resulted in many additional challenges. Although it is not
possible to fully return to the format of pre-pandemic times, we are extremely grateful to be able to welcome you in person to the 24th FJS at the Leibniz University Hannover in the beautiful Welfenschloss!

This event would not be possible without the GDCh, our collaborators, helpers and of course our sponsors and supporters. We especially thank Leibniz University for hosting the conference. The JCF Hannover and JCF Göttingen wish you many fruitful discussions, networking opportunities and a lot of fun in general at the conference.

With Best regards,

Janina Carolin Höner
Head of Conference

Maxim Gindele
Head of Conference

Karen Hindricks
Head of Conference

Greetings
Greetings of Dr. Karsten Danielmeier  
President of the GDCh

In the name of the entire Board of Directors of the GDCh a very warm welcome to the JCF Spring Symposium. Although the “Frühjahrssymposium” is a meeting of young chemists, it already has a remarkable tradition, as this year the 22nd anniversary of the meeting takes place. What started as a small event in Berlin in 1999 has developed into one of the largest conferences in Europe organized by young scientists for young scientists. This year for the first time researchers from other scientific societies will be part of the spring symposium to promote interdisciplinary connection.

"Communicating the Future" is this year’s motto and this is more important than ever in times of the Covid pandemic. Even if we are all fed up with this topic: Especially as natural scientists who create facts not fake news, we must not stop to elucidate again and again what contribution science has made already to help overcome the pandemic. Interdisciplinary research was the key to developing the Corona vaccine, without which the healthcare systems worldwide would have collapsed long ago.

Additionally of course, science plays an essential role in many other global challenges that are at least as important as the pandemic: the energy transition and the associated climate change, feeding more and more people on this planet, controlling plastic waste, just to name a few.

We all know that we cannot solve these challenges without modern chemistry. But we have to keep communicating this to people who are not as devoted to science as we are: we need to get out of our labs and present ourselves and our science to the outside world.

For that, we have to learn how to communicate chemical facts in a generally understandable way to people who are not experts in the field. We all can give lectures or talks and discuss scientifically challenging topics with colleagues. But only a few of us have learned how to present scientific topics in a way that lay people can understand. When I studied chemistry, this was not a topic at all, and unfortunately even today it still occurs far too little in chemistry studies, while media to communicate widely has dramatically changed. But if there’s one thing that characterizes us, it’s that we’ve learned to learn and to acquire new things on our own.
All of us, whether young or old, male, female or diverse, university, industry or otherwise, have two things in common: our passion for chemistry and our striving for excellence in science. If we can manage to get both of these things across, then we convince others thereof as well. Let’s get started.

Unfortunately, at the time of printing this Book of Abstracts, we do not know yet whether we will be able to meet in person in Hannover or whether the pandemic will once again throw a spanner in the works. But I will not finish this preface without thanking the organizers of this symposium and also those of the last two years for their extensive volunteer work under such difficult conditions: you did a fantastic job!

Last but not least I wish all participants an exciting conference with excellent science, new inspiring contacts and a lot of fun. Go ahead and “Communicate the Future”.

Dr. Karsten Danielmeier
GDCh President 2022 & 2023
Greetings of Prof. Dr. Volker Epping
President of Leibniz University Hannover

Dear participants,

It is my great pleasure to welcome you to the 24th JCF Spring Symposium.

The Spring Symposium is taking place under the motto “Communicating the Future”, emphasizing science communication and interdisciplinarity. Science communication and interdisciplinarity are very important for Leibniz University Hannover, as the biggest university in Lower Saxony with more than 29,000 students enrolled in 180 degree programmes and joint degree programmes, offered by 9 faculties and with approximately 3,100 researchers.

As one of the nine leading Universities of Technology in Germany, LUH is aware of its responsibility to seek sustainable, peaceful and responsible solutions to the key issues of tomorrow. Our expertise for this stems from the broad spectrum of subjects, ranging from engineering and natural sciences to architecture and environmental planning, from law and economics to social sciences and humanities. We embody interdisciplinarity in the same way as our namesake Gottfried Wilhelm Leibniz. For 40 creative years of his life, Gottfried Wilhelm Leibniz was associated with Hannover. He made major contributions to all areas of contemporary knowledge – including chemistry. His universality and inspiration have created an example and set a commitment for LUH. We see ourselves as a community striving for scientific and academic insight, seeking sustainable, peaceful and responsible solutions to central issues concerning the future.

The Faculty of Natural Sciences at LUH offers a broad spectrum of programmes and research areas in chemistry and biochemistry – some in conjunction with the biochemistry centre of Hannover Medical School. Our chemistry institutes are closely linked to other institutes in order to take advantage of interdisciplinary co-operation. It is our goal to create flexible structures to facilitate the highest level of interdisciplinary teaching and research. Outstanding results within the disciplines are essential for sustainable interdisciplinary achievements. Therefore, we are very pleased, that some of the chemistry institutes are able to successfully participate in the clusters of excellence at LUH.
It is of great importance for us to communicate our findings and successes such as the clusters of excellence to society. Therefore, we see science communication as an indispensable tool to promote interest in science and to generate understanding for scientific findings. We strive to provide society with relevant knowledge, to promote transparency and to create acceptance. Meetings, such as the JCF Spring Symposium, are important for expanding the network and promoting exchange among each other. However, they are also a way to promote science communication internally and externally. Take advantage of this good opportunity.

Lastly, we are delighted that this conference can take place in person. LUH is always striving to enable on-campus teaching and understands the importance of talking and networking face to face. We all look forward to returning to normal times with teaching and working on campus, being able to experience personal exchange, face-to-face conversations and meeting in person.

I hope that you enjoy the conference, the stimulating presentations and lively discussions. I wish you immense fun and a pleasant stay in the city of Hannover and LUH in general.

Prof. Dr. Volker Epping  
President of Leibniz University Hannover
Greetings of Lorin Steinhäuser
Chairperson of the JCF National Board

Dear Participants,

After the cancellation of our Spring Symposium in 2020 and the online conference in 2021 - with all the advantages and disadvantages of virtual exchange - I am honoured to welcome you to the first "regular" Spring Symposium in 3 years. Naturally, there are still limitations, but I very much hope that these will not diminish the benefit and, above all, the fun of the event.

In these trying times, it is vital to look forward. The conference motto hits the mark there. As natural scientists, we will take on a huge role in solving - or at least improving on the many problems of our time. A sustainable, even completely circular economy seems very much possible, but we are faced with an enormous amount of work to get there. Many challenges lie ahead that we cannot take on individually. Science is teamwork, and teamwork requires communication. Events like the spring symposium are essential to furthering scientific discussion and fostering collaboration and innovation.

Meanwhile, science is exploited more and more for political purposes. Scientific evidence is denied, from the effects of climate change to the earth’s shape. And many institutions are plagued by systemic problems like a severe lack of diversity and precarious working conditions. As scientists, we are often used to viewing ourselves as apolitical. But we can still act by communicating our research to combat science denialism, and we can call out misconduct and injustice among our peers. The German chemical society and the young chemists' network want to stand for scientific rigour and transparency, equal opportunity and an inclusive, respectful and tolerant scientific community, but this also requires us to communicate this stance all around. The conference offers a chance to discuss these topics as well.

Despite the challenges our future holds, I am very optimistic. If the young chemists I have had the pleasure of meeting so far (and this, of course, includes the FJS organisation team) constitute a representative sample, I am confident that we will overcome all obstacles. We are looking forward to a future that will be very bright and more colourful in every respect. In this spirit, I hope that the symposium will kickstart many exciting discussions on that future and
will spark lots of fresh ideas and new insights.

Realising an event like this necessitates gratuitous support from our office, our industry partners and most importantly, our many volunteers who take the time besides their lectures, theses, and dissertations to choreograph this fantastic conference. I want to end with a huge thank you in the name of the entire JCF and the other national board members to everyone involved in making the 24th Spring symposium possible. Let us all take this opportunity to communicate the future!

Lorin Steinhäuser
Chairperson JCF National Board
Conference Site

The conference site is located in the main building of the LUH campus (1101), which is also referred to as the "Welfenschloss". The registration desk and the poster session as well as snacks and drinks during the lunch breaks will be found in the entrance hall. The oral presentations, plenary lectures and other talks are taking place in the university’s biggest lecture hall, the Audimax (room E415). The workshops, on the other hand, are taking place in different rooms on the chemistry campus, which is located on the other side of the Welfengarden.

Networking Evening by Covestro

Instead of the classic “Welcome reception” we invite you to the Networking Evening which sets the stage for the opening of the conference. A finger food buffet and cooled drinks provide the optimal opportunity to get to know each other, have a glance at the sponsor booths and network.

Conference Dinner by BASF

This year’s conference dinner will be a small food truck festival with three different kinds of food you can choose from. The trucks will be located at the entrance of the Welfenschloss. We will offer asian and american street food as well as Crêpes, both savory and for dessert. There will also be vegetarian and vegan options and a special treat for the celebration of 25 years JCF.

Evening Event

After the dinner, a science slam with young scientists presenting their work with entertaining presentations will take place and also a little experimental show “Communicationg the Past” for our 25th anniversary.
**Poster Session**

On the 24th of March, a poster session is taking place from 18:15 to 20:00 in the entrance hall of the university's main building (1101, Welfenschloss). As every year, you will be able to vote for the best poster. Each participant will receive a personalized link per mail, which operates as a ballot paper. The poster awards will be given during the closing ceremony. The abstracts to every poster can be found in our digital Book of Abstracts.

**Oral Presentation**

In addition to the plenary lectures held by research experts from different research fields, the oral presentations held by the participants of FJS2022, are the heart of the conference. There will be 12 talks with 15 minutes each, divided into four sessions on Thursday and Friday. A committee will also decide on the best oral presentation award, which will be given during the closing ceremony.

**Meme Competition**

During the beginning of 2022, you had the opportunity to hand in a self-made scientific meme to become the FJS’ first meme master ever known. The submitted memes were evaluated by a jury and the two most hilarious ones will be awarded during the closing ceremony.

**FJS Passport**

At the beginning of the conference you will receive a FJS 2022 Passport. Do not worry, you will not have to fly out of the country but maybe cross the borders of your own peer group. The idea is that you collect signatures from four sponsors or exhibitors, one member of the FJS team and six people from different regional sections other than your own or Hannover/Göttingen to complete the challenge and receive a special prize.

**WiFi Connection**

You can connect to Eduroam Wifi on the whole LUH campus. If you don’t have access to Eduroam, you can also connect to our separate WiFi Hotspot.

Name: UHEvent
Password: D5jWn9Ly
**Nightlife**

On Thursday night, we invite you to discover the nightlife of Hannover. There are plenty of places to enjoy a nice drink while discussing the comprehensive program of the day. In here, we have gathered information about some places in the northern city as well as the city center. We will meet at 19:45 in front of the Welfenschloss.

**Social Activities**

In the afternoon of Saturday, 26.03.2022, you will have the opportunity to end the last day of the conference with some fun activities such as visiting the Herrenhausen Gardens, taking a guided tour through the city of Hannover, enjoying pieces of modern art in the Sprengel museum or the Hannover Zoo. Meeting points are the respective entrance areas at 14:30.

**Questions?**

If you have questions during the conference, please do not hesitate to ask one of the helpers who all wear distinctive black shirts and green FFP2 masks. If the question is not answered then, you will be referred to the Registration desk, which is located in the Lichthof (Welfenschloss, building 1101).
The conference takes place at two different sites: The workshops will take place at the Chemistry Campus (buildings 2501, 2504 and 2505), whereas the rest of the events are located at the Welfenschloss (building 1101), which is the main building of the university. You will get from one site to the other via the Welfengarten.

You can get to the conference site by bus with the lines 100 and 200 (exit Kopernikusstraße) or by train with the lines 4, 5 (exit Leibniz Universität, Schneiderberg/Wilhelm-Busch-Museum) or lines 6, 11 (exit Kopernikusstraße).
Welfenschloss

You can enter the Welfenschloss through the main entrance which leads you via a flight of stairs directly to the Lichthof on the first floor where most of the program points take place. Alternatively, you can also enter via the ground floor and take the stairs to your left to get to the Lichthof. One workshop will be in Room A320 which you can find on the third floor. If you still have problems finding the right room, ask the helpers or use the Standortfinder of the University.
Chemistry Campus

The Chemistry Campus is the location for the workshops. Here you can find buildings 2501, 2504 and 2505. Registration for the workshops is the entrance hall of the Institute for Organic Chemistry (building 2505).

Institute for Organic Chemistry (building 2505):
Institute for Inorganic Chemistry (building 2501):

Institute for Physical Chemistry (building 2504):
In 2022, the Spring Symposium takes place in Hannover, the capital of Lower-Saxony in northern Germany. With about 540,000 citizens it is one of the 15 most populated cities in Germany.

It is one of the most green cities due to its extensive city forest 'Eilenriede', many parks and short ways into recreational landscapes such as the city lake 'Maschsee' and following along the rivers 'Leine' and 'Ihme'. Moreover, Hannover has also been named as city of music by UNESCO in 2014. This is due to its diverse cultural scene with international festivals and street art all over the town. The most famous festival is the Maschsee festival, taking place annually for three weeks in the summer evolving around the lake in the southern part of the city.

Even the so-called 'new city hall' is accompanied by its own small park and is located right between the Maschsee and the city center. This castle-like building was finished in 1913 and its dome can be visited by a special elevator with an arcuate driving path. Even though there might be a queue, the beautiful view over the city from above is totally worth it.

An internationally well-known part of Hannover might be the fairgrounds, which is the largest exhibition ground of the world and even held the EXPO 2000. Every year, international fairs, like the industrially focused Hannover Messe in April, are hosted on these grounds. Up to this day the fairly large area is host to large events, concerts and conventions.
When arriving in Hanover at the central station, you might have the pleasure to pass the Niki de Saint Phalle promenade that connects the station and the city center. It is a semi underground shopping street named after the French artist and Hanoverian honorary citizen Niki de Saint Phalle. Among others, she is the designer of the famous Nanas. The sculptures represent colorful and voluminous female bodies, which are a symbol for femininity and the beauty of all body shapes. Three of them – Sophie, Charlotte and Caroline – can be found at the Leibniz shore of the Leine.

At the end of the promenade, the Kröpcke clock can be found in the city center. This landmark is not only a clock but also a showcase for small art exhibitions or announcements and a popular meeting point for citizens as well. It was built in 1885 from donations of the citizens as a multifunctional weather column. During the second world war, there was a ban on meteorological equipment, thus the column was more and more used for advertisement and propaganda. After a restoration in 1977, the clock celebrated its 130th anniversary in 2015.

Hannover is also known for its universities. The Hannover medical school 'MHH' for example is one of the leading medical schools in Germany. In 1983, it was the first clinic to receive an MRI scanner for human bodies in Europe and is today internationally recognized for its expertise in transplantation, neurology and cardiology amongst others. On the other side of the city, the Gottfried Wilhelm Leibniz University, hosting the FJS 2022, is located in the northern part of Hannover. Its department buildings are spread across the district. Yet, the center of every student’s life is the Guelph Castle, which is the main building. The university is named after the German polymath Gottfried Wilhelm Leibniz. He was a mathematician, philosopher, scientist, and a diplomat and had great impact on natural science, linguistics and geology, as well as psychology, law and even computer science until long after his death.

The Herrenhausen Gardens are stretched out around the university. The park consists of four separate English gardens, which are the 'Großer Garten', the 'Berggarten', the 'Georgengarten' and the 'Welfengarten' in which the Guelph Castle is located. They were all built in the 17th and 18th century and the Großer Garten is also one of the most famous baroque gardens in Europe. In 2015, the gardens were even awarded with the European garden prize for the best
development of a historic park. Moreover, annually, between May and September, the international fireworks competition takes place above the stunning scenery. Several destinations in and around the parks host art exhibitions, such as the ‘Orangerie’ and the Wilhelm-Busch museum. While admission must be paid in the Großer Garten and the Berggarten, the Welfen- and Georgengarten are free to enter by everyone and often used by students as recreational area.
Leibniz University Hannover is one of the biggest universities in Lower Saxony with 29,000 students from 119 countries. Approximately 3,100 researchers work in more than 150 institutes with subjects ranging from engineering and natural sciences to architecture and environmental planning, from law and economics to social sciences and humanities. LUH is one of the nine leading institutes of technology in Germany and leader of two clusters of excellence: PhoenixD and QuantumFrontiers. Additionally, it is a co-applicant of Hearing4all with Oldenburg University and cooperates with TU Braunschweig on the SE²A project.
Chemistry at LUH

The chemistry department at LUH is subdivided into five institutes, all located on one campus. The Institute of Inorganic Chemistry (ACI) is located in a historic building that was opened in 1909 and is currently the oldest building in Germany that has been continuously used as a chemistry institute since its inauguration. Here you can find the Kali-Chemie-Hörsaal, the oldest lecture hall of the whole university. The working groups are mainly concerned with solid state and material chemistry as well as molecular chemistry and polymers. As part of the excellence clusters Hearing4all and PhoenixD researchers contribute their expertise in multidisciplinary projects.

The Institute of Organic Chemistry (OCI) is located right next to the ACI in a modern glass and steel building. In total nine research groups work here in the main building as well as the Centre of Biomolecular Drug Research (BMWZ) that can be found right down the street. The working groups focus primarily on organic synthesis, biological chemistry and structural biology. It aims to discover new active substances and elucidate their mechanisms of action. The main pillars of this research can be divided into the following categories: Organic synthesis, synthetic biology, medicinal chemistry, chemical biology and structural biology. Most of the research groups are involved in the BMWZ where they cooperate with different groups from the Hannover and Braunschweig areas.

The Institute of Physical Chemistry and Electrochemistry (PCI) conducts research in the areas of energy, nanostructured functional materials for energy conversion, development of functional nanomaterials from colloids, separation, complex interfaces and molecules, and heterogeneous surface catalysis.

The Institute for Food Chemistry (LCI) covers a large spectrum of topics from food chemistry, biotechnology, life science and related fields.
At the Institute of Technical Chemistry (TCI) biotechnological research in many areas is carried out. This covers mammalian cell culture as well as tissue engineering, microbial cell culture and the cultivation of microalgae. Furthermore we are focusing on downstream processing and on the biotechnological characterization of the targeted products, as well as developing and employing multiple sensory means for monitoring and controlling the bioprocesses. Another focus is on microsystem engineering to downscale processes to a miniature size and on additive manufacturing of lab technologies. Further research is dedicated to photocatalysis, medical biotechnology, digitalization of lab infrastructure and bioinformatics.
The FJS 2022 is organized by the local groups of Hannover and Göttingen. However, as this year’s motto “Communicating the Future” puts emphasis on communication, we aim to also include neighboring fields into the conference. This being said, we are happy to announce that the FJS 2022 will also feature program points from the jDPG (young German Physical Society), the Junior GBM (Society for Biochemistry and Molecular Biology) and the yPC of the DBG (German Bunsen Society for Physical Chemistry).

**jGBM**

The ‘Gesellschaft für Biochemie und Molekularbiologie e.V.’ (GBM) was founded in 1947 and is one of the leading German professional societies for life sciences. With 5,000 members, including 1,500 young members, the non-profit GBM forms a national network of researchers supporting e.g. further education, research and teaching. Additionally, the GBM displays a platform for an interdisciplinary exchange at congresses and conferences for scientists. Since April 2011, the young members of the GBM have been established, who are locally anchored in city groups, namely Junior-GBM. These young GBM members organize regional and nationwide scientific symposia and provide insight into the pharmaceutical industry by e.g. company visits. All in all, the GBM membership is an opportunity for (young) scientists establishing national academic and industrial contacts extending the potential of good interacting scientific research.
jDPG
The Young DPG (jDPG) is a part of the German Physical Society (DPG) where students who are interested in physics can meet and share their fascination for the subject. The Young DPG currently has around 4000 members and is divided in more than 30 regional groups that are spread all over the country.

There are many national events such as excursions, competitions, lectures and conferences. Programs especially for doctoral and teaching students, as well as vocational orientation events are also offered. Moreover there is a pupils’ conference for high school students every year. In total the Young DPG organizes around 200 events every year that have a large variety of topics.

The regional group in Hanover consists of around twelve active members. Its local events are open to everyone who is interested in physics. There are monthly group meetings, as well as excursions and talks. Especially for university students vocational orientation events, workshops and networking events are offered. The aim of the regional group is to share the joy of physics and to connect people.

yPC
The young Physical Chemists (yPC), are part of the German Bunsen Society for Physical Chemistry (Deutsche Bunsen-Gesellschaft für physikalische Chemie, DBG), which was founded in 1894 and are representing the interests of young DBG members within the society as well as outside. They provide a network for young members to connect, and are organizing several events each year focused on topics such as career opportunities.

Their last event was an online lecture series “yPC meets industry - online” focused on career development in November 2021 with very exciting speakers from different fields ranging from laser technology and spectroscopy, to publishing, artificial intelligence, and modern challenges in chemistry. For more information, visit their website https://bunsen.de/ypc.
The workshop participants will be guided to the corresponding rooms from the reception desk by a member of the organizing committee.

1) Career Talk: What is it like to be part of the Research and Development team at BASF?

**Date:** 03/23/2022; 4:30 PM - 6 PM  
**Location:** Building 2505 - Room 335 (Schneiderberg 1B, 30167 Hannover)  
**Organizer:** BASF  
**Language:** English

**Description:**

At BASF, we create chemistry for a sustainable future. We combine economic success, social responsibility and environmental protection - and our employees are the most important factor in this! Our competitive advantage lies in the different business and research fields as well as in our size: This gives you the most diverse, international career opportunities within the company as well as a secure and reliable employer.

You always wanted to know why you should work for BASF, how the recruiting process works and how the everyday life of an employee in Research and Development (R&D) looks like?

Our career talk with colleagues from R&D as well as Human Resources will include general information about BASF, career opportunities in R&D and the recruiting process. Insights into the daily routine e.g., as a research scientist and the work packages will be given and additionally some current research topics will be highlighted.

Join us if you want to know what makes working at BASF special and what it is like to be part of our team.

We are looking forward to meeting you!
2) Let's talk transformation: how to make #fullycircular happen

**Date:** 03/23/2022; 1:30 PM - 4 PM  
**Location:** Building 2505 - Room 335 (Schneiderberg 1B, 30167 Hannover)  
**Organizer:** Covestro  
**Language:** English

**Description:**

We all know that in order to be more sustainable, we have to change the way we are living and doing business. The way to success is transforming to a circular economy. But the question is: how?

We want to enlighten the future with you: Who are the main stakeholders that need to be addressed? What defines a sustainable product? And what has to be changed to achieve it? We are looking forward to discussing with you - the scientists of tomorrow - how to shape this transformation.

3) How does drug discovery work? Ask Boehringer Ingelheim scientists anything you like!

**Date:** 03/23/2022; 1:30 PM - 3 PM  
**Location:** Building 2501 - Room 101 (Callinstraße 9, 30167 Hannover)  
**Organizer:** Boehringer Ingelheim  
**Language:** English

**Description:**

Finding and developing new medications for humans and animals is a complex and highly interdisciplinary endeavor. In order to provide insights into this challenging but rewarding process, we offer a round table discussion with scientists from different departments and different sites within Boehringer Ingelheim. You will have the chance to connect to chemists, biochemists, biologists and pharmacists and learn about their tasks, responsibilities and everyday work life.
4) Skillworkshop: Effektiv kommunizieren

Date: 03/25/2022; 9:45 AM - 11 AM
Location: Building 1101 - Room A320 (Welfengarten 1, 30167 Hannover)
Organizer: McKinsey & Company
Language: Deutsch

Description:

Verschaffe dir in entspannter Atmosphäre einen persönlichen Eindruck von McKinsey und gewinne einen Einblick in unsere Arbeitsweise.

Lerne die Grundlagen effektiver Kommunikation kennen und erfahre zudem wie sich deine Botschaften wirkungsvoll visualisieren lassen. Im Rahmen praktischer Übungen zum Storylining kannst du das Gelernte im Anschluss anwenden.

Nutze auch die Gelegenheit, persönlich mit uns ins Gespräch zu kommen und Tipps für deine weitere Karriereplanung zu erhalten.

5) Altana: Digital Excursion to ACTEGA Terra

Date: 03/23/2022; 1:30 PM - 4 PM
Location: Building 2504 - Room 007 (Callinstraße 3a, 30167 Hannover)
Organizer: Altana
Language: English

Description:

Discover your career plus in specialty chemicals at ALTANA: Join an digital excursion to our site in Lehrte (near Hanover) and get to know ACTEGA Terra – Experts in Coatings. ACTEGA Terra is a European market leader for overprint varnishes. As a specialist for water-based, UV and effect coatings as well as coatings based on renewable resources, ACTEGA Terra provides a comprehensive portfolio for Paper-based Packaging, Flexible Packaging, Labels and Publication & Commercial. We offer you a virtual tour through our laboratory and production facilities as well as exciting presentations about our product portfolio and the entry and career opportunities. Curious? Then register for the event. We are looking forward to seeing you!
6) Professionelles Bewerben: Todsünden und Tugenden

Date: 03/23/2022; 1:30 PM - 4 PM  
Location: Building 2501 - Room 219 (Callinstraße 9, 30167 Hannover)  
Organizer: MLP SE  
Language: Deutsch

Description:

Nach dem Seminar werden die Teilnehmer:

- Bessere Bewerbungen schreiben können.  
- Sich gezielter und Präziser ausdrücken können.  
- Stellenausschreibungen richtig lesen und interpretieren.  
- Mehr Einladungen zu Vorstellungsgesprächen haben.  
- Im Vorstellungsgespräch punkten.
7) Gehaltsverhandlung - Wie verdiene ich mehr Geld?

Date: 03/23/2022; 4:30 PM - 6:30 PM
Location: Building 2501 - Room 219 (Callinstraße 9, 30167 Hannover)
Organizer: MLP SE
Language: Deutsch

Description:

Jeder sollte verdienen, was er wert ist. 85% der Jobeinsteiger verhandeln falsch oder gar nicht. Studien belegen, dass Absolventen, die gut verhandeln können, bis zu 10.000 € mehr Einstiegsgehalt bekommen. Kennen Sie die Verhandlungs-Basics? Kennen Sie Ihren Marktwert? Haben Sie die richtige Einstellung als Absolvent? Wenn Sie mindestens eine der Fragen mit NEIN beantworten, gehören Sie zu den 85%.

Wenn Sie zu den 15% gehören möchten: Herzlich Willkommen im Workshop!

Nach dem Seminar werden die Teilnehmer:

- Ihr Einstiegsgehalt sympathisch und kompetent verhandeln.
- Den Aufbau und die Spielregeln einer Gehaltsverhandlung kennen.
- Das Gespräch mit der richtigen Verhandlungsstrategie führen.
8) Berufseinstieg in der Chemie

Date: 03/24/2022; 4 PM - 5 PM  
Location: Building 1101 - Room A320 (Welfengarten 1, 30167 Hannover)  
Organizer: VAA Führungskräfte Chemie  
Language: Deutsch

Description:

Mit welchen Gehaltsvorstellungen gehe ich in ein Vorstellungsgespräch?  

Wie entwickeln sich die Gehälter in der Chemischen Industrie?  

Was ist beim ersten Anstellungsvertrag zu beachten? 

9) Synthesis - Retrosynthesis - Analytical Methods - Patents in research

**Date:** 03/23/2022; 4:30 PM - 6:30 PM  
**Location:** Building 2504 - Room 007 (Callinstraße 3a, 30167 Hannover)  
**Organizer:** CAS  
**Language:** English  
**Additional information for participants:** Please bring a Laptop with you if possible

**Description:**

In this course you will learn how to use SciFinder<sup>n</sup> in the most efficient way for your synthetic and analytical research. We are going to discuss the different options to control your structure searches for substances, as well as for reactions to remove noise in the most effective way. Map visualizations of structure search results offer a fresh new viewpoint on your research, e.g. are great for poster presentations. SciFinder<sup>n</sup> further offers an automated way to create retrosynthesis plans, either based on published literature, or predictively. We will also discuss different ways to find analytical data and review analytical methods.

In the second part, we discuss new functionalities of SciFinder<sup>n</sup> to explore the information contained in and associated with patents. For example, SciFinder<sup>n</sup> enables the efficient comparison of synthesis steps published in patents with those in scientific journals and to intuitively use citations as stepping stones to find and analyze associated technologies. A recently implemented AI-based prior art search technology enables users to automatically retrieve the closest published patent and non-patent literature.

This class will allow newbies to quick-start searching with SciFinder<sup>n</sup> while seasoned users will learn how to enhance their search efficiency.
10) Reference Text Searching - Biosequence Searching - Searching materials - Patents in research

Date: 03/23/2022; 4:30 PM - 6:30 PM
Location: Building 2504 - Room 010 (Callinstrasse 3a, 30167 Hannover)
Organizer: CAS
Language: English
Additional information for participants: Please bring a Laptop with you if possible

Description:

This free-of-charge course will be valuable for everyone who performs text reference searches to retrieve scientific or patent literature. Dedicated segments will highlight best-practice examples to search biosequences and materials on SciFinder®.

We will explain and exemplify how to efficiently retrieve relevant substance and reference information in Medline and the CAS reference database. You will understand how to exploit the value of intellectual indexing in SciFinder® with keywords, substances and roles to get faster to relevant results.

We will discuss new functionalities of SciFinder® to explore the information contained in and associated with patents. For example, SciFinder® enables the efficient comparison of scientific knowledge in patents with those in scientific journals and to intuitively use citations as stepping stones to analyze associated technologies. A recently implemented AI-based prior art search technology enables users to automatically retrieve the closest published patent and non-patent literature. Map visualizations of structure and sequence results offer a fresh new viewpoint on your research, e.g. are great for poster presentations.

This class will allow newbies to quick-start searching with SciFinder® while seasoned users will learn how to enhance their search efficiency.
11) Startups in Chemistry - how does that work? (Keynote & Practical Workshop)

**Date:** 03/23/2022; 1:30 PM - 4 PM  
**Location:** Building 2504 - Room 010 (Callinstraße 3a, 30167 Hannover)  
**Organizer:** chemstars.nrw  
**Language:** English

**Description:**

Do you find startups exciting? Then this workshop session is for you. No matter if you have a solid startup idea already or if you’d like to find out if your research is suited for a startup? This session will help you with that.

In our keynote we will explain what really matters when starting a business, which mistakes you should avoid and showcase some real-life examples.

During the workshop part, you will analyze the startup potential of your research. Alone or in a team, you brainstorm potential customer groups and deal with the question of how they can benefit from your research. You think about possible applications for your research, define a product or service. Step by step, you will develop a startup idea or bring your existing idea to the next level.

Please note: chemstars happily offered a lengthy Q&A session as part of their workshop. If you have specific questions or topics you’d like chemstars to cover, please send them to fjs-program@jcf.io no later than 11th March 2022.

About chemstars.nrw: chemstars is an initiative of market-leading companies from the chemical industry, the German chemical industry association (VCI) NRW and the Ministry of Economics, Innovation, Digitalization and Energy of the State of North Rhine-Westphalia. We’re on a mission to empower scientists to build successful chemistry-related businesses. The chemstars team has long-standing experience in helping founders bring ideas to life and research to market. For more information visit www.chemstars.nrw
Social Activities

1. Royal Garden Ensemble

Discover the splendor of the gardens in the Herrenhausen Gardens, including the Georgengarten, which is directly adjacent to the Welfenschloss, the Berggarten and the Great Garden. Wander through this remarkably well preserved Baroque garden in an one and a half hour guided tour of the Great Garden.

How to get there: Starting at station Kröpcke, use the tram lines 4 Garbsen or 5 to the Herrenhausen Gardens stop

Meeting point: Main entrance to the Museum and Great Garden, 26.03., 14:20

Price: 17 € - 24,50 €

2. Hannover - walkabout

Take a stroll through the charming Old town of Hanover and let yourself be enchanted by alleys and sights of bygone times. The two-hour tour goes along the half-timbered houses of Hanover’s old town between the Marktkirche and the banks of the Leine.

How to get there: Use the tram lines 4, 5, 6 or 11 to the tram station Kröpcke or tram lines 1, 2, 3, 7, 8 or 9 to the central station and walk to the Hanover Tourist Information Center

Meeting Point: Hanover Tourist Information Center at Ernst-August-Platz, 26.03., 14:20

Price: 5 € - 11 €
3. Sprengel museum

Located on the north bank of the Maschsee is the Sprengel Museum Hannover, which is one of the most important museums of art of the 20th and 21st centuries. The tour shows you the world’s largest collection of Max Ernst and Kurt Schwitters, as well as other important modern artists and numerous changing exhibitions.

**How to get there:** Use tram lines 1, 2, 4, 5, 6 or 11 to the station Aegidientorplatz and take a short walk towards the Maschsee (about 10 min.) or use the bus line 100 or 200 and get off at the station Maschsee/Sprengel-Museum

**Meeting point:** Main entrance of the Sprengel museum, 26.03., 14:30

**Price:** 7 € - 11 €

4. Hannover Zoo

Visit the Hanover Zoo and discover the seven themed worlds that are based on the natural habitat or culture of the animals. During the two and a half hour tour with a zoo scout, you will learn exciting facts about the life of the zoo animals and experience the zoo from new perspectives.

**How to get there:** Use the tram line 11 Zoo and get off at the final station Zoo

**Meeting point:** Main entrance area of the Hanover Zoo, 26.03., 14.20

**Price:** 15 € - 25 €
Thursday evening, you get a chance to experience the nightlife of Hannover in different bars next to the university as well as in the old town next to the city center. We will meet in front of the Welfenschloss at 19:45.

**Northern City**
The Bars in the northern city can be reached by foot from the university.

1) **Gaststätte Kaisers**  
*Open: 17:00 to 01:00*  
A corner pub with a rustic bar that offers German cuisine, whiskeys and board games.

2) **Kuriosum**  
*Open: 18:00 to 00:30*  
An Irish pub that offers whiskeys and also German drinks.

3) **Extrakt**  
*Open: 12:00 - 02:00*  
A restaurant with a bar where you have a wide choice of food.

4) **Klein Kröpke**  
*Open: 16:00 to 00:00*  
A small pub with a beer garden opposite of the Department of Inorganic Chemistry.

5) **Santana Bar**  
*Open: 16:00 to 01:00*  
A Cocktail Bar that also offers small snacks directly opposite of the Department of Inorganic Chemistry.
Old Town / City Center
The bars in the city center can be reached by taking the subway 4 (Roderbruch) or 5 (Anderten) to Steintor or Kröpke.

6) Café BarCelona
Open: 09:00 to 00:00
A cozy café and bar in the old town that offers a wide choice of drinks and food and also Cocktails.

7) Stadtliebe Hannover
Open: 12:00 to 00:00
A Cocktailbar that also serves German food and Pizza.

8) Alt Hannovera
Open: 16:00 to 03:00
An Irish pub that offers a wide choice of beer and also snacks.

9) Brauhaus Ernst August
Open: 11:00 to 00:00
Traditional brewery with beer garden, traditional German cuisine and live music.

10) Dublin Inn
Open: 17:00 to 00:00
Irish pub with a table quiz night on Thursdays. They offer whiskeys and Irish beer as well as snacks.

11) Boga Beef&Bar
Open: 09:00 to 01:00
A steak restaurant that also serves breakfast and cocktails.

12) Schateke
Open: 17:00 to 00:00
Old town restaurant in rustic ambience and convivial atmosphere. They offer home-style cooking and burgers.
I experiment because I work on innovative projects that improve millions of lives.

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Markus Antonietti is director of the Max Planck Institute of Colloids and Interfaces. Starting 35 years ago with polymer science, he now drives modern materials chemistry, where sustainable processes and materials are a central theme. Carbon and Carbon-Nitrogen Materials indeed exert a special fascination to him. He published around 700 Papers and issued 90 patents, his H-index is 147. Besides being a devoted scientist and a higher academic teacher (about 55 of his former students hold leading professorships, worldwide), he also is a passionate chef specialized in fusion cuisine and plays in a Rock’n’Roll band.

**From CO$_2$-negative chemical products to Waste Plastic recycling: A Chemistry setting the base of possible global sustainability cycles**

Markus Antonietti*

Max Planck Institute of Colloids and Interfaces Research Campus Golm, D-14424 Potsdam, Germany
e-mail office.cc@mpikg.mpg.de

You do not necessarily have to watch TV to see that humanity has messed up planet earth: anthropogenic changes of the atmosphere, altered land use schemes, or oceans full of plastic waste: we all might feel helpless or depressed in face of these “technology traps”. This is however not the tenor of my talk. I rather want to point to the fact that for every problem related to molecules a solution of conversion can be found, and this is our “chemistry”. It is just that “chemistry” should not only be used to create the beauties of civilization, but also to tackle the serious downsides of the non-closed global cycles.

In a fictive world of circularity and sustainability, it will become difficult to earn money with the “fossil” business schemes, and biomass as a source of molecules is one obvious alternative of dense high energy carbon products. But: biomass usually comes with water and chemical functionality, making our current synthetic toolbox rather poor.
Hydrothermal reforming (HTR) and hydrothermal carbonization (HTC) are chemical processes to turn carbohydrates (including crude forestry side products, but also waste biomass in general) into products which –depending on reaction conditions- can result in hydrochar, but also in value chemicals. All these processes also occur naturally, but can be highly accelerated with minor chemical engineering.

HTC is a classical process, and the coalification (when compared to geology) is boosted down to about 1 – 24 h reaction time by employing elevated temperatures (up to 230 °C) and appropriate catalytic schemes. The processes not only work with a broad variety of “waste biomasses” and thereby represent an end-of-pipe technology, but they are also exothermic and therefore weakly dependent on outer energy sources. With a slight bend of conditions, we end up with “hydrothermal humification”, and the product turns out to be extremely useful for agriculture and soil remediation. Two billion hectares of arable land are actually affected by moderate to severe soil degradation and need two billion tons of humic substances, which in return then probably sequester up to 350 billion tons of CO₂ through the return of soil biology. That is no less than the equivalent to the amount emitted by humanity in the last ten years.

The hydrothermal catalysts developed for biorefinery also have secondary uses, as they tolerate water and biology. I will show that an acidic, metal-free carbocatalyst can split waste plastic into value molecules under moderate conditions, which is a potential paradigm change for the polymer industry.

If time allows, I will dare a discourse on creativity and scholastic restrictions. The question is why it is so difficult to see the sometimes most nearby solutions and why a broader education also outside the core disciplines is to be requested.
Prof. Dr. Michèle Heurs
Leibniz University Hannover

Since 2016 Michèle Heurs is professor for experimental physics at Leibniz Universität Hannover, where she works in the fields of nonclassical laser interferometry and quantum optomechanics for interferometric gravitational wave detection and quantum technologies. After her PhD on novel stabilisation schemes for solid state lasers for gravitational wave detection in 2004, she was a PostDoc first at the Max Planck Institute for Gravitational Physics in Hannover and then at the University of New South Wales in Australia. She returned to Hannover to take up a junior professorship in 2010 within the Centre of Excellence QUEST (Quantum Engineering and Space-Time Research). She is a long-term member and council member of the LIGO Scientific Collaboration (LSC). In 2017 she received the teaching award of Leibniz Universität Hannover. She is principal investigator in the Centres of Excellence “QuantumFrontiers” and “PhoenixD”. Her main research interests are nonclassical light sources („squeezed light“), quantum radiation pressure noise reduction techniques, precision metrology, novel methods for laser stabilisation, optomechanics, and metamaterials.
Gravitational wave astronomy — a new window to the universe

Prof. Dr. Michèle Heurs
Max-Planck-Institute für Gravitationsphysik, Hannover; Germany

Since the first direct detection of gravitational waves in September 2015 our knowledge of the Universe has expanded by virtue of this new form of astronomy. Now we can not only “look at” the universe with electromagnetic telescopes and with neutrino detectors, but we can “listen” to some of the most cataclysmic astrophysical events, such as binary black hole mergers, with gravitational wave detectors. Observations from all these different types of instruments gives rise to true multi-messenger astronomy.

To achieve ever-higher detection rates for meaningful gravitational wave astronomy, ever-greater detection sensitivity is required. In this talk I will introduce the principle of interferometric gravitational wave detection, and highlight some of the advanced technologies employed in Advanced LIGO. Current-generation gravitational wave detectors are already limited by quantum noise of the laser light over wide ranges of their detection band. One sophisticated technique that is already routinely being employed to increase the quantum-limited sensitivity of gravitational wave detectors is the use of non-classical (fixed-quadrature squeezed) light. I will conclude my talk by showing some recent results and further possibilities.
Prof. Dr. Deborah Kays

University of Nottingham

Deborah Kays completed both her MChem in Chemistry and her PhD in Inorganic Chemistry at Cardiff University, Wales, UK. After postdoctoral research, also at Cardiff University, she began her independent research career as a Junior Research Fellow at the University of Oxford (2005-2007). Following this, she was appointed as Lecturer in Inorganic Chemistry at the University of Nottingham and was subsequently promoted to Associate Professor in 2014 and Professor in 2019. Her research interests involve the stabilisation of low-coordinate and highly reactive main group and transition metal complexes, and the investigation of their reactivity under stoichiometric and catalytic regimes. The analysis of these complexes through spectroscopic, structural, magnetism and computational studies, and the investigation of fundamental patterns of reactivity, leads to their exploitation in catalysis, small molecule activation and magnetochemistry. She was the recipient of the 2018 Chemistry of the Transition Metals award from the Royal Society of Chemistry for outstanding recent contributions to the development of very low coordinate, electronically unsaturated compounds of the transition metals.
Small molecule activation and catalysis using highly unsaturated complexes
Deborah L. Kays
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The use of sterically demanding ligands enables the isolation of highly unsaturated complexes that can exhibit very unusual reactivity towards small molecules.1 Our research group are particularly interested in the use of m-terphenyl ligands (2,6-Ar₂C₆H₃⁻) for this purpose, the steric bulk of which can be conveniently manipulated through the flanking aryl substituents. Low-coordinate iron(II) terphenyl complexes react with carbon monoxide at ambient temperature and pressure, cleaving the CαO bond to afford novel squaraines where the C₄ core is derived completely from carbon monoxide, through a selective homologation reaction.2 Combined spectroscopic, structural and theoretical investigations allow us to develop a postulated mechanism for this reaction and to elucidate the properties of the squaraine products.

Transition metal m-terphenyl complexes are also able to act as precatalysts for a growing number of reactions, such as cyclotrimerisation, hydrofunctionalisation and dehydrocoupling.3-6 Remarkably, hydrophosphination using low-coordinate iron(II) precatalysts affords phosphinodicarboxamides, asymmetric phosphorus analogues of biuret, through a formal isocyanate coupling and P–H addition with high selectivity.4 We are now expanding P–H addition to P(V) chemistry, where we demonstrate that hydrophosphinylation can occur in solvent-free or low-added solvent conditions without the need for a catalyst.7

Prof. Dr. Matthias Preller

*University of Applied Sciences Bonn-Rhein-Sieg*

Since September 2020, Matthias Preller is Professor for Structural Biology and Chemical Analytics at the University of Applied Sciences Bonn-Rhein-Sieg. He graduated in Chemistry at the Technical University Braunschweig, and received his PhD in Biophysical Chemistry from the Leibniz University Hannover in 2011, working on molecular motors. In 2012 he was appointed as assistant professor at the Centre for Structural Systems Biology in Hamburg and Hannover Medical School. In addition, he was a member of the Biomolecular Drug Research Centre in Hannover from 2012 to 2020. His research focuses on cytoskeletal motility, and small effector molecules modulating protein dynamics in order to counteract disease mechanisms.
Exploring the Infinitely Small of Diseases and their Treatment

Matthias Preller
Institute for Functional Gene Analytics, University of Applied Sciences Bonn-Rhein-Sieg, Rheinbach, Germany

A multitude of severe human diseases result from small modifications in the composition of the building blocks of life. These alterations originate in the fundamental atomic level and eventually manifest at the level of cells and organisms.

Single point mutations in protein-encoding, human genes can lead to diverse pathologies, including disorders of the sensory and central nervous system, cardiovascular diseases, and cancer, the major causes of death in developed countries. The consequences of these disease-associated mutations are shown to frequently affect the atomic structures and conformational dynamics of the corresponding proteins, the working machines in our bodies.

Likewise, infections with pathogens, such as viruses and tropical parasites, rely on complex molecular interactions and processes on a submicroscopic scale in order to enable the pathogens to invade our cells.

The use and future development of hybrid approaches, combining high-resolution structure determination with sophisticated computational simulations, and functional analysis, is key to understanding the complex mechanisms of disease development, and to allow targeted treatments.

The presentation will provide insights into the smallest, atomic world of biological molecules and their mechanisms of disease development, as well as strategies of using structure-based, de novo design to modulate pathological effects.
Prof. Dr. Mischa Bonn
Max-Planck-Institute for Polymer Research, Mainz

Mischa Bonn serves as Max Planck Director and professor by special appointment in Amsterdam (Physics) and Mainz (Chemistry). The overall aim of Bonn’s research is to reveal the structure and dynamics of molecules and intermolecular interactions at interfaces, as well as the transport of molecules and charge across those interfaces. This is of fundamental interest, but also highly relevant for environmental processes (e.g. chemical conversion on ice surfaces), biophysics (e.g. water, lipids and proteins at membrane interfaces) and energy conversion (e.g. photocatalytic water splitting at interfaces and charge carrier dynamics across semiconductor nanostructures). To achieve these goals, Bonn develops and implements state-of-the-art, laser-based spectroscopic tools. He has won several awards and prizes for his work.
Chemical activity of water interfaces

Mischa Bonn
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Water interfaces differ from the bulk, in both their physical structure and chemical composition. In particular, the role of charges at interfaces and the effect of charges on the arrangement of counterions and water is much debated. These charges also affect the chemical dynamics occurring at water interfaces. For instance, charge is relevant for “on-water chemistry” – chemistry at the open water surface, relevant for both technologies and chemical processes in the atmosphere. Water-mineral interfaces are also typically charged, and the dissolution chemistry occurring at these interfaces changes the charged state.

My presentation will show how we can follow chemical conversion at water surfaces and interfaces in great detail using surface-specific vibrational spectroscopies. These spectroscopies reveal reaction intermediates for the on-water synthesis of organic 2D materials, and provide detailed insights into mineral dissolution.
Markus Kalesse is Professor of Organic Chemistry at the Leibniz University Hannover since 2003. Additionally, he is the head of medicinal chemistry at the HZI in Braunschweig. He studied Chemistry at the Leibniz University Hannover, where he obtained his Ph.D. under supervision of Dieter Schinzer. Afterwards he became a postdoctoral fellow at the University of Wisconsin in Madison (USA) in the working groups of Steven D. Burke (1991-1992) and Laura L. Kiessling (1992). In 1997 he habilitated at the Leibniz University Hannover, while working with Ekkehard Winterfeldt. From there he became a deputy professor at the University of Wisconsin in Madison (USA) and the Christian-Albrechts-University of Kiel between 1998 and 2000. After spending 2 more years in Hannover, he filled the position of a full professorship at the Freie Universität Berlin in 2002 in Organic Chemistry, after returning to Hannover in 2003 to occupy his current position. His research is focused on the synthesis of complex natural substances, especially polyketides and polyketide-peptide-hybrids as well as the development of methods for stereoselective synthesis.
Stereoselective Sparteine-free 1,2-Metallate Rearrangements in Natural Products Syntheses

M. Kalesse,1 Y. Linne,1 M. Birkner,1 D. Lücke,1 D. Lohrberg,1 M. Aursnes,2 A. Kipper,1 E. Bonandi,3 J. Geldsetzer4

1Institute of Organic Chemistry, Leibniz Universität Hannover, Germany
2University of Oslo, Norway
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4Helmholtz-Zentrum für Infektionsforschung, Braunschweig, Germany

The stereoselective synthesis of two natural products relied at pivotal C-C disconnections on an Aggarwal 1,2-metallate rearrangement as an advancement of the work originally developed by Hoppe and Matteson. This 1,2-metallate rearrangement of vinyl boronates yields stereoselectively allylic alcohols which are usually constructed through a Nozaki-Hiyama-Takai-Kishi (NHTK) reaction, of which stereo as well as enantioselective variants are available. However, in the context of complex natural product syntheses it often provides unsatisfactory yields and/or selectivities. The two projects for which we had to overcome these obstacles were the syntheses of chondrochloren and meridamycin. We will not only describe our endeavors towards these two natural product but discuss a set of polyketidal substrates and their diastereoselective transformation in 1,2-metallate rearrangements in order to provide a general concept for its use in total syntheses.

At the beginning of the lecture, I would like to describe a typical working day in the 1980s and 1090s at the institute of organic chemistry and Professor Winterfeldt’s participation in it.

Jun.- Prof. Dr. Anna Krawczuk

Georg-August University Göttingen

Anna Krawczuk obtained her PhD in chemistry in 2009 at the Jagiellonian University in Krakow, Poland, investigating the optical properties of chiral crystalline compounds. From 2009 to 2020 she was appointed lecturer at the Podhale State College of Applied Sciences where she founded a new curriculum of cosmetology studies. At the same time, she continued her scientific research with stays at the universities of Bern and Lorraine before she started her independent research as a research associate back in Krakow in 2012. Since October 2020 Anna Krawczuk is Junior Professor at the Georg-August University in Göttingen, Germany. Her research focuses on the investigation of structure-property correlations with an emphasis on mechanical and optical properties. For this, advanced experimental techniques such as high resolution and high-pressure single crystal x-ray diffraction are combined with theoretical methods within the Quantum Crystallography framework to gain insights into intermolecular interaction and their influence on the macroscopic crystal. She pioneered the use of atomic polarizabilities for the prediction of physical properties and is currently developing a software to make them accessible within a database approach.

25.03., 17:30-18:00
Audimax (E415), Welfenschloss (Building 1101)
In recent years an increasing attention on the design of new crystalline materials with enhanced molecular and thus physical properties is observed, in particular in the field of materials science. It is of great importance to understand how molecules interact which each other in a solid-state and which of the interactions may be at the origin of a given property. For example, if one wants to design efficient optical device, high polarizability of the constituting molecules must be assured, typically tuned by modifying their structure with different substituent groups. Adopting advanced theoretical and experimental techniques within the framework of Quantum Crystallography\textsuperscript{[1,2]} seem to be an efficient way to yield precise insights on potentially functional materials and give the possibility of direct identification of reproducible structural features, transferable among different systems which, in turn, leads to better understanding of molecular self-assembly processes promoting specific crystal packing and thus prominent material property.

Here we present the interplay between experimental and theoretically derived data towards better prediction of optical, electrical and mechanical properties of solid-state materials. Special attention will be put on distributed atomic polarizability approach\textsuperscript{[3]} which proved to be an efficient and simplified way in estimating accurate electrostatic\textsuperscript{[4]} and linear optical properties of materials\textsuperscript{[5]}.

\textsuperscript{[2]} A. Genoni & P. Macchi Crystals 2020, 10, 473.
1. BASF

*Sustainable Materials for a Circular Economy*

**Date:** 24.03. 17:15

**Speaker:** Dr. Bernhard von Vacano

**Place:** Building 1101, Room E415

**Abstract:** All industrial sectors face the challenge to transition into a Net Zero world, that achieves climate neutrality in 2050, as laid out, for example, in the EU Green Deal. Polymers play a crucial role in enabling sustainable applications and emission reduction. As structural materials: by weight saving in transportation, in composites for wind turbine blades, or for insulation of buildings. As functional materials: replacing solvent-based formulations by water-based ones, or helping save energy by enabling cold-water laundry in your washing machine. Being carbon-based organic compounds, polymeric materials themselves need further innovation: A sustainable circular economy for polymeric materials will decouple their economic value from emissions and resource consumption. Feedstocks will increasingly be based on recycled or biobased carbon sources. At end of life, polymers need to be collected and recycled, or should be biodegradable if they are dispersed in the application. This is an exciting field for research and development, and will pave the way to achieving comprehensive sustainability.
2. Covestro

*Sustainable Development through continuous improvement*

**Date:** 25.03., 15:15  
**Speaker:** Rolf Albach, Covestro Deutschland AG, Performance Materials R&D, 51365 Leverkusen, email: rolf.albach@covestro.com  
**Place:** Building 1101, Room E415

**Abstract:** A 2012 Harvard Business Review started with “Big companies are really bad at innovation because they’re designed to be bad at innovation”. While this has been debated a lot, there is hardly a debate about their competence in continuous improvement. If directed well this can be extremely powerful to transform the chemical industries and their partners into a sustainable future.

Polyurethanes, the 6th important polymer by volume, give a wealth of examples for this from elimination of side effects in thermal insulation [1], improving vehicle indoor air quality through the Knoevenagel reaction [2], longevity through eliminating polymer-polymer aggression [3], and more.

The polyurethane industry in 2000 stopped work on the chemical recycling after 30 years of work [4] and restarted recently [5]. This will serve as an example how much chemists are essential but not sufficient parts of innovation ecosystems.

3. Boehringer Ingelheim

**Using digital tools for drug design**

**Date:** 24.03., 14:45  
**Speaker:** Dr. Theodor Peez, Research Scientist Medicinal Chemistry, Boehringer Ingelheim Pharma GmbH & Co. KG  
**Place:** Building 1101, Room E415  
**Abstract:** Everyone is talking about the transformative power of digitalization & AI, but how do things look like from the user’s perspective? How do scientists in 2022 come up with ideas for new molecules that could become drugs one day? In this talk from a medicinal chemist’s perspective, you will get a glimpse of how scientists at Boehringer Ingelheim collaborate with each other as well as machines by using a variety of digital tools to generate ideas for the drugs of tomorrow.

4. International Sustainable Chemistry Collaborative Centre (ISC3)

**Let’s discuss Sustainable Chemistry! - But what even is Sustainable Chemistry?**

**Date:** 24.03., 15:05  
**Speakers:** Kiana Frank, Jens Krol  
**Place:** Building 1101, Room E415  
**Abstract:** The ongoing international debate on Sustainable Chemistry shows that the expectations towards the term differ widely. By taking different viewpoints into account, the ISC3 will use this session to discuss existing frameworks in this field and map out key goals that Sustainable Chemistry aims to achieve.
5. BCNP Consultants

**Supporting decision-maker in tech companies and tech-related institutions**

**Date:** 24.03., 15:25  
**Speaker:** Tobias Kirchhoff  
**Place:** Building 1101, Room E415

**Abstract:** Feeling insecure about strategic decision making, need of a carefully prepared strategy or access to new customers and cooperation partners – these are the main triggers why tech companies work together with BCNP Consultants.

BCNP, founded back in 2002, is a consultancy company specialized on the branches Biotech, Chemistry, Nanotech and Pharma. BCNP offers market analyses, technology scouting and business planning for making strategic decisions (BCNP Strategy) and brings clients together with new potential customers (BCNP connect). Furthermore, BCNP is initiator and organizer of the European Chemistry Partnering (ECP), connecting start-ups and SME with Corporates and Investors. BCNP’s customers appreciate the simultaneous understanding of technology and economy.

There are various types of customers with different kinds of needs and challenges working together with BCNP: Big Industry, SME, Start-ups, Investors as well as Non-Profit Organizations.

Holger Bengs, chemist and founder of BCNP, and Tobias Kirchhoff, business chemist and head of the Cologne office, are the VCW regulars table organizers for Frankfurt and Cologne.

BCNP is always looking for interns in the BCNP strategy unit.
6. Evonik

**Evonik Health Care - Career Talk**

Date: 25.03., 11:15  
Speaker: Dr. Ulrich Kloeckner  
Place: Building 1101, Room E415

**Abstract:** In this industry lecture, Ulrich Kloeckner, group leader at Evonik Health Care, will give insights into his journey from his studies in Frankfurt, Tuebingen and at Urbana-Champaign Illinois in the U.S. to working for Evonik Health Care, including for the “speed of light” project. What will the world look like in 10 or 20 years? What will humankind need? What challenges might we face? What solutions might help us to overcome them?

At Evonik, we are exploring ways to make the world—and everyday life—better by finding answers to questions like these. In more than 100 markets, about 33,000 people work to improve people’s lives by creating innovative, profitable and sustainable solutions.

One key example was the approval of the first mRNA vaccines, which was an important step in fighting the coronavirus pandemic and saving lives all over the world. In these vaccines, the active mRNA is encapsulated in so called lipid-nanoparticles (LNPs), which consist of a specific lipid composition that allow the intracellular delivery of mRNA and the subsequent release to unfold the mode of action. At Evonik, we recognized the crucial role of lipids in these formulations and we continue to support our clients with custom lipid projects by combining this understanding with decades of expertise in process development, analytics, scale up, validation and GMP manufacturing.

Opportunities to work on exciting projects like these at Evonik Health Care are plentiful! We can support a wide range of innovative projects and products with expertise. Join this talk to find out more!
7. Altana

**ALTANA Innovations for a Sustainable Future: Selfdiagnostic Polymers**

**Date:** 25.03., 11:35  
**Speakers:** Dr. Christian Schaumberg, Head of Science Relations, ALTANA AG  
**Place:** Building 1101, Room E415

**Abstract:** As a specialty chemical company, ALTANA strives to find innovative solutions, helping our customers to develop more sustainable products. A significant contribution to innovation comes from our partnerships with academic research groups under the umbrella of the ALTANA Institute.

One example is the collaboration between ELANTAS and the Martin Luther University Halle-Wittenberg. A fluorescence sensor was developed to detect the degradation of polymers under thermal stress.\(^1\)\(^2\) This will facilitate the development of a sensor system which allows to follow the aging process of electrical motors and generators. An increased service time of these devices will be significant contribution to a sustainable future.

\(^1\) A. Funtan, P Michael, S. Rost, J. Omeis, K. Lienert, W. Binder *Advanced Materials* 2021, 2100068.  
\(^2\) W. Binder, A. Funtan *Nachrichten aus der Chemie* 2022, 70, 40 - 41.

8. McKinsey & Company

**Why McKinsey?**

**Date:** 25.03., 11:55  
**Speakers:** Alexander Graf, Andy Rinaldi  
**Place:** Building 1101, Room E415

**Abstract:** Who are we, how do we work, what do we offer our consultants, and why could joining McKinsey be exactly right for you?

Wide-ranging topics: Who are our clients? What questions do we advise them on? And what core competence do we contribute?  
Inspiring colleagues: What can McKinsey offer you specifically and what matters most to you?  
What kind of environment will you find when you join McKinsey?  
Your career: What options do you have for joining McKinsey and what opportunities for advancement do we provide?
Selective modification of unprotected carbohydrates for cross-linking in waterborne coatings

S.C. Massmann¹, M.D. Witte¹, A.J. Minnaard¹, K. van den Bergen², D.J. van Dijken³

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Coatings for paints, inks and lacquers on an environment-friendly and non-toxic basis are highly desired. Therefore, I am working on the novel functionalization of bio-polymers such as carbohydrates (oligo- and polysaccharides). The group of Prof. Minnaard already showed the selective oxidation of α-methyl-β-glucose at the C3 position with a palladium-neocuproine-catalyst and benzoquinone in methanol in high yield. This method was demonstrated in the end term oxidation of 1,4-linked glucans up to the 7-mer as well. Through this carbonyl moiety within the carbohydrates, further functionalization is much more accessible and has a wide spectrum of possibilities. During my PhD, I aim to oxidize carbohydrates and especially polysaccharides with the same selectivity but in a sustainable and greener way. Many screenings were already done focusing on the one hand on stabilizing the Pd catalyst, which has the tendency to decompose due to a hydrogen abstraction from the ligand during the oxidation cycle, and on the other hand on the susceptibility for C3-selective oxidation of different oligo- and polysaccharides. Other oxidizing metal catalysts with less toxicity will also be tested in the near future.

Switching Selectivity in HMF Oxidation with CTF Photocatalysts

Daniel Ditz 1, Nina Sackers 1, Florian Wisser 2, Regina Palkovits 1

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2 University of Regensburg, Institute of Inorganic Chemistry, 93053 Regensburg
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The ongoing endeavour towards more sustainable chemical processes drives research in photocatalysis. Photocatalysis holds the potential to combine direct usage of the most abundant alternative energy resource, sunlight, with chemical valorisation. Hereby, covalent triazine-based frameworks (CTFs) excel as photocatalysts due to their chemical and thermal robustness, their highly conjugated and nitrogen rich nature, facile syntheses, and most important unprecedented structural variability. This allows the design of tailor-made photocatalysts. [1]

In this work, we present how a slight modification of the CTF network triggers a switch in selectivity in 5-hydroxymethylfurfural (HMF) oxidation. HMF remains as one of the most promising biogenic platform molecules and finally approaches commercialisation. [2] We designed a phenyl- and a naphthyl-based CTF that each catalyse one distinctive reaction pathway in HMF valorisation. Either HMF is directly oxidised to 2,5-diformylfuran (DFF) or molecular oxygen is activated to singlet oxygen which then undergoes a [4+2] cycloaddition with HMF. Extensive characterisation of the optoelectronic properties combined with detailed knowledge of the reaction mechanism allowed us to understand this switch in selectivity which adds another tool to the toolbox of CTF photocatalysts. [3]

Visible Light Initiated Hydrooxygenation of Unactivated Alkenes — A Strategy for Anti-Markovnikov Hydrofunctionalization

Linda Quach¹, Subhabrata Dutta¹, Philipp M. Pflüger¹, Frederik Sandfort¹, Peter Bellotti¹, Frank Glorius*¹

¹ Westfälische Wilhelms-Universität Münster, Organisch-Chemisches Institut, 48149 Münster, Germany

Hydrofunctionalization of unactivated alkenes is an indispensable mean in synthetic chemistry. Given that addition of electrophilic species into alkenes intrinsically follows the Markovnikov rule, a regioselectivity switch presents a major challenge. Herein, we present a visible light promoted strategy for the selective anti-Markovnikov hydrooxy-genation of unactivated alkenes. Therefore, an innovative reagent was carefully designed to release a highly reactive and strongly underdeveloped alkoxycarbonyloxy radical upon reduction, which selectively adds into alkenes. Hydrogen atom abstraction from 2-phenylmalononitrile is the key to form the product. We believe that this protocol is a significant addition to existing hydrofunctionalization reactions and further highlights the importance of rational reagent design towards the development of methods to tackle challenging synthetic transformations.¹ We are convinced that such radical approaches will find broad application in the future.


Figure 1: This work about the Anti-Markovnikov selective hydrooxygenation of unactivated alkenes utilizing an innovative pyridinium salt and 2-phenylmalononitrile as H atom donor.¹
Untangle the Intertwined: What Happens During Colloidal \(\text{MoS}_2\) Nanosheet Syntheses?

André Niebur\(^1\,2\), Aljoscha Söll\(^1\), Onno Strolka\(^1\), Dominik Rudolph\(^1\), Philipp Haizmann\(^3\), Heiko Peisert\(^3\), Marcus Scheele\(^3\) and Jannika Lauth\(^1\,2\,4\)

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\(^2\) Cluster of Excellence PhoenixD (Photonics, Optics, and Engineering – Innovation Across Disciplines), Hannover, Germany
\(^3\) University of Tübingen, Institute of Physical and Theoretical Chemistry, 72076 Tübingen, Germany
\(^4\) Leibniz University Hannover, Laboratory of Nano and Quantum Engineering (LNQE), 30167 Hannover, Germany

Ultrathin two-dimensional (2D) transition metal dichalcogenides (TMDCs) provide a toolbox for physical phenomena with compelling properties for emerging optoelectronic technologies. This includes excitonic devices, single-photon emitters, and silicon-free photovoltaics. Colloidal synthesis is a wet-chemical fabrication method for these TMDC nanosheets (NS) and offers straightforward material control by precursor and ligand chemistry.\(^1\) Although colloidal TMDC NSs in various shapes have been reported, a thorough understanding of the reaction mechanisms guiding the colloidal syntheses is still missing.\(^2,3\) Here, we investigate the colloidal synthesis of \(\text{MoS}_2\) NSs in terms of their crystal phase and shape over the course of the reaction. With X-ray photoelectron spectroscopy we found that regardless of the reactivity of the Mo precursor, a mixture of the stable semiconducting crystal phase and the metastable metallic crystal phase forms initially. The NSs are then transformed into the semiconducting phase during reaction, following the Ostwald step rule. Consistently, we obtain semiconducting \(\text{MoS}_2\) NSs with a lateral size smaller than the exciton diameter in 2D \(\text{MoS}_2\). The optoelectronic properties of these NSs thus not only depend on the 2D character of the TMDCs but also on their lateral confinement.\(^4\) Our findings add to the understanding of colloidal \(\text{MoS}_2\) syntheses and will help to make TMDC NSs with tailored properties.

A mutant-selective inhibitor for inositol hexakisphosphate kinases

Tim Kröber $^{1,2}$, Martin Neuenschwander $^1$, Anja Schütz $^3$, Jens Peter von Kries $^1$ and Dorothea Fiedler $^{1,2}$

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Inositol pyrophosphates (PP-InsPs) are key messengers involved in many important cellular processes at the intersection of signaling and metabolism, $^{[1]}$ including insulin and glucose homeostasis $^{[2]}$, tumor metastasis $^{[3]}$ and spermatogenesis $^{[2]}$ in mammals. Their signaling functions have mainly been defined by genetic perturbation of the inositol hexakisphosphate kinases (IP6Ks), which are responsible for PP-InsP synthesis. In this work, a chemical genetic method called ‘bump-hole’ approach $^{[4,5]}$ was implemented to find specific mutant kinase/inhibitor pairs to pharmacologically perturb PP-InsP biosynthesis. Due to the introduction of a new gatekeeper mutant in the IP6Ks (LàV), a high-throughput-screen (HTS) was performed to identify new inhibitors or inhibitor scaffolds. A compound with good selectivity for the mutant over the wild type kinase was identified and validated biochemically. This molecule will serve as lead compound for further dissecting the individual functions of IP6K isozymes to enable a more granular view on their role in signaling and metabolism.

Funding: Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy – EXC 2008 – 390540038” – UniSysCat.

$^{[2]}$ Bhandari R. et al., PNAS, 2008, 105, 2349-2353
$^{[3]}$ Jadav R. S. et al., Cell Signal., 2016, 28, 1134-1136
$^{[5]}$ A. C. Bishop et al., JACS, 1999, 121, 627-631
Direct Synthesis of Enamides via Electrophilic Activation of Amides

Philipp Spieß, Martin Berger, Daniel Kaiser, Nuno Maulide*
University of Vienna, Institute of Organic Chemistry, Währinger Straße 38, 1090 Vienna, Austria

Enamides (N-alkenyl amides) are highly versatile synthetic building blocks which can be seen as stable enamine surrogates. As reactants, enamides can be applied in a variety of settings, including (asymmetric) transition-metal catalysis or photochemistry. [1,2] However, the preparation of enamides has remained a major challenge, relying to a large extent on prefunctionalized starting materials. [3,4] In order to address this issue, a protocol for direct N-dehydrogenation of N-alkylamides is a highly desirable scenario. However, only a few specialized methods have been reported to date. [5,6]

Informed by our group’s extensive experience in the field of electrophilic amide activation, we speculated whether the in-situ generated species I might enable a novel pathway to access enamides (Figure 1). [7] Assuming that the proton α to nitrogen in intermediate I is highly acidified, we anticipated that combination with a strong, non-nucleophilic base might trigger the desired N-dehydrogenation event. Herein, we present the deployment of the unusual combination of triflic anhydride and LiHMDS to this end. The scope and limitations of the transformation, its mechanism and the utility of the synthesized enamides shall be discussed in this presentation.

Figure 1: a) Concept of Tf₂O-enabled N-dehydrogenation of amides; b) Sample subset of the scope.

Configurational Lability at Tetrahedral Phosphorus: syn/anti-Isomerization of a P-Stereogenic Phosphiranium Cation via Intramolecular P-Epimerization

Like the analogous tetrahedral C, Si, and N compounds, P-stereogenic phosphonium cations are configurationally stable. In contrast to this well-known behavior, we report here that P-epimerization of chiral phosphiranium cations occurs under mild conditions. Heating either syn- or anti-[Mes*P(Me)CH2CHPh][OTf] (Mes* = 2,4,6-(t-Bu)3C6H2) at 60 °C in CD2Cl2 resulted in isomerization to give a syn-enriched equilibrium mixture. Ion exchange with excess [NBu4][Δ-TRISPHAT] (Δ-TRISPHAT = Δ-P(ο-C6Cl4O2)3) followed by chromatography on silica gel removed [NBu4][OTf] and gave mixtures of syn- and anti-[Mes*P(Me)CH2CHPh][Δ-TRISPHAT]-x[NBu4][Δ-TRISPHAT]. NMR spectroscopy showed that isomerization proceeded with epimerization at P and retention at C. On the basis of DFT calculations, we propose a mechanism consistent with this stereochemistry, involving P–C cleavage to yield a hyperconjugation-stabilized carbocation, pyramidal inversion promoted by σ-interaction of the P lone pair with the neighboring cation, and ring closure with inversion of configuration at P. The unusual configurational lability at pyramidal phosphorus and configurational stability in a carbocation can be rationalized by the cooperative effects of strain in the three-membered phosphiranium ion, hyperconjugation in the ring-opened cation, and stabilization of the planar inversion transition state by the pendant Lewis acid carbocation. DFT calculations comparing the ring-opened cation [Mes*P(Me)CH2CHPh]+ and its neutral analogue Mes*P(Me)CH2CH2Ph suggested that the σ-interaction with the cation reduced the P-inversion barrier by 13 kcal/mol.
Water-in-Oil Microemulsions as Soft-Templates for the Self-Assembly of Nanoparticle Clusters into Filament Networks

Rebeca Fortes-Martín 1, Joachim Koetz 1.

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Self-Assembly of nanoparticles into ordered structures constitutes a promising bottom-up approach to larger-scale nanomaterial-based devices. For this purpose, soft-templates of self-organized dispersions containing nanoparticles and surface-active agents can mediate the formation of self-assembled nanostructures upon solvent evaporation.

In our research, reverse, water-in-oil microemulsions were formulated by using Aerosol-OT (dioctyl sodium sulfo succinate, AOT) as surfactant. Oleyl-capped nanoparticles can be incorporated in the continuous oil phase, while polyethylenimine-stabilized nanoparticles where confined in the dispersed water droplets. Thin films of ordered nanoparticles as filament-like networks were formed after drop casting and solvent evaporation of the upper water-in-oil phase from a biphasic Winsor type II system. [1] More detailed studies proved an initial nanoparticle clustering and a microemulsion droplet elongation, which should guide the subsequent formation of the final filament-like network of interconnected nanoparticle filaments over a surface (Scheme 1). [2]

Thus, a new application of microemulsions as soft-templates is shown, which enables the hierarchical ordering of spherical nanoparticles into thin films of anisotropic nanostructures, extended to several µm over a surface. [1,2] This method might contribute to the development of surface-assembled nanomaterials on larger scale.

Direct copper deposition from copper(II) oxide in ionic liquid

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One of the main problems of metal production is that, typically, the processing of the according oxidic ores or minerals requires high temperatures of around 1000 °C. Against the backdrop of climate change and fossil fuels running low, there is a growing need for more energy-efficient methods for ore processing.

A suitable approach for more energy- and resource-efficient metallurgical processes could be low temperature metal extraction with the aid of ionic liquids, so-called ionometallurgy. In the first stage of this approach, metal oxides are dissolved at low temperature. [1] In the second stage, metals are electrochemically deposited from the resulting solution. Here, we show that this approach can be successful, using the example of copper. [2] Copper coatings are widely applied, e.g. as conductive layers in circuit boards. In comparison to the energy-intensive and water-consuming conventional electroplating process, with our approach, a more efficient process could proceed from the mineral tenorite or copper(II) oxide residues from pyrometallurgy.

In the first stage of our approach, upon the dissolution of copper(II) oxide, four complexes with varying coordination geometries and ligands were obtained. In the second stage, the resulting copper-betaine compounds were used as starting materials for the direct electroplating of steel. Both stages reveal an influence of various reaction parameters, such as chloride concentration, temperature, solvent and impurities. Altogether, copper(II) oxide can be dissolved in ionic liquid, allowing for a subsequent direct copper electrodeposition. The model system copper gives a proof of concept for the general feasibility of our ionometallurgical approach for the direct metal production from metal oxides using ionic liquids. This could also be applicable to the processing of other industrially highly relevant oxidic ores. Future research will also involve the optimization of this process as well as a recycling strategy for the ionic liquid.

Communicating Particles: Identification Taggant and Temperature Recorder in One Single Supraparticle

Jakob Reichstein¹, Franziska Miller¹, Susanne Wintzheimer¹,², Karl Mandel¹,²

¹ Friedrich-Alexander-University Erlangen-Nürnberrg, Professorship for Inorganic Chemistry, 91058 Erlangen, Germany
² Fraunhofer-Institute for Silicate Research ISC, 97082 Würzburg, Germany

Flexibly applicable smart additives could render random objects conscious. More precisely, they enable passive matter to communicate and thereby, contribute to the realization of sustainable, innovative concepts, like Industry 4.0 or Circular economy. [1]

Here, we introduce micron-scaled communicating particles (CPs) as smart additives that unite the functionalities of an identification (ID) taggant and a thermal history recorder within their luminescent signal characteristic. [2] Key to unite these two functionalities in a single particle is the hybrid inorganic-organic nature and the chosen nano-architecture of the CPs. Three differently colored luminescent nanoparticle (NP) types, acting as optical information carriers, are assembled into supraparticles with a hierarchical core-satellite structure via spray-drying (Figure 1a). The resulting tunable inorganic ID functionality, is environmentally inert, while the organic temperature recorder is irreversibly quenched upon thermal events that exceed a specific adjustable threshold temperature (Figure 1b). Both functionalities can be read out simultaneously using single-wavelength excitation.

In summary, the presented CPs and their conceptual design give rise to an entire new family of smart additives to foster materials’ intelligence.

Figure 1: a) Design of a micron-scaled communicating particle (CP);

b) Temperature-dependent luminescent signal characteristic of the CP: temperature stable ID signal (green and red wavelength area), thermal history recorder that is irreversibly quenched upon specific thermal events (blue wavelength area).

Investigating an asset-based approach to teaching undergraduate general chemistry

Klaudja Caushi 1, Hannah Sevian 2

1 University of Massachusetts Boston, Chemistry Department, Boston, MA, 02125, United States
2 University of Massachusetts Boston, Chemistry Department, Boston, MA, 02125, United States

Many universities and colleges in the United States encounter a universal problem of high failure and withdrawal rates in introductory chemistry courses 1,2. At the University of Massachusetts Boston, up to half of the students do not pass first-semester general chemistry. The University has also become increasingly diverse, now at 72% underrepresented racial minorities among undergraduates in the College of Science and Mathematics. The literature suggests that there is a relationship between diversity of students and drop, fail, or withdrawal (DFW) grades in science, technology, engineering, and mathematics (STEM) getaway courses 3. Supplemental academic support greatly improves students’ persistence and success in initial mathematics and science courses, particularly for students who are underrepresented in STEM disciplines, but most supplemental support occurs in the form of remediation. Unfortunately, major studies have shown that the long-term effects of remediation with students are indistinguishable from no remediation with peer comparisons 4. Instead of focusing on remediating students perceived deficits, this study utilizes students’ strengths by developing, implementing, and studying an asset-based supplemental chemistry course. The curricular goals of the course include practice with mathematical, chemical, and calculator skills necessary for general chemistry; strengthening of study skills that are important for general chemistry as well as other courses; and work with chemistry representations, specialized language in chemistry, and scientific reasoning employed in chemistry. In this presentation we present findings on which elements of the course design are productive in supporting students and discuss the implications that the course has had on students’ success in general chemistry. Through this work we aim to demonstrate how focusing on students’ assets opens new possibilities for designing chemistry courses.

(2) Bunce, D. M.; Bauer, C. F.; Bentley, A. B.; Gellene, G. I. A Six-Year Study of the Effects of a Remedial Course in the Chemistry Curriculum; 2005; Vol. 82.
Synthesis of a proline-derived module and its application in the development of α-helical peptides as potential SARS CoV-2 inhibitors

Pascal M. Engelhardt 1, Sebastian Florez-Rueda 2, Ines Neundorf 1, Ronald Kühne 2 and Hans-Günther Schmalz 1

1 University of Cologne, Department of Chemistry, 50939 Cologne, Germany
2 Leibniz-FMP, Department for Chemical Biology II, 13125 Berlin, Germany

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We developed a toolkit of Proline-derived Modules (ProMs), which consist of rigidified diproline units inducing conformational preorganization in peptidic constructs. While the original ProM units were used in the construction of PPII-helical peptides as inhibitors of the EVH1 domain,[1] further constructs using Ac-[HAsp]-ProM-5 as an N-cap were designed to induce α-helices in short peptides.[2] This α-helix inducing effect of ProM-5 was initially proven for idealized short peptides and now applied further to a more complex biological system by attempting to mimic the α1-helix found in ACE2, which SARS-CoV-2 and other corona viruses employ for cell entry. [3] Short α-helical peptides derived from α1 may directly serve as inhibitor ligands for this specific interaction (Figure 1) and may therefore be a promising therapeutic strategy for COVID-19. While the α-helix inducing effect of ProM-5 could be proven by comparison to proline containing reference peptides, a stronger increase in helicity was achieved by replacing non-binding amino acids by alanine, which is an established strategy in the preparation of helical peptides. [4] Binding affinities were measured by microscale thermophoresis for all prepared peptides and a binding to the SARS-CoV-2 Spike protein could be observed for ProM-5 containing peptides. Interestingly, the best binding affinity of 610 nM was observed for an alanine-enriched reference peptide N-capped by Ac-[HAsp]-Pro-Pro unit.

1. **Carl-Roth Award**

**Dr. Jacob Schneidewind**

Institute for Technical and Macromolecular Chemistry  
RWTH Aachen University

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**Curriculum Vitae**

<table>
<thead>
<tr>
<th>Year</th>
<th>Position/Institution</th>
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<tbody>
<tr>
<td>since 2022</td>
<td>Junior research group leader at Institute for Technical and Macromolecular Chemistry, RWTH Aachen University (Liebig fellow)</td>
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<tr>
<td>2021</td>
<td>Postdoc at Institute for Technical and Macromolecular Chemistry, RWTH Aachen University (Prof. Walter Leitner)</td>
</tr>
<tr>
<td>2021</td>
<td>Postdoc at Leibniz Institute for Catalysis (Prof. Matthias Beller)</td>
</tr>
<tr>
<td>2017–2021</td>
<td>PhD at Leibniz Institute for Catalysis/University of Rostock (Prof. Matthias Beller)</td>
</tr>
<tr>
<td>2016–2017</td>
<td>Chemistry studies at University of Rostock (B.Sc. und M.Sc.)</td>
</tr>
<tr>
<td>2015</td>
<td>Research stay at University of Toronto (Prof. Robert H. Morris)</td>
</tr>
<tr>
<td>2014–2015</td>
<td>Undergraduate studies (liberal arts) and research (Prof. Kang Hway Chuan) at Yale-NUS College, Singapore</td>
</tr>
<tr>
<td>2012–2014</td>
<td>Dual enrolment studies (Schülerstudium, chemistry) at University of Cologne</td>
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**Awards and Scholarships**

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<tr>
<td>since 2022</td>
<td>Liebig Fellowship by Fonds der Chemischen Industrie</td>
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<tr>
<td>2021</td>
<td>„summa cum laude“ distinction for PhD at University of Rostock</td>
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<tr>
<td>2018 – 2020</td>
<td>Kekulé PhD fellowship by Fonds der Chemischen Industrie</td>
</tr>
<tr>
<td>2014 – 2017</td>
<td>Fellow of the Studienstiftung des deutschen Volkes (German Academic Scholarship Foundation)</td>
</tr>
</tbody>
</table>
Production and use of green hydrogen for a sustainable chemical economy

Jacob Schneidewind

1 RWTH Aachen University, Institute of Technical and Macromolecular Chemistry, 52074 Aachen, Germany

To create a fossil-free chemical economy, bulk chemicals will have to be produced from sustainable raw materials such as hydrogen and carbon dioxide. An important target in this regard is methanol, which can be produced via direct CO₂ hydrogenation. However, this reaction typically requires high temperatures, which lowers energy efficiency. Using a combination of Co(acac)₃ and Triphos, it was possible to create a homogeneous, non-noble metal catalyst for CO₂ hydrogenation to methanol that enables the reaction at only 100 °C.[1] Hence, this system can serve as the basis to develop energy efficient and non-noble metal-based catalyst to produce methanol directly from CO₂ and hydrogen. The availability of sustainable (green) hydrogen, however, is one of the major bottlenecks for realizing such processes. Photocatalytic water splitting is an interesting pathway to low-cost green hydrogen.[2] To enable cost-competitive hydrogen production, solar-to-hydrogen efficiency has to be improved from the current state-of-the-art of 2% to at least 6-10% while the catalyst concentration needs to be reduced at least five-fold.[2] These improvements are challenging because of the high complexity of the water splitting reaction, requiring at least four photons per catalytic cycle. Furthermore, efficiently utilizing visible light has been a major obstacle. A new mechanism for light-driven water splitting was discovered (see Fig. 1),[3] in which only two-photons are required for the reaction. Furthermore, a wide range of wavelengths can be utilized since the two photons are absorbed by two different species. Two-photon water splitting may thus form the foundation to create a new class of efficient and active photocatalysts that enable low-cost green hydrogen production.

Figure 1: Overview of two-photon water splitting mechanism mediated by a molecular ruthenium complex.

2. Dres.-Volker-und-Elke-Münch Award

Award Winners

Rainer Ostermann studierte Chemie und Materialwissenschaften in Aachen und Paris und promovierte 2011 an der JLU Gießen.

Nach einigen Jahren in der Material- und Polymerforschung bei BASF in Ludwigshafen und Lemförde lehrt und forscht er seit 2016 an der Westfälischen Hochschule in Recklinghausen.

Zu seinen Interessen gehören mikro- und nanostrukturierte Materialien, wie Nanofasern, Aerogele und Schäume, sowie übergeordnete Themen wie energieeffiziente Prozesse und Nachhaltigkeit.

Er ist seit dem Studium GDCh-Mitglied und seit 2018 Vorsitzender der OV Marl-Recklinghausen.

Johannes Limberg studierte dual Chemieingenieurwesen an der Hochschule Niederrhein und war währenddessen bei Rüters Novares tätig. Nach seinem Master in Polymerchemie an der Westfälischen Hochschule blieb er dort und ist aktuell in verschiedenen Forschungsprojekten eingebunden. Parallel studiert er derzeit berufsbegleitend BWL und Wirtschaftspychologie an der FOM Hochschule in Essen.

Seine Forschungsschwerpunkte liegen in der Prozessentwicklung und der Aerogelsynthese. Außerdem gilt sein Interesse der Automatisierungstechnik und dem 3D-Druck.

Bereits seit seinem Studium ist er in der GDCh und nun seit mehreren Jahren aktives Vorstandsmitglied des JCF Marl-Recklinghausen.
Felix Leven begann 2012 nach seiner Ausbildung zum CTA ein Chemiestudium an der Westfälischen Hochschule (WHS) in Recklinghausen. Im Anschluss daran absolvierte er das vertiefende Masterstudium mit dem Schwerpunkt Polymerchemie der WHS in Kooperation der Universität Duisburg-Essen (DUE), welches er 2017 mit Auszeichnung beendete. Derzeit ist Felix Leven Wissenschaftlicher Mitarbeiter der Westfälischen Hochschule und promoviert im Bereich der Nanostrukturierung von Polymeren an der DUE. Hierbei stehen energieeffiziente Prozesse zur Herstellung von Dämmmaterialien und Wärmespeicher im Focus der Arbeit.
Energy efficient production of aerogels via liquid-solid-drying

Rainer Ostermann¹, Johannes Limberg¹, Felix Leven¹

¹ Westfälische Hochschule, Technische und Makromolekulare Chemie, 45665 Recklinghausen, Germany

Aerogels are highly porous solids with many interesting properties such as high surface area and low thermal conductivity.¹ Many potential applications have been proposed and demonstrated, for example SiO₂ aerogels as thin, non-flammable and high-performance insulation.²

However, widespread application is still limited due to the high energy consumption and production costs of aerogels. Accordingly, the carbon footprint of aerogels is much higher than of other insulation materials.³

The main challenge in the production of aerogels is to remove the solvent from the synthesis without pore collapse and massive shrinkage.

In this presentation, the state-of-the-art for the production of SiO₂ aerogels (supercritical drying, surface modification, freeze drying) will be briefly reviewed before we demonstrate a new approach of using liquefied camphor to replace the aqueous alcohols initially present in the gel. By carefully controlling the process, water and alcohols can be removed at moderate pressures by distillation before the camphor is solidified inside the pores. A sublimation is then possible with low shrinkage of the aerogel and complete recovery of the camphor whose high freezing point depression and high vapor pressure can be successively exploited to achieve an energy- and cost-efficient process.

Figure 1: Monolithic and granular SiO₂ aerogels produced by liquid-solid-drying

3. FAIR4Chem Award

The NFDI4Chem is part of the German National Research Data Infrastructure (NFDI) and aims both to implement the technical means as well as to foster the cultural change towards modern, digital research data management (RDM) in chemistry. An important set of criteria for good RDM are the FAIR guiding principles, demanding that research data should be Findable, Accessible, Interoperable, and Reusable.

The FAIR4Chem Award is given for published chemistry research datasets that best meet the FAIR principles and thus make a significant contribution to increasing transparency in research and the reuse of scientific knowledge. The prize money is kindly provided by the Fonds der Chemischen Industrie (FCI).

During this session, NFDI4Chem will present the FAIR4Chem Award 2022 to the winners.


Dr. Robert Tobias Giessmann
2013  B.Sc. Chemistry, University of Rostock
2016  M.Sc. Chemistry, University of Marburg
2019  part-time work in Research Data Management at Bayer AG
2020  Ph.D. Biotechnology, Technical University of Berlin
2021  Affiliated as independent researcher at the Institute for Globally Distributed Open Research and Education

Niels Krausch
Studied Biotechnology in Brunswick and Berlin
M.Sc. in Biotechnology from TU Berlin (2018)
International research experience from DTU Lyngby (DK), ETH Zurich (CH) and Imperial College London (UK)
Currently PhD student at TU Berlin, focusing on bioprocess engineering and computer-aided process engineering
“The FAIRest dataset in chemistry” award: UV/Vis spectra acquired while monitoring reaction progress of thymidine phosphorolysis

Niels Krausch 1, Robert T. Giessmann 1,2,3

1 Technische Universität Berlin, Department of Biotechnology, Chair of Bioprocess Engineering, Berlin, Germany
2 Bayer AG, Berlin, Germany
3 Institute for Globally Distributed Open Research and Education (IGDORE)

The FAIR4Chem Award honors researchers in chemistry who publish their research data conforming to the FAIR guiding principles (Findability, Accessibility, Interoperability, and Reusability) and thus make a significant contribution to increasing transparency in research and the reuse of scientific knowledge.

Here we present version 1.0.0 [1] of the dataset we acquired in the course of investigating an enzyme-catalyzed reaction. The investigated pyrimidine-nucleoside phosphorylases have the potential to be used for the efficient and ecological production of modified nucleosides, which have several useful applications in research and pharmacy. In our study, we developed a dynamic model for the production of pentose-1-phosphate, which had to be fitted to the obtained data. [2] We deposited the data into the general-purpose repository Zenodo to make them publicly available and to keep changes trackable. We included a README file about the dataset as a whole, free-text descriptions as well as structured data about the experiments and the deposited files, scans of the paper lab notebook to provide provenance information, the raw instrument output in its proprietary format as well as in open csv format, and finally licensed the data openly with a CC-BY license.

Our dataset can serve as an exemplar of data being considered a first class citizen, instead of mere supplementary material to a narrative. Although our dataset already adheres somewhat well to the FAIR guiding principles, we want to show how much work is still needed to ensure that chemical research data fully follow the ideas of FAIR.

Christopher Keßler

Educational Background

01/2019 - present  | University of Stuttgart, Faculty 4 – Energy-, Process- and Bioengineering PhD Chemical Engineering
“Molecular Simulation of Adsorption and Diffusion in Functionalized Mesoporous Materials“

Specialisation: Natural Sciences, Process Engineering and Fluid Mechanics

Specialisation: Water and Soil Protection, Supply and Waste Disposal


06/2009  | Werratalschule Heringen (Werra)
Higher Education Entrance Qualification

Professional Experience

10/2018 - present  | University of Stuttgart, Institute of Thermodynamics and Thermal Process Engineering, Stuttgart Germany
Scientific Coworker in Collaborative Research Center 1333: “Molecular Heterogeneous Catalysis in Confined Geometries“

01/2018 - 09/2018  | University of Stuttgart, Institute of Combustion and Power Plant Technology, Stuttgart Germany
Scientific Coworker
FAIR Data: Classical Density Functional Theory and Grand Canonical Monte Carlo Simulation

Kessler, C. 1, Eller, J. 1, Gross, J. 1, Hansen, N. 1
1 University of Stuttgart, Institute of Thermodynamics and Thermal Process Engineering, 70569 Stuttgart, Germany
E-mail: kessler@itt.uni-stuttgart.de

Grand Canonical Monte Carlo (GCMC) simulations and classical Density Functional Theory (cDFT) are methods to predict adsorption properties in porous media (e.g., zeolites and covalent organic frameworks). In classical Density Functional Theory based on a PC-SAFT equation of state this is achieved by minimizing the grand potential. GCMC is a stochastic simulation approach relying on atomistic models of adsorbate and adsorbent. We present remarkable agreement between cDFT and GCMC for pure components and mixtures.\(^1\)

![Figure 1: Density plot obtained by cDFT in a covalent organic framework.](image)

To publish the generated data according to FAIR data principles we chose the Data Repository of the University of Stuttgart (DaRUS). Therefore the publication is supported by a dataset denoted by a unique DOI.\(^2\) This leads to findable, accessible, interoperable and reusable but also reproduceable results and additional information. We briefly introduce the novel 3D cDFT method and then focus on the published data.

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Communication 101

How do I introduce myself?

**DOs**
„Moin, I enjoyed your talk very much! My name is ___ by the way, I am coming from the University of ___ / Institute of ___ / …”
(The “Moin” is obligatory, the rest is up to you)

**DON'Ts**
“My name is Bond. James Bond.”
“I’m Batman!”
“The name is Sherlock Holmes and the address is 221B Baker Street.”

Which topics can I use for small talk?

**DOs**
the weather, the lovely University of Hannover, names of your lab equipment, funny group traditions, your most surprising moment at a conference so far, the one (two/three) skill(s) you would like to master

**DON'Ts**
“How long have you been studying up to now?”, “Herri is not a beer!”, pineapple on pizza, “GoT season 8 was fantastic!”, “anyone can speak high German”, “everything except AC/OC/PC is not important”

How do I applaud in the lecture hall?

**DOs**
Knock appreciatively on the desk in front of you

**DON'Ts**

Questions for sponsors:

**DOs**
remember: sponsors are also human!, “What was your career path like?”, “What is it you like most about your job?”

**DON'Ts**
Don’t just walk by! Use the opportunity to get insights into future career options
Your Organizers

Heads of Conference

Janina Carolin Höner
Karen Hindricks
Maxim Gindele

Finance

Karen Hindricks
Simon Homölle
Jan Gerstenberger

Program

Denis Pluta
Maxim Gindele
Jan Flormann
Sina Nolte

Cong Duc Tran
Guest Service

Janina Carolin Höner  Felix Lücke  Elena Krauskopf

Your Organizers
1) **Altieri, Roberto**: Bismuth-based perovskite nanocrystals for photoelectrochemical/photocatalytic applications

2) **Arsenie, Laura**: Bioinspired self-assembled nucleobase polymers: from self-assembly formulation to description of dynamic properties

3) **Asma, Umme**: Kinetic adaptation of the ORAC (Oxygen Radical Absorbance Capacity) assay

4) **Baars, Julian**: Enantioselective Total Synthesis and Structural Revision of Dysiherbol A

5) **Biesterfeld, Leon**: Surface Treatment of Colloidal 2D PbSe NPLs for Emission Enhancement at Telecom Wavelength

6) **Block, Inga**: New adsorbents for the removal of methylene blue and methyl orange from spent coffee

7) **Bordewick, Sven**: Biocatalytic Production of Bioactive Dipeptides

8) **Borodin, Oleg**: Amidinium exchange: expanding the toolbox of dynamic covalent chemistry

9) **Boyce, Hannah**: Ingestible Carbon Monoxide Systems to Treat Inflammation

10) **Brutui, Bogdan-Razvan**: Stable and easily available sulfide surrogates allow a stereoselective activation of alcohols

11) **Caliskanyürek, Volkan**: Electrochemical and spectrophotometric investigations of a bimetallic Re catalyst for electro- and photocatalytic CO2 reduction.

12) **Chachula, Sarah**: Rhodium-Catalyzed Asymmetric Dehydrocoupling: Enantioselective Synthesis of P-Stereogenic Diphosphines and Phosphines via Formation of P-P and P-C Bonds

13) **Chumakovski, Michael**: Synthesis and characterization of (MgaNi1-a)12(CO3)8(OH)6O·x H2O (x=6-8) as a catalyst precursor

14) **Debes, Paul**: Molecular Rectifiers: Diamantane-Fullerene Adducts

15) **Del Rosario, Cathlene**: Synthesis and Characterization of {Nb(pinF)} Complexes

16) **Dilanas, Melina**: Accessing Cationic α-Silylated and α-Germylated Phosphorus Ylides

17) **Ding, Yubin**: The antioxidant compounds from Olea Europaea detected by HPLC-CoulArray-MS

18) **Donnelly, Dan**: Exchange Site Dipole Polarization in Perfluorosulfonated Ionomers: An FTIR Study

19) **Döttinger, Florian**: Exploring the Tunability of Photophysics and Electrochemistry of Cu(I) Photosensitizers with a Library of Electronically Diverse Ligands
20) **Drögemüller, Patrick**: Continuous electroorganic synthesis: a tool for sustainable fine chemical and fuel production

21) **Dzemski, Martin**: Novel bioinspired dinuclear copper TACN/pyrazolate complexes for the activation of dioxygen

22) **Ecke, Alexander**: An Imunosensor for Pharmaceutical Contaminants in Drinking Water

23) **Effnert, Philipp**: Chemie Industrie Forum des JCF Münster

24) **Eisele, Niklas**: Anionic Polymerization Observed by Electrospray-Ionization MS

25) **Elfert, Jonas**: Diastereoselective Intramolecular Mukaiyama Hydration

26) **Escobar, Giamper**: Molten-flux synthesis of plate-like La2NiO4+δ ceramic particles

27) **Fortes, Rebeca**: Water-in-Oil Microemulsions as Soft-Templates for the Self-Assembly of Nanoparticle Clusters into Filament Networks

28) **Fresia, Marvin**: Synthesis of the ABCD ring system of the tremorgenic Janthitrem B from *Penicillium janthinellum*

29) **Friedrichs, Teresa**: Using Immobilized Bio- and Organocatalysts under Continuous Flow Conditions

30) **Gey, Marten**: Anodic generation of a bio-based monomer: On the base-free oxidation of 5-(Hydroxymethyl)-furfural to 2,5-Furandicarboxylic acid

31) **Gindele, Maxim**: Composition and structure of polymer stabilized amorphous calcium carbonates

32) **Graupner, Tim**: Lanthanum-Iron/Nickel-Perovskites as Precursors for Ammonia Decomposition Catalysts

33) **Graw, Nico**: Ducks in space groups! Students grasping 3D-arrangement of symmetry elements with hands-on models

34) **Groß, Jonathan**: Computer-Aided Natural Product Structure Elucidation and Xylochemical Synthesis of Selected Examples

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36) **Häusler, Felix**: Late phase changes of calcium silicate hydrates at 200 °C

37) **Hayes, Justin**: Engineering *E. coli* for gut-on-chip systems to investigate the mechanistic role of H2S in the gut

38) **Heintz, Chris**: Direct Observation of Charged Droplet Signatures within ESI-MS Systems

39) **Hemmersbach, Lars**: Bifunctional Enzyme-Triggered CO-releasing molecules (ET-CORMs) as potential anti-inflammatory medicinal agents

40) **Herrmann, Niklas**: Mechanistic insights by multimodal analysis of a 2D imine COF synthesised at the solid/liquid interface using a two-in-one approach

41) **Hielscher, Maximilian**: Get into Flow: Optimization Strategies for the Anodic Phenol-Phenol Cross-Coupling Reaction in Flow Electrolyzers

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46) Jurado, David: Theoretical studies investigating the mechanism of methanol formation over Cu/ZnO(Al) based catalysts

47) Katzenburg, Felix: JCF Team Sustainability

48) Keppler, Nils: Large refractive index changes in Metal-organic frameworks

49) Sönmez Şafak: Investigation and Antioxidant Properties of Transition-metal dichalcogenides (TMDs) Molybdenum Disulfide-Reduced Graphene Oxide (MoS2/RGO) Nanohybrid Materials

50) Efkan Uzunoglu, Nuri: Performing click reactions of acetylene-substituted phthalocyanine molecules of new kinds of azide-derived insecticide carbamates

51) Selen, Bedirhan: Preparation and Characterization of Molybdenum Disulfide-Reduced Graphene Oxide (MoS2/RGO) Nanomaterials for energy application

52) Keskin, Bahadir: Production of high energy capacity hybrid material containing Reduced Graphene Oxide-Quinoline Zinc Phthalocyanine (rGO/KZnPc)

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54) Klepzig, Lars: Colloidal 2D Nanoplatelets with Tuneable Optical Properties and Efficient Emission from the Visible to the Infrared

55) Köble, Kerstin: The Effect of Thermal Treatment on Carbon Felt Electrodes for Vanadium Redox Flow Batteries

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59) Schilling, Monja: Development of a battery seminar for pupils

60) Schilling, Monja: Distribution of Relaxation Times (DRT) Study on the Positive Half Cell of a Vanadium Redox Flow Battery

61) Kruppa, Katharina: Microstructural and thermoelectric characterization of electrospun Ca3Co4-xO9+δ ceramics from nanofiber mats

62) Kwesiga, George: Applications of Suzuki-Miyaura Coupling/Cross Metathesis Reactions for the Total Synthesis of Prenylated Isoflavone Natural Products

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64) Lübkemann, Franziska: Functional Nanostructures – Bridging the Nano- and the Macroscale
65) **Lüert, Daniel:** Lithium, Sodium, or Potassium precursors? Alkali Metal Based Trimidosulfite Cages as Versatile Precursors for Single-Molecule Magnets

66) **Marschall, Rahel:** CO2 as a tuning parameter for the head group properties of non-ionic E0-surfactants

67) **McLernon, Bailey:** C–H Bond Activation via Series of Small Molecule Manganese Catalysts

68) **Meier, Nils:** Casein as Release System and Blocking Layer for Implant Coatings

69) **Millard, Caroline:** Optimization of a cinnoline scaffold against *Plasmodium falciparum*

70) **Miller, Lukas:** Formylation as key step for new tandem reactions – Towards BODIPY dyes

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Bismuth-based perovskite nanocrystals for photoelectrochemical/photocatalytic applications

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Metal halide perovskites have been widely studied in the fields of optoelectronics, due to their tunable optical and electronic properties. The typical structure, ABX₃, involves a large mono-valent cation (A) like Cesium or Rubidium, a divalent metal cation (B) (where Pb stands out for the optical properties)[1], and a halogen (X).

A relatively novel application involves the use of dimensionally reduced perovskite nanocrystals (PNCs) in photocatalysis and photoelectrochemistry, where H₂ evolution[2] and CO₂ reduction[3] have been already demonstrated.

Due to the Pb toxicity and limited stability to standard environmental conditions, research is now focusing on developing lead-free halide perovskites, like the Bi-based vacancy-ordered perovskites (A₃B₂X₉) or the double perovskites (A₂B(I)B(III)X₆), where Pb²⁺ is replaced by a combination of +1 and +3 cations (such as Ag⁺ and Bi³⁺).

Our work is focusing on the synthesis and characterization of bismuth-based PNCs, where multiple candidates are being studied, such as the Cs₃Bi₂X₉ and Cs₂AgBiX₆ (X=Cl, Br) PNCs, improving their optical properties through metal ion doping. In addition, we aim at preparing hybrid heterostructures with other low-dimensional materials, such as graphene-based materials, carbon nanotubes, 2D carbon nitrides and 2D transition metal dichalcogenides employing covalent and non-covalent hybridization methods, in order to improve stability and activity in photo(electro)catalysis.

Bioinspired self-assembled nucleobase polymers: from self-assembly formulation to description of dynamic properties

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The double helix DNA structures are formed by self-assembly via H-bonds between complementary nucleobases. These structures inspired the synthesis of nucleobase copolymers. Their self-assembly attracted a particular interest as they form various architectures via H-bonds between nucleobases and solvophobic interactions.\cite{1} Nevertheless, self-assembly of nucleobase copolymers in water faces two important challenges: low solubility of the copolymers in water, and difficult control of the dynamics of the system (e.g. kinetics of the association/dissociation of nucleobase-containing polymer chains, strength of H-bonds between nucleobases, etc.).\cite{2} The water insolubility limits the application of these systems in biology. Gaining control over the dynamic of self-assembly opens the possibility to finely tune the size or morphology of the self-assembled structures. Moreover, dynamic structures are sensitive to stimuli of the environment. Since drug delivery or cellular transfection require a fine control over particle size, a better understanding of the dynamics of self-assembled nucleobase polymers is fundamental for their use in biology.

This talk aims at presenting the approaches used to answer these two major issues. Advanced polymer synthesis techniques enabled the preparation of well-defined nucleobase polymethacrylate copolymers. The tuning of the hydrophobic/hydrophilic balance led to original macromolecular structures with high water solubility. SLS/DLS, TEM and ITC characterisations showed that nucleobase density and polymer structure had a strong effect on the size and dynamics of the self-assemblies and governed the formation of self-assembled structures. This work presents original attempts to elucidate the dynamics of hydrosoluble self-assembled nucleobase architectures, and paves the way towards new stimuli responsive biomimetic systems.

\[2\] Arnaud, A.; Bouteiller, L. Isothermat Titration Calorimetry of Supramolecular Polymers. Langmuir 2004, 20, 6858-6863
Kinetic adaptation of the ORAC (Oxygen Radical Absorbance Capacity) assay

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A widespread method for assessing the antioxidant capacity of biological samples is the oxygen radical absorbance capacity (ORAC) assay \[1\]. In this work we would like to extend the usefulness of the ORAC assay, providing further information about the activity of antioxidants to trap peroxyl (R•) radicals \[2\]. For this purpose, we develop a kinetic approach based on the transient signal of the ORAC assay. Through the simulation and fitting of the experimental data with our model, we have been able to express the radical scavenging activity of water-soluble extracts based on an apparent second order rate constant. In details, the ORAC’s kinetic model consists of a system of three reactions \[1\] as follows:

\[ R \rightarrow 2R^+ + N_2 \quad \text{.................} k_i \quad (1) \]
\[ R^+ + FH \rightarrow ROOH + F^+ \quad \text{.................} k_f \quad (2) \]
\[ R^+ + AH \rightarrow ROOH + A^+ \quad \text{.................} k_{\text{inh}} \quad (3) \]

Where R, FH and AH refers to azo-dye radical generator (AAPH), fluorescein, and antioxidant respectively. Similarly, R• corresponds to the peroxyl radicals, while F• and A• are radical products. Based on numerical fitting, the three rate constants, respectively, \( k_i \), \( k_f \) and \( k_{\text{inh}} \) could be determined. The model has been applied first to 13 antioxidant standards, giving rate constants values ranging from 2000 M\(^{-1}\)s\(^{-1}\) to 20000 M\(^{-1}\)s\(^{-1}\). Finally, the model has been applied to measure the antioxidant activity of fruits and vegetables. This study provides a new protocol to determine the antioxidant activity of foods in terms of kinetic values.

Table 1: Determination of total phenolic content, antioxidant activity of different apple pomace using ORAC assay based on kinetic approach

<table>
<thead>
<tr>
<th>Apple variety</th>
<th>Total Phenol Concentration mg GA/g of extract</th>
<th>Kinetic of ORAC assay ( k_{\text{lim}} ) (M(^{-1})s(^{-1}))</th>
<th>( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granny smith</td>
<td>2.585</td>
<td>3000</td>
<td>0.9998</td>
</tr>
<tr>
<td>R201-kissabel</td>
<td>1.295</td>
<td>3500</td>
<td>0.9994</td>
</tr>
<tr>
<td>Pink lady</td>
<td>1.837</td>
<td>3500</td>
<td>0.9993</td>
</tr>
</tbody>
</table>


\[2\] Dorta, E.; Fuentes-Lemus, E.; Aspee, A; Atala, E.; Speisky, H.; Bridi, R; Lissi, E.; Lopez-Alarcon, C. The ORAC index does not reflect the capacity of antioxidants to trap peroxyl radicals. RSC Advances 2015, 5, 39899–39902
Enantioselective Total Synthesis and Structural Revision of Dysiherbol A

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Dysiherbol A, a meroterpene from the marine sponge *Dysidea* sp., has proven to be a strong NF-κB inhibitor, capable of affecting inflammatory, immunological and carcinogenic processes. Dysiherbol A furthermore possesses a novel 6/6/5/6-carbocyclic skeleton exhibiting five continuous stereocenters with three quaternary carbon atoms. [1]

This work describes the total synthesis of the unnatural (−)-enantiomer of dysiherbol A featuring a AuCl₃-catalyzed double cyclization reaction to assemble the tetracyclic carbon skeleton. Interestingly, the synthesis of (−)-dysiherbol A resulted in a revision of both the constitution and absolute configuration of the originally proposed structure, which was secured by X-ray crystallography and CD spectroscopy. [2]

**Scheme 1:** Total synthesis of (−)-dysiherbol A.

**References:**
Surface Treatment of Colloidal 2D PbSe NPLs for Emission Enhancement at Telecom Wavelength

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The direct synthesis of 2D lead chalcogenide (PbX, X = S, Se, Te) based nanocrystals, so-called nanoplatelets (NPLs), yields photoluminescent materials with strong excitonic effects at room temperature and high potential for optoelectronic applications in the telecommunication window. [1]

We report a facile and direct wet chemical approach toward colloidal 2D PbSe NPLs with high emission efficiency. [2] The NPLs exhibit exciton features in the range of 800 – 1000 nm and photoluminescence in the range of 900 - 1500 nm, with the respective positions being precisely tuneable by adjusting the NPLs lateral size via the reaction conditions. Postsynthetic surface treatment with metal and organic halide compounds results in increased photoluminescence quantum yields up to 50 % and strongly pronounced optical features, ascribed to a reduction of non-radiative recombination in the NPLs as well as a stabilization of the band-edge state, by saturation of undercoordinated surface sites.

References:
New adsorbents for the removal of methylene blue and methyl orange from spent coffee

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Water is a highly valuable resource and economically viable. Efficient methods to produce clean water for the growing world population are of ever-increasing importance. Although quite expensive, activated carbon (AC) is commonly used for pollutant removal by adsorption. Spent coffee (SC) is an alternative, abundant and cheap, raw material for AC production and is known for removing of e.g. heavy metals and dyes from water[2].

Figure 1: Synthesis of adsorbents based on spent coffee for dye removal.

This work focuses on the preparation of AC adsorbents from SC utilizing new activation and separation strategies, aiming for a cheap alternative to commercial activated carbon. First, we present ACs activated with CaCO₃ during pyrolysis. The materials were characterized via IR spectroscopy, electron microscopy, X-ray diffraction, and N₂ sorption. The potential to remove dyes from water is evaluated for methylene blue (MB) and methyl orange (MO). All ACs show significant dye removal[1]. Second, we present a new approach using magnetic ACs. These ACs combine the high adsorption capacities with the possibility of magnetic separation from the treated water phase. Although preliminary, initial experiments show that these ACs are quite efficient adsorbents for MB and MO while at the same time they can also be recovered with a simple magnet. All in all, several materials with high adsorption properties are created which may present another promising alternative to commercially available AC.

References:
Biocatalytic Production of Bioactive Dipeptides

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In ancient times, salt was scarce and a valuable trade item due to its flavor-enhancing properties, important physiological functions and for the preservation of food. However, similar to the availability and consumption of sugar, our modern world has gone from scarcity to excess. A high salt intake is correlated with cardiovascular diseases like hypertension and an increased risk for other chronic diseases in predisposed patients. [1] Despite a general awareness in the population about the risks of salt, the actual intake in most western countries of above ten grams far surpasses the maximum recommended amount of five grams by the WHO. A reduced salt content of food is generally not tolerated well due to the importance of salt to the overall taste of food and previous salt substitution strategies tend to introduce irritating off-flavors. Arginyl dipeptides like Arg-Ser, Arg-Ala, and Arg-Gly are salt-taste enhancers and can potentially be used to reduce the salt content of food without introducing these off-flavors. [2] A novel biocatalytic approach for the synthesis of dipeptides is the usage of l-amino acid ligases (LAL), which synthesize them from their respective amino acids. However, the industrial applicability of these enzyme was prevented by the usage of stoichiometric amounts of the expensive cofactor adenosine triphosphate (ATP). To alleviate this problem, a coupled reaction system was created consisting of the LAL RizA from B. subtilis for the specific synthesis of N-arginyl dipeptides and acetate kinase (AckA) from E. coli providing ATP regeneration from acetyl phosphate. [3] In a next step, 21 RizA variants were created by site-directed mutagenesis of eight amino acids in the substrate binding pocket. [4] The combination of RizA variants and AckA enables biocatalytic production of different bioactive arginyl dipeptides while drastically reducing the need for ATP. In the next step towards preparative production, immobilization will be conducted to improve the stability and reusability of the enzyme system. The results obtained from this approach so far will be presented and discussed.

References:
Amidinium exchange: expanding the toolbox of dynamic covalent chemistry

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Due to its adaptive nature, dynamic covalent chemistry (DCvC) has found widespread applications in the discovery and development of new drugs, “smart” materials and molecular sensors.[1] In the toolbox of DCvC comprising more than two dozens of dynamic covalent reactions, one, however, remains underexplored – amidinium exchange (Fig. 1a).[1,2] A unique combination of the net positive charge, the ability to donate hydrogen bonds and dynamic covalent nature makes amidinium ions particularly interesting for the self-assembly of supramolecular architectures. Recently, we showed that amidinium exchange can afford the iconic class of mechanically interlocked compounds – [2]rotaxanes (Fig.1b).[3] To further unleash the potential of the amidinium exchange, we currently explore anion-assisted amidinium metathesis (Fig. 1c) and amidinium exchange in aqueous media. These studies are the very first steps towards applications of amidinium exchange in materials science and biomedical fields.

Figure 1: a) General scheme of the amidinium exchange. b) Key species under dynamic covalent exchange affording the amidinium [2]rotaxanes. c) General scheme of amidinium metathesis.

References:
Ingestible Carbon Monoxide Systems to Treat Inflammation

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Currently it is estimated that six in ten adults in the US have a chronic disease, which range from diabetes to Inflammatory Bowel Disease (IBD) to arthritis. These inflammatory diseases are typically caused by autoimmune responses, where the immune system targets normal cells as foreign matter, resulting in an upregulation of inflammatory cytokines. [1] A new method to treat inflammation includes administering low levels of carbon monoxide (CO), which causes activation of the Heme Oxygenase-1 (HO-1) gene that results in anti-inflammatory productions downstream. Current carbon monoxide treatments are limited by physiologic differences between patients, liabilities of CO tanks in hospitals, and transition metals with toxicity limits from carbon monoxide releasing molecules (CORMs). [2] As such, we developed a carbon monoxide foam that has a high level of carbon monoxide encapsulation about 50 times greater compared to other CO containing systems. [3] Carboxyhemoglobin (CO-Hb), a marker of CO exposure, was measured in mice after dosage of CO through varying foam formulation, as well as the pressure within the loading canister. CO-Hb in mice and in vitro CO release rates were able to be controlled through different formulations. There was a significant increase in CO-Hb in mice, pigs, and rats, as well as effective treatment of Acetaminophen induced acute liver injury (APAP) in mice, dextran sodium sulfate (DSS) induced colitis model in mice, and radiation induced proctitis in rats. Our carbon monoxide system allows for a smaller total volume of treatment, and a controlled rate of gas release and gas encapsulation through formulation changes, as well as targeted delivery to either the rectum or mouth to treat different areas of disease.

References:
Stable and easily available sulfide surrogates allow a stereoselective activation of alcohols

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Sulfur is the 5th most abundant element (after C, H, O and N) in pharmaceuticals and agrochemicals. More than 20% of recently approved drugs contain at least one sulfur atom.[1] Thioethers (or sulfides) are traditionally synthesized via a SN2-type strategy starting from the corresponding alcohol and thiol. However, thiols are notoriously malodorant compounds, susceptible to oxidation and very few are commercially available.

In contrast, isothiouronium salts are odorless, stable and easily accessible compounds, which can function as an activator for the hydroxyl group. Kajigaeshi reported a general one-pot two-step strategy for preparation of thioethers from primary alcohols and isothiouronium salts.[2] We report the use of isothiouronium salts as versatile deoxasulfenylation agents enabling a stereoselective, thiol-free protocol for synthesis of thioethers from alcohols.[3] This method is applied to biologically relevant compounds.

References:
‡ and § authors contributed equally
Electrochemical and spectroelectrochemical investigations of a bimetallic Re catalyst for electro- and photocatalytic CO₂ reduction.

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Global warming is one of the greatest challenges currently facing society and science. The efficient production of solar fuels is a promising option to address this issue. Therefore, suitable catalysts for the photo- and electrocatalytic reduction of CO₂ are required. In this respect, bimetallic Re catalysts were investigated and an unexpected reaction mechanism has been found.[1,2,3] The two Re-centres form dimers after reduction of the catalyst.[1,2,3] Similar to these catalysts a novel Re-based catalyst, which bridges two (bpy)Re(CO)₃Cl moieties via an organic backbone is studied (see figure). As demonstrated by electrochemical and spectroelectrochemical studies the given structure can also undergo Re-Re-dimerization. A short outlook of future experiments is given.

References:
Rhodium-Catalyzed Asymmetric Dehydrocoupling: Enantioselective Synthesis of P-Stereogenic Diphosphines and Phosphines via Formation of P-P and P-C Bonds

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P-stereogenic phosphines are valuable ligands for metal complexes used in asymmetric catalysis. We investigated new routes to these compounds via metal-catalyzed asymmetric dehydrocoupling of phosphines bearing P–H groups, leading to P–P or P–C bond formation. Rh-catalyzed enantioselective dehydrocoupling of the bis(secondary phosphine) PhHP(CH₂)₃PHP gave the C₂-diphospholane PhP(CH₂)₃PPh. The meso-diphospholane was observed as a catalytic intermediate and identified by trapping with the metal fragments W(CO)₅, AuCl, and [Pd((S)-C₆H₄CHMeNMe₂)Cl]₂ and ³¹P{¹H} NMR spectroscopy. Rh- or Co-catalyzed dehydrocoupling of the bulky primary or secondary phosphines PHRMes* (R = H, Ph; Mes* = 2,4,6-(t-Bu)₃C₆H₂) resulted in activation of a t-butyl C–H bond and P–C bond formation to yield cyclophosphinated products. We are now studying the diastereoselectivity and enantioselectivity of these catalytic transformations.

Scheme 1: a) Conversion of rac/meso mixture of bis(secondary phosphine) to an enantioenriched C₂- phospholane either directly or via a meso-phospholane intermediate. b) Rh- or Co-catalyzed dehydrocoupling of PHRMes* (Mes* = 2,4,6-(t-Bu)₃C₆H₂) to give the cyclophosphinated product.
Synthesis and characterization of \((\text{Mg}_{x}\text{Ni}_{1-x})_{12}(\text{CO}_3)_8(\text{OH})_6\text{O} \cdot x \text{H}_2\text{O}\) \((x=6-8)\) as a catalyst precursor

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The isothermal coprecipitation at constant pH of a 1 M \(\text{Mg(NO}_3\text{)}_2/\text{Ni(NO}_3\text{)}_2\) solution with 1.6 M \(\text{Na}_2\text{CO}_3\) solution at low temperatures and pH = 9 yielded a nanocrystalline precursor with the sum formula of \((\text{Mg}_{x}\text{Ni}_{1-x})_{12}(\text{CO}_3)_8(\text{OH})_6\text{O} \cdot x \text{H}_2\text{O}\). The optimal ageing temperature under hydrothermal conditions was found to be 100 °C. The calcination temperature to obtain a \((\text{Ni,Mg})\text{O}\) mixed oxide is dependent on the \(\text{Mg}^{2+}\) content in the sample. It was determined to be between 290 and 370 °C with higher temperatures correlating to a higher \(\text{Mg}^{2+}\) content in the sample. The biggest surface area was reported for the calcined \((\text{Mg}_{0.3}\text{Ni}_{0.7})_{12}(\text{CO}_3)_8(\text{OH})_6\text{O} \cdot x \text{H}_2\text{O}\) precursor at 184 m²g⁻¹. It was observed that with a lower content of \(\text{Mg}^{2+}\)-ions a drastic change in morphology occurred. The \(\text{Ni}_{12}(\text{CO}_3)_8(\text{OH})_6\text{O} \cdot x \text{H}_2\text{O}\) precursor had an undefined morphology before the calcination and formed spheres with a diameter of approx. 22 nm after calcination. This effect was not observed for the \((\text{Mg}_{0.3}\text{Ni}_{0.7})_{12}(\text{CO}_3)_8(\text{OH})_6\text{O} \cdot x \text{H}_2\text{O}\) precursor and no change in morphology was seen after calcination. The precursors resemble mesoporous solids with typical H3 and H2(a) hysteresis loops. Two hypotheses were formed regarding the crystallization process using \textit{in situ} IR-spectroscopy and \textit{ex situ} ICP-AES. The first proposes a substitution reaction for the \(\text{Ni}^{2+}\) with \(\text{Mg}^{2+}\) at hydrothermal conditions. The second suggests a gradient like crystallization regarding the incorporation of \(\text{Mg}^{2+}\) ions into the crystal structure.
Molecular Rectifiers: Diamantane-Fullerene Adducts

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Molecular rectifiers convert alternating current into direct current and consist of a donor and an acceptor separated by a sigma-bound tunnel bridge. A prerequisite for a rectifier is the restricted movement of electrons only in one direction. Similar to a solid state p-n junction, organic rectifiers possess the same properties.[1]

The molecular rectifier of Randel et. al. is synthesized via a Diels-Alder reaction to a diamantane-fullerene adduct.[2] Due to the occurrence of the retro-Diels-Alder reaction back to the starting materials, the goal was to synthesize a similar diamantane-fullerene adduct via the Prato-Maggini reaction to avoid the back reaction.[3]

The Prato-Maggini reaction yields in a pyrrolidine ring between the diamantane and the fullerene which should act as a sigma-bound tunnel bridge. (see Figure 1) 1D and 2D NMR together with MALDI-TOF and TGA was used to verify the compound. Thermogravimetric analysis furthermore yields in a temperature of 227 °C at which the compound starts to decompose. This leads to the assumption that the compound is more stable than the Diels-Alder adduct.[3]

To determine the rectifier properties of the synthesized adduct, scanning tunnelling spectroscopy will be carried out in the future. The challenge to overcome is to obtain a layer of the fullerene-diamantane adduct on a gold surface to measure its properties. During the measurement, current in only one direction should be detected to confirm the adduct as a molecular rectifier and promising stable alternative for the Diels-Alder adduct from Randel et. al.[3]

Figure 1: As a potential molecular rectifier the pyrrolidine adduct via the Prato-Maggini reaction is depicted as a further stage of the Diels-Alder adduct from Randel et. al.[2,3]

References:
Synthesis and Characterization of \{\text{Nb}(\text{pin}^\text{F})\}_2\} Complexes

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Over the past 15 years, the Doerrer group has synthesized a variety of d-block metal and p-block metalloid complexes with fluorinated alkoxide ligands, such as OArF (OC$_6$F$_5$)-, perfluorotributoxide (OC$_4$F$_9$)-, and perfluoropinacolate, denoted as pin$^\text{F}$, (OC(CF$_3$)$_2$)$_2$.$^1$ These ligands are strategic for catalysis because they lack C–H bonds that can render a catalyst sensitive to oxidation, additionally important for isolating C–H bond activation to targeted substrates. A series of Nb(V) complexes with fluorinated alkoxide ligands are being studied for dehydration chemistry, analogous to Nb$_2$O$_5$ (Figure 1).$^2$

Figure 1: Proposed reactivity of 4-coordinate Nb(V) complexes, \{Nb(pin$^\text{F}$)$_2\}_2\}, transforming target substrates with water in hydration and dehydration reactions.

References:


Accessing Cationic $\alpha$-Silylated and $\alpha$-Germlyated Phosphorus Ylides

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Frustrated Lewis pairs (FLPs) have been studied in great detail in recent years. [1] Most commonly, a combination of a sterically hindered Lewis acid and a Lewis base are applied, leading to "frustration" by preventing Lewis acid/base adduct formation. Moreover, so-called hidden FLPs were reported, [2] which seem to be not frustrated at first glance, as a bond between acidic and basic site is formed. However, ring strain or steric strain can still enable dissociation of the acidic and basic site and promote the reaction towards small molecules such as H₂, CO or CO₂. Our group recently reported on $\alpha$-borylated phosphorus ylides ($\alpha$-BCPs) that readily reacted with NH₃, CO, CO₂ and other heteroallenes. [3, 4] The synthesis and full characterization of $\alpha$-silylated ($\alpha$-SiCPs) and $\alpha$-germylated ($\alpha$-GeCPs) phosphorus ylides bearing one chloride substituent $R_3PC(R^1)E(Cl)R^2$ (R = Ph; R¹ = Me, Et, Ph; R² = Me, Et, iPr, Mes; E = Si, Ge) is presented. The molecular structures were determined by X-ray diffraction studies. The title compounds were applied in halide abstraction studies in order to access cationic species. Carrying out the halide abstraction reaction in the sterically demanding ether $i$Pr₂O afforded the protonated $\alpha$-SiCP $[Ph_3PCH(Et)Si(Cl)Pr_2][B(C_6F_5)_4]$ by sodium mediated basic ether decomposition, whereas successfully synthesized $[Ph_3PC(Et)SiPr_2][B(C_6F_5)_4]$ readily cleaves the F–C bond in fluorobenzene. Thus, the ambiphilic character of $\alpha$-SiCPs is clearly demonstrated. The less reactive germanium analogue $[Ph_3PC(Me)GeMes_2][B(3,5-(CF_3)_2C_6H_3)_4]$ was fully characterized including X-ray diffraction analysis. Structural parameters indicate a strong $\text{C}_{\text{ylide}}$–Ge interaction with high double bond character, and consequently the C–E (E = Si, Ge) bonds were analyzed with NBO and AIM methods.

References:
The officinal herb Olea Europaea is widely applied in food and pharmaceutical industries due to the high antioxidant capacity. [1] However, its antioxidant compound profile was remaining unknown. This work demonstrates the use of the coulometric array detector (CoulArray) coupled to liquid chromatography, diode array detector (DAD) and mass spectrometry (MS) for screening of antioxidants in Olea europaea. The CoulArray detector can assess the potential of molecules to oxidize and determine their electrochemical behaviour based on multiple channels poised at different potentials. [2] In this research, the Coularray was applied to select the main antioxidant compounds from Olea europaea with charge transfer ability higher than 5 μC. Meanwhile, the DAD was applied to first screen all the bioactive compounds from the extracts. Finally, the MS was used to identify all the selected compounds. From the result, the oleuropein was determined as the bioactive compound with the highest antioxidant capacity, followed by hydroxytyrosol. The transferred charge accumulated from the multichannel was used to quantify the main antioxidant compounds with the application of the Faraday's law. [3] The content of oleuropein and hydroxytyrosol was 7.36 and 3.44 mg per gram of dried herb, respectively. A hydrodynamic voltammogram, which shows the electrochemical behaviour of Olea europaea, was drawn and compared with other officinal herbs and antioxidant standards to further analyse the antioxidant activity of Olea europaea. In conclusion, the applied triple detector system presented a swift way for analysis of antioxidant compounds in Olea europaea and can be further applied to different natural herbs.

References:
Exchange Site Dipole Polarization in Perflurosulfonated Ionomers: An FTIR Study

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Perflurosulfonated ionomer (PFSI) membranes are well recognized among the electrochemical community as the canonical solid electrolyte and separator in energy-storage and -conversion devices (Figure 1). Metal-ion exchanged PFSIs (PFSI-M) are additionally employed in ion-polymer metal composites to achieve biomimetic actuation. Tuning the conditions that affect the performance of ionomers require a thorough understanding of their dynamic structure in their normal operating environments (operando). Fourier-Transform infrared spectroscopy (FT-IR) is commonly used for nondestructive analysis of complex molecular architectures because it requires little to no modification of the sample during analysis. We have used FTIR to validate the influence of solvation sphere waters to the vibrational spectra of group-I cation exchanged PFSI-M (i.e., Li, Na, K, Rb and Cs)

PFSI-M retain three-fold local exchange site symmetry (C3V) at all states of hydration. In the totally dehydrated (dry) state, exchange site (sulfonate, SO3-) band frequencies are observed to monotonically decrease with cation principal quantum number, n. This spectral down-shift suggests that the sulfonate dipole moment is less sensitive to softer cations (weaker polarizing strength). Highly polarizing cations (e.g. Li+, Na+) more effectively withdraw electron density from sulfonate sites, causing S-O bonds to strengthen and vibrate with higher frequency. Upon hydration, the exchange site band frequencies are not monotonic with n. Cation solvation is enhanced with increasing humidity and their proximity to exchange sites are reduced. We attribute the non-monotonic behavior to the impact of solvation sphere waters on non-occupied d-orbitals of exchange cations.

Figure 1. General perflurosulfonated ionomer or ion-exchange polymer (PFSI) structure in the anionic form.
Exploring the Tunability of Photophysics and Electrochemistry of Cu(I) Photosensitizers with a Library of Electronically Diverse Ligands

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Heteroleptic diimine–diphosphine Cu(I) complexes of the type \([P^P]Cu[N^N]\)⁺ (see below) are a viable alternative to noble-metal containing photosensitizers like \([Ru(bpy)₃]^{2⁺}\) or \([Ir(ppy)₃]\). A major drawback of such Cu(I) systems, however, is their limited ability to efficiently absorb visible (sun)light. [1]

To tackle this issue, several studies already dealt with the introduction of fused aromatic rings in 5,6-position at the phenanthroline moiety (see below). [2,3,4]

As a promising alternative we recently tested the introduction of different alkynyl-based (blue) and phenyl-based (green) substituents in 5,6-position. Consequently, a systematic series of 11 novel Cu(I) complexes was prepared and thoroughly investigated by different photo- and electrochemical methods. [5]

In consequence, distinct differences between both ligand classes were revealed. [5] Also a correlation between luminescence quantum yield and the steric demand of the substituents could be deduced. Furthermore, emission lifetimes are strongly dependent on the electronic characteristics of the substituents and more than doubled for some examples, demonstrating the tunability of these diimine based photosensitizers. [5]

References:
Continuous electroorganic synthesis: a tool for sustainable fine chemical and fuel production

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The progressive abandonment of fossil raw materials and the associated conversion of the production economy and mobility towards renewable resources are changing the basis on which the existing chemical industry was developed. This in part necessitates new processes, which on the one hand have to do justice to the changed properties of the raw material and on the other hand to society’s demands for sustainability. As a suitable means of combining both, electroorganic reactions are to be investigated and made industrially usable by carrying them out in flow reactors. These are generally easier to scale up and advantageous for large production quantities. [1] For this purpose, the conversions of a suitable model substance are considered. Using the reduction of the potential platform chemical levulinic acid and the kolbe electrolysis of the resulting product valeric acid to n-octane, as a potential biofuel, the transferability of the reactions from the standard laboratory batch reactors to a continuously operated flow reactor will be examined, and the associated advantages and disadvantages evaluated.

Figure 1: Scheme of an a) electrochemical flow reactor and b) H-cell type batch reactor

References:
Novel bioinspired dinuclear copper TACN/pyrazolate complexes for the activation of dioxygen

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The activation of small molecules like O2 by bioinspired copper model complexes is of great interest in bioinorganic chemistry research. Especially, the isolation and investigation of the primary reactive dioxygen adducts (peroxido, superoxido, hydroperoxido species) have helped to gain valuable insight into the mechanism of dioxygen activation at the active sites of copper containing enzymes. Moreover, these species are key intermediates in catalytic substrate oxygenation and oxidation reactions.[1] In the last years, we have been investigating highly preorganized dinuclear copper complexes which are based on symmetrical and asymmetrical pyrazolate/TACN hybrid ligands with bulky substituents. These allowed to isolate important reactive intermediates in the shielded bimetallic cleft.[2-5] Now we introduce two modified ligand scaffolds 1 and 2 with the intend to increase reactivity via reducing steric hindrance at the dinuclear core of the corresponding copper complexes. The resulting new dicopper/O2 intermediates, their syntheses and properties will be presented.

References:

Figure 1: Molecular structures of the novel pyrazolate/TACN hybrid ligand scaffolds 1 and 2.
An Immunosensor for Pharmaceutical Contaminants in Drinking Water

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Contamination of drinking water with pharmaceuticals is an emerging problem and represents a potential threat to human health that demands for fast and reliable detection techniques. To overcome time-consuming and expensive mass spectrometry-based methods that are commonly used to detect pharmaceuticals in water, immunochemical techniques appear promising as they enable fast and cost-effective point-of-care analyses. Such competitive immunoassays require an analyte-specific antibody and a competitor (mimicking the analyte) one of which bearing a quantifiable label (here: the enzyme horseradish peroxidase).

In this context, we are developing an immunosensor based on magnetic beads to detect two relevant contaminants of water: the nonsteroidal anti-inflammatory drug diclofenac and the broad-spectrum antibiotic amoxicillin. The magnetic bead-based immunoassays alone represent a timesaving and more versatile alternative to the conventional ELISA (enzyme-linked immunosorbent assay).[1] Furthermore, they allow for implementation of the detection unit into an online setup for on-site analysis. Together with an electrochemical readout module, this will enable the automated online drinking water analysis for pharmaceutical contamination directly in the water supply pipes (Figure 1).

![Figure 1: Application of the integrated immunosensor on a water supply pipe.](image-url)

References:
Chemie Industrie Forum des JCF Münster

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The Chemie Industrie Forum (ChInFo) is the largest regular event organized by the JCF Münster. To start the fair, the company representatives introduce themselves at a small breakfast. Next there will be animated company presentations where the companies will introduce themselves in front of an auditorium. For refreshment, a lunch buffet will be offered between the presentations, which all participants can enjoy. Companies can present themselves like at a job fair or conference event with a lecture or a poster. Possible career opportunities are presented. Through the direct contact between company representatives and students, a personal exchange can take place. Companies like ASI, BASF, Altana, Eurofins, Thescon, P&G, Merck and Biesterfeld have already happily participated in the event. At the end of the participants will meet in a get-together for a relaxed end with some coffee and cake. The ChInFo is not only the biggest event of the JCF. Every year, the Bachelor, Master and PhD students, as well as the professors, enjoy the opportunity to get in touch with the industry and to establish new relationships. Due to the variety of industry subfields, all interests can be covered and there is something for everyone.

It provides a good transition for students from academic life to industry and shows you the many possibilities for your future. You can also get a taste of what is to come in an internship, which is welcomed by the students. It is an event that you should have visited no matter if you are a Bachelor or a Posdoc.
Among polymerization reactions, anionic mechanisms are most commonly associated with living polymerization conditions. Usually the active species are highly reactive, resulting in fast propagation but also an extreme sensitivity to impurities. The Penelle working group have investigated substituted cyclopropanes as monomers, whose ring-opened product forms stable anions and thus show reduced propagation rate and sensitivity.[1] Using one such monomer, we have applied electrospray-ionization mass spectrometry to observe the growing chains during the first few steps of propagation directly (Fig. 1).

In order to mitigate mass bias often encountered when using ESI-MS, the instrument settings were changed successively for the various chain lengths. The resulting mean molecular masses were in agreement with those determined by NMR.

Using the mass distribution, we have simulated the reaction kinetics assuming irreversible, second order reactivity.[2] The optimized rate constants begin at 0.25 M$^{-1}$s$^{-1}$ for the initiation, then gradually decrease by a factor of ca. 100 over the first 4 propagation steps, after which the reaction rate remains unchanged.

The mass spectra also gave insight into a termination side-reaction that may impact the living character of the polymerization, though it occurs sufficiently slow as to be negligible during regular reaction conditions.

References:
Diastereoselective Intramolecular Mukaiyama Hydration

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Mukaiyama hydrations using Oxygen as an oxidant have become a staple method for the Markovnikov hydration of Alkenes. The high chemoselectivity and mild conditions are ideal for late-stage functionalizations, but the usage of oxygen bears some problems. Air sensitive substrates can’t be used, the reaction is diffusion limited and the use of oxygen is a safety risk as Hydrogen is also a side product of the reaction mixture. Mukaiyama hydrations also typically have barely any diastereoselectivity. [1]

Our group published a paper in 2020 where Nitroarenes have been used as an oxidant, circumventing oxygen while giving high yields and improving the diastereoselectivity up to dr>20:1 for some tertiary alkenes. [2]

Building upon this we have been working on an intramolecular variant, with the goal of improving diastereoselectivity. By installing a Nitroarene we can carry out the Hydration in high diastereoselectivity and remove it again afterwards. We have found that sulfonamides are ideal for the intramolecular reaction and easy to synthesize from allylic and homoallylic amines, though the removal of the group afterwards proved to be a challenge. The reaction proceeds much faster than other protocols and only one diastereoisomer is observed. Other Methods did not work for these substrates.

![Figure 1: (a) General procedure for the intramolecular Mukaiyama hydration (b) proposed mechanism.](image)

References:
Molten-flux synthesis of plate-like La$_2$NiO$_{4+\delta}$ ceramic particles

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Due to its high chemical stability in CO$_2$ atmosphere and its anisotropic crystal structure, the Ruddlesden-Popper phase La$_2$NiO$_{4+\delta}$ has attracted considerable attention in the research area of oxygen-transporting membranes. To produce ceramic La$_2$NiO$_{4+\delta}$ membranes with asymmetric microstructure, the templated grain growth process can be used. For this, anisotropic plate-shaped La$_2$NiO$_{4+\delta}$ template particles are required. Since the morphology of the templates plays a crucial role in the preparation of textured membranes, they can be obtained by molten-flux synthesis. This method enables the production of powders with anisotropic particles at lower temperatures. Here, we report on the synthesis of plate-like La$_2$NiO$_{4+\delta}$ particles from a NaOH melt. For this purpose, the products of a sol-gel process from the nitrate precursors at 500 °C were used as reactants. [1] Using X-ray diffraction, the sol-gel products were identified as a mixture of La$_2$CO$_5$ and NiO. The existence of NiO was also confirmed by transmission electron microscopy in combination with electron energy-loss spectroscopy. The reactants were then mixed with NaOH and additional water in crucibles and heated to 400 °C for 6-18 hours. The chemical reactions in the air during the molten-flux synthesis were examined by thermogravimetric analysis. X-ray diffraction patterns indicated a K$_2$NiF$_4$-type tetragonal structure with I4/mmm space group for the product powder. Scanning electron microscopy showed plate-like La$_2$NiO$_{4+\delta}$ particles with lateral sizes of 1-30 µm and varying aspect ratios while energy-dispersive X-ray spectroscopy revealed a homogeneous distribution of lanthanum and nickel in the powder. The influence of reaction parameters on size and morphology of the La$_2$NiO$_{4+\delta}$ particles was systematically investigated.

References:
Water-in-Oil Microemulsions as Soft-Templates for the Self-Assembly of Nanoparticle Clusters into Filament Networks

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Self-Assembly of nanoparticles into ordered structures constitutes a promising bottom-up approach to larger-scale nanomaterial-based devices. For this purpose, soft-templates of self-organized dispersions containing nanoparticles and surface-active agents can mediate the formation of self-assembled nanostructures upon solvent evaporation.

In our research, reverse, water-in-oil microemulsions were formulated by using Aerosol-OT (dioctyl sodium sulfosuccinate, AOT) as surfactant. Oleyl-capped nanoparticles can be incorporated in the continuous oil phase, while polyethylenimine-stabilized nanoparticles where confined in the dispersed water droplets. Thin films of ordered nanoparticles as filament-like networks were formed after drop casting and solvent evaporation of the upper water-in-oil phase from a biphasic Winsor type II system. [1] More detailed studies proved an initial nanoparticle clustering and a microemulsion droplet elongation, which should guide the subsequent formation of the final filament-like network of interconnected nanoparticle filaments over a surface (Scheme 1). [2]

Thus, a new application of microemulsions as soft-templates is shown, which enables the hierarchical ordering of spherical nanoparticles into thin films of anisotropic nanostructures, extended to several µm over a surface. [1,2] This method might contribute to the development of surface-assembled nanomaterials on larger scale.

Scheme 1: Proposed steps for the self-assembly of nanoparticles into filament-network films.

References:
Synthesis of the ABCD ring system of the tremorgenic Janthitrem B from *Penicillium janthinellum*

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The tremorgenic mycotoxins janthitrems A – G (B: 1) from *Penicillium janthinellum* cause tremors in mice and exhibit anti-insect activity. [1,2] Their biological activity and intriguing structure makes the janthitrems interesting targets for total synthesis.

Our first approach entailed the synthesis of 5,6-disubstituted indolines, inspired by the plausible biosynthesis of the western hemisphere from a 5,6-diprenylated indole species. However, the envisioned gold-catalyzed cyclization failed for all substrates. We wondered, whether the Lewis acid promoted cyclization of an ortho-dihydropyranyl benzaldehyde by Magnus and coworkers [3] could be applied for the first time to indoline-based systems 2. Gratifyingly, the reaction proceeded smoothly and provided tetracyclic diene 3 in good yield (48%).

![Scheme 1: Structures of janthitrem B (1), aldehyde 2 and tetracyclic diene 3.](image)

Already, pyranocyclopentaindole 3 represents the western hemisphere of the natural product JBIR-137 [4] and hydroboration/oxidation thereof afforded the western hemisphere of janthitrem B (1). Additionally, the western hemisphere of shearinine G was prepared.

References:


Using Immobilized Bio- and Organocatalysts under Continuous Flow Conditions

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Flow chemistry is a rapidly growing research field with a multitude of application established. While the combined use of supported bio- and organocatalysts under continuous flow conditions might lead to a sustainable and efficient production of enantiomerically enriched compounds, their successful implementation is still underrepresented. [1]

We are working on the immobilization of different bio- and organocatalysts in order to combine them in a flexible manner. Different factors need to be considered for obtaining suitable packed bed reactors. This includes the choice of the right immobilization strategy, the matrix material or the stability in organic solvents. [2] Additionally, the well-known rapid deactivation of heterologous organocatalysts in flow mode is a challenge that must be met. [3] We will present a modular approach and demonstrate how we circumvented some of the major limitations also compared to the batch mode processes, especially in onepot-synthesis. Precise reaction control, solvent-change and automation opens up possibilities for new reactions and can lead to improved catalyst reactivity and efficiency. [4]

Figure 1: Modular catalyst-system in continuous flow mode (a) with different mixers (b) and a toolbox of immobilized catalyst in packed-bed reactors (c).

References:
Anodic generation of a bio-based monomer: On the base-free oxidation of 5-(Hydroxymethyl)-furfural to 2,5-Furandicarboxylic acid

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In the last few years, biomass-derived furan components like 5-(Hydroxymethyl)-furfural (HMF) have gained a lot of attention as platform chemicals for the synthesis of value-added products which can be applied in the polymer industry, for instance. Therefore, the oxidation of HMF to 2,5-Furandicarboxylic acid (FDCA) is currently of great interest, since the product is an attractive substitute for the PET monomer terephthalic acid. [1] Among the various possibilities to perform this reaction, aqueous electrochemistry is a sustainable method which eliminates the need of stoichiometric chemical oxidants or the use of O2 at high pressures. Additionally, the anodic oxidation of an aqueous HMF solution can be combined with the reduction of water to gain hydrogen gas as a second product of value (Scheme 1). [2]

It has been shown in numerous studies that anodic oxidation can be used to generate FDCA from alkaline HMF solutions in high yields. However, the instability of the reactant at high pH values and the need to lower pH in order to separate the product by protonation are problems that make these methods unfit for industrial upscaling. [2] Hence, base-free methods are needed. Accordingly, experiments in acidic and pH neutral solutions with varying reaction conditions (different electrode materials, use of redox catalysts etc.) have been made in the context of this study.

Scheme 1: Combined electrochemical oxidation of HMF to FDCA and reduction of water to hydrogen.

References:
Composition and structure of polymer stabilized amorphous calcium carbonates

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The mechanisms by which organisms control the structure and stability of amorphous and crystalline calcium carbonate species are not fully understood.[1] It has been shown that proteins with aspartic- and glutamic acid rich sequences are associated with calcium carbonate formation in biomineralization.[2] Surprisingly, although the chemical structures of glutamic acid and aspartic acid are similar, they are usually associated with different calcium carbonate species. For example, in corals, glutamic acid rich proteins (CARP2) are upregulated during amorphous calcium carbonate (ACC) formation, and aspartic acid rich proteins (CARP1, 3 and 4) are associated with the formation of crystalline calcium carbonates.[3] The effect of aspartic- and glutamic acid rich proteins on CaCO₃ mineralization can also be seen in in vitro studies on calcium carbonate crystallization, where they usually show strong stabilizing effects on liquid- and amorphous mineral precursor phases.[4,5]

We systematically investigate the effect of poly(aspartic acid) and poly(glutamic acid) on the calcium carbonate crystallization using in situ and ex situ characterization techniques to gain insights into additive controlled crystallization processes. Potentiometric titration allows to quantitatively access the amount of bound calcium and bound carbonates in the prenucleation regime,[6] suggesting the polymer additives facilitate bicarbonate binding in prenucleation species. This is supported by thermogravimetric analysis coupled with mass spectrometry and FTIR spectroscopy (TGA-FTIR-MS) on the isolated polymer stabilized ACCs.

References:
Lanthanum-Iron/Nickel-Perovskites as Precursors for Ammonia Decomposition Catalysts

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A constant pH coprecipitation method was used to synthesize amorphous precursor materials of the composition La(Fe₁₋ₓNiₓ)(OH)ₓ(CO₃)₂ with 0 ≤ x ≤ 1. The samples were afterwards calcined at 800 °C for 3 h, to obtain La(Fe₁₋ₓNiₓ)O₃ perovskite materials. For values up to x = 0.4, samples with a phase pure orthorhombic LaFeO₃ structure were obtained. For values larger than x = 0.6, the hexagonal structure of LaNiO₃ was obtained, with secondary phases of La(OH)₃ and NiO. Changes in the unit cell size were observed for the introduction of nickel into the orthorhombic cell by a shift of the PXRD reflections. The experimental iron to nickel ratio was confirmed to be close to the theoretical values by ICP-OES. The particle size of calcined samples decreases with higher x values. Sorption measurements showed a strong decrease in total pore volume and surface area during calcination, but no clear trend was observed for different x values.
Ducks in space groups! Students grasping 3D-arrangement of symmetry elements with hands-on models

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Symmetry considerations are vital in chemistry and even more so in crystallography. Learning and teaching about molecular symmetry naturally requires spatial imagination. To develop and refine this, models and model kits are of outmost importance and are readily available for a broad range of purposes. However, the description of crystalline matter from a crystallographer’s point of view necessitates translational symmetry to be considered. From our teaching experience this introduction of translational symmetry components is difficult and something students struggle with. These difficulties culminate when it comes to the assembly of symmetry elements to give space groups.

We herein present large scale (i.e. typically 50 x 50 x 50 cm), physical 3D models of complete space groups (Fig. 1) to promote student’s spatial imagination and to help understanding the construction of space groups by symmetry elements. The models were designed and built to fulfil three basic requirements: (1) to be accurate space group representations containing the symmetry symbols, (2) to visually resemble the conventional 2D space group notation if viewed along the respective crystallographic axis and, (3) to allow students to assemble asymmetric units within the unit cell by themselves.

Grabbing fosters grasping!

References:
Computer-Aided Natural Product Structure Elucidation and Xylochemical Synthesis of Selected Examples

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A current approach in drug discovery is the identification of pharmacologically active compounds from natural sources (plants, roots, sponges, fungi, etc.), some of which have been known for their biological activity for centuries. An important part of this workflow is the elucidation of the correct structure of unknown, recently isolated natural products.

By combining spectroscopic methods with quantum mechanical calculations on the DFT-level, we were able to predict and confirm the exact chemical structure of several small molecules of such examples using NMR- and CD-spectroscopy as well as polarimetry. [1]

Figure 1: A) Structure elucidation using a combination of spectroscopic techniques and DFT.
B) The synthesis of 2-Aminophenoxazinone natural products via a novel xylochemical approach. [3]

Today's starting materials for organic chemistry and in particular for the total synthesis of natural products are commonly derived from petrochemical resources. Due to the geological process of kerogenesis being involved in their formation, petrochemicals are poorly functionalized so that lengthy procedures are required to reintroduce heteroatoms and other chemical functionalities. [2]

Herein, we present the use of wood-derived starting materials, the so-called xylochemicals which offer a higher degree of functionalization such as heteroatom substituents, [3] for the synthesis of complex molecules in the form of 2-amino-phenoxazinone-type natural products.

In addition to the use of eco-friendly starting materials, we developed a new eco-friendly oxidative coupling reaction to construct the 2-aminophenoxazinone nucleus. [4]

References:
The amide bond is amongst the most prevalent structural motifs found in natural products, it represents the key connection in proteins and is encountered in high value products like polymers or pharmaceuticals. [1,2] Although the importance of this moiety is well recognized, amide bond formation remains a contemporary challenge in organic chemistry as highlighted by the ACS Green Chemistry Institute Pharmaceutical Roundtable (ACS GCIPR), who called out for “amide bond formation avoiding poor atom economy”. [3] Well-established methods to forge amide bonds typically rely on pre-activation of carboxylic acids or by the utilization of a coupling reagent like carbodiimides or uronium salts. [2,4] Alternatively, redox approaches starting from carboxylic acid surrogates like alcohols or aldehydes have been reported. [5] Unsurprisingly, a recent growing interest in electrochemical transformations, has led to the use of electric current as clean oxidant in such reactions, however, methods for direct condensation of a carboxylic acid and amine remain scarce. [6]

We developed a mild and robust electrochemical methodology based on the Garegg-Samuelsson reaction to condensate carboxylic acids and amines to form amide bonds.

**Figure 1:** a) general procedure for electrochemical amide bond formation using PPh₃, b) three selected examples of the substrate scope.
Late phase changes of calcium silicate hydrates at 200 °C

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The system Ca(OH)2-SiO2-H2O was the object of numerous investigations, regarding its role as the binder phase system for ordinary Portland cement (OPC). Especially the application of OPC in radioactive waste repositories requires a reliable understanding of phase formation within varying conditions (e.g. up to 200 °C in salt repositories [1]) over a long period. Hydrothermal syntheses in literature are often executed over hours to at most a few days not allowing reliable predictions concerning long-term safety. [2,3,4]

Figure 1: Single Pulse 29Si-MAS-NMR of a CSH sample with Ca/Si ratio of 2.50 at 200 °C.

However, phase changes occur even after months at elevated temperatures as Fig. 1 shows exemplarily. Thus, systematic observations of CSH samples varying in Ca/Si = 0.50-3.00 via PXRD and 29Si-MAS-NMR were executed. The temperature-dependent formation of crystalline calcium silicate hydrates was shown and their time-dependent stability up to one year was investigated. While some phases like Xonotlite and Hillebrandite remain unchanged at their respective Ca/Si ratio, other samples like Trabzonite and Reinhardbraunsite form fast, but decompose over time, indicating their metastable state at the given conditions. Furthermore, some phase formations occur after multiple month revealing the complexity of the assumed simple ternary system.

References:
Engineering E. coli for gut-on-chip systems to investigate the mechanistic role of H$_2$S in the gut

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The human gut microbiota is a complex biological system composed of trillions of bacteria and their interactions with the host. Hydrogen sulfide (H$_2$S), a by-product of microbial metabolism, has been correlated with diseases such as IBD but has also been shown to protect tissue from oxidative stress and act as a signaling molecule in the central nervous system. [1,2] It has been proposed these effects are concentration dependent. Elucidating the mechanistic role of molecules such as H$_2$S is important in advancing our understanding of human health. Traditionally, static epithelial cultures and animal models are used to study the gut but are plagued by low transcriptomic similarity, high drug failure rates, and ethical issues. [3] In vitro flow systems, such as the gut-on-chip (GoC), designed with human-derived tissue are easier to probe than animal models and more genetically representative than static cultures.

In this research, we engineer the bacterium E. coli to modulate the production of H$_2$S to study its role in a GoC system. Native H$_2$S production genes were knocked out via the CRISPR-Cas9 system and the heterologous gene cdl from F. nucleatum was cloned onto plasmids with varying promoter strengths (tet, lacuv5, T7). In Hungate tubes, it was shown the production of H$_2$S is tunable and has a 32-fold dynamic range in the biologically relevant range (25 to 800 $\mu$M H$_2$S). Our tunable strain will be used to investigate the effects of different H$_2$S concentrations on epithelial cells in a GoC system. In recent experiments we show control of H$_2$S production levels in GoC, co-culture Caco-2 cells with RFP-expressing E coli for real-time imaging (Figure 1.), and assays to report effects of H$_2$S. Unlike static cultures and animal models, our system allows the direct study of microbial metabolism on human epithelial cells under flow conditions. These results will give insight into the role of H$_2$S in the human gut microbiome.

References:
Electrospray Ionization (ESI) is the most common atmospheric pressure ionization (API) technique in modern analytical mass spectrometry (MS). A liquid solution of the analyte is sprayed in a strong electric field which generates a spray of charged droplets containing the analyte. In the common model of analyte ion generation from the droplets, they shrink primarily due to evaporation of solvent molecules. Consequently, the coulomb forces between the analyte ions overcome the droplet surface tension at some point and the droplet fissions into smaller droplets. This shrinking mechanism repeats until there are only bare analyte ions. However, experimental evidence \cite{1} shows that at least for a significant fraction of these droplets, this evaporation and fission mechanism is not completed in the ion source region. Therefore, they are aspirated into the vacuum system of the MS, which can have adverse effects for analytical performance.

The presented experiments were done with a Bruker microTOF. A Rhode & Schwarz Oscilloscope was connected to an ion detector (secondary electron multiplier - SEM), which is located downstream the TOFs acceleration stage, to directly observe the signatures of large, charged aggregates penetrating the TOF mass analyser region. We observed the characteristics of these signatures in terms of appearance frequency, their shape, dependence on ion source parameters and long-term stability.

The observed droplet signatures are temporally highly correlated and remarkably intensive bursts of ions with pulse widths of hundreds of µs, each possibly generated from single aspirated large liquid droplets. Furthermore, we recorded single (non-summed) mass spectra. Analysis of the intensity distribution of this data reveals a group of single spectra with intensities remarkably higher than the average. This would be expected for intensive individual ion bursts reaching the TOF analyser region.

The frequency of ion burst appearance clearly depends on the analytical conditions: We see strong dependence between the observed signal intensity and shape of the individual bursts (e.g., occurrence of exclusively double peaks) and the ESI conditions. Generally, the ion burst frequency tend to decrease with time. However, changing the polarity from positive to negative measurement mode and back, recovers the ion burst frequency to a significant higher level. Remarkably, we did not observe ion bursts signals in negative measurement mode at all.

References:
Bifunctional Enzyme-Triggered CO-releasing molecules (ET-CORMs) as potential anti-inflammatory medicinal agents

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Despite its toxicity, carbon monoxide (CO) exhibits extraordinary beneficial physiological effects at low concentrations. Among those are anti-inflammatory, cytoprotective and other activities,\textsuperscript{[1]} making CO a promising candidate for therapeutic use. However, the administration of gaseous CO bears also many risks such as headache, vomiting, loss of consciousness or even death.\textsuperscript{[2]} To circumvent these general toxicity problems, so-called CO-releasing molecules (CORMs) have been developed by several research groups to provide a more selective supply of CO into the affected tissue.\textsuperscript{[3]}

In our own laboratory, we have developed oxy-substituted cyclohexadiene-Fe(CO)\textsubscript{3} complexes as enzyme-triggered CORMs (ET-CORMS), which are equipped with esterase-, amidase-, protease- or phosphatase-labile functionalities.\textsuperscript{[4,5,6,7]}

Scheme 1: General concept of bifunctional lipoxin based ET-CORMs. Upon enzymatic cleavage of the ester moiety in 1A, CO and 2 are released, which could lead to a feed forward cycle that causes a rapid resolution of an inflammation.

The concept of bifunctional ET-CORMs is currently expanded with the synthesis of lipoxin based ET-CORMs (1A, Scheme 1). Specialized pro-resolving mediators (such as analogues of 2 \textsuperscript{[8]}) play a key role in the resolution of inflammation. In addition, they upregulate the expression of heme-oxygenase 1 leading to an increase of the CO-release.\textsuperscript{[9]} The combination of both concepts is expected to induce a feed-forward cycle causing a fast resolution of an inflammation.

References:
Mechanistic insights by multimodal analysis of a 2D imine COF synthesised at the solid/liquid interface using a two-in-one approach

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Among the many two-dimensional materials (2DMs) which gained attention within the last decade, covalent organic frameworks (COFs) are promising because of their possible application in optics, catalysis, energy storage and electronics. The bottom-up synthesis of 2D COFs enables the tuning of the geometry, linkage type, and pore size using reticular chemistry and classical organic syntheses from molecular precursors. When synthesised at the solid/liquid interface, finding the optimal precursor concentration and ratio leading to 2D COFs with a large domain size and low number of defects is often challenging. Further understanding of the 2D COF formation mechanism is also highly necessary to optimise the reaction conditions. To tackle these challenges, we made use of a monomolecular two-in-one precursor, carrying both amine and aldehyde moieties, which forms an imine-based 2D COF.  

After drop casting of a monomer solution, 2D imine COF flakes were obtained at the liquid/solid (highly oriented pyrolytic graphite (HOPG)/octanoic acid (OA)) interface under ambient conditions. Scanning tunnelling microscopy (STM) was used to image the COF nanoflakes and to determine their unit cell size and geometry. Interestingly, higher monomer concentrations hinder the interfacial 2D COF formation. UV-vis spectroscopy gave access to kinetic data of the system, which were consistent with the formation of COF flakes in solution at room temperature showing a low activation energy and fast kinetics in octanoic acid. The covalent bond formation on surface was proven by X-ray photoelectron spectroscopy (XPS). Both the visual appearance of the COF flakes in STM and the fast kinetics point towards a direct monomer-to-COF mechanism without an amorphous polymeric intermediate. All in all, the use of the two-in-one approach simplifies the optimisation of reaction parameters and enabled the analysis of the resulting 2D COF and its formation at various length scales.

References:
Get into Flow: Optimization Strategies for the Anodic Phenol-Phenol Cross-Coupling Reaction in Flow Electrolyzers

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For the formation of symmetrical or non-symmetrical biaryls, the anodic C,C–coupling represents a sustainable and efficient synthetic pathway. In contrast to established approaches such as reductive coupling reactions the generation of reagent waste can be completely avoided, since there is no need for leaving groups and transition-metal catalysts. Recently, our group developed a wide range of synthesis protocols for various biaryl systems. Nevertheless, the optimization of the numerous reaction parameters, such as current density, supporting electrolyte, choice of electrode material, poses a challenge, as these parameters usually correlate with each other. Recently, we reported an optimized protocol for the phenol arene cross-coupling, enabling high current densities and increased cell loadings of up to 5 mmol for ortho as well as para coupling reactions in 25 mL beaker-type cells. When the reaction is transferred from the batch cell to an electrochemical flow cell, additional parameters such as the flow rate increase the complexity of the parameter space even further. Classical optimization approaches such as the one-factor-at-a-time method (OFAT) often fail to quantify the relevant correlations between the individual parameters and fail to address the global optimum of yield or selectivity. Using design of experiments (DoE), we optimized multiple reaction parameters at once by means of 35 experiments, resulting in highly efficient reaction condition with an almost threefold increase in space-time yield in contrast to time-consuming linear optimization.

References:
Photochemical Reactions and 3D-Structuring in Metal-Organic Frameworks

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Two-photon lithography (2PL) is well established for the precise three-dimensional (3D) nanostructuring of photoresponsive materials. The introduction of 2PL technologies to nanoporous metal-organic frameworks (MOFs) closes the gap of versatile and customizable materials, which are needed to exploit the full potential of the powerful structuring technique. Although multiphoton absorption in MOFs has already been reported, 3D structuring is to date limited to incorporated guest molecules or bond cleavage.¹ We focus our work on the synthesis and preparation of photoreactive MOFs based on benzophenone (bzp) linker molecules. Benzophenone units are widely used as photo-initiators for polymerization and in resins for 2D and 3D writing processes in polymers (2PP). When MOFs containing the bzp units are irradiated with UV light, photo-induced reactions can take place in the crystalline nanoporous materials. Using two-photon excitation of the bzp unit, three-dimensional structures can be written into the crystals or thin films. Thus, a photo-induced local change of material properties, such as the refractive index, colour or polarity is feasible by the choice of modification agent. However, only few bzp-MOFs have been investigated for photochemical modifications so far.²,³ The transfer of MP techniques for the 3D-structuring of optimized bzp-based MOFs might open the way for the additive manufacturing of optical components from MOF single crystals or thin films.

Figure 1: Possibilities of 2PL nanostructuring of a bzp-MOF single crystal for various application.

References:
Electrochemical Synthesis of Pyrazoles and Pyrazolines via Iodine-mediated [3+2] Dipolar Cycloaddition

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Highly biologically active pyrazole and pyrazoline derivatives are widely featured in pharmaceuticals as well as agricultural chemistry as pesticides, anti-cancerogenics or antimicrobics. [1] Conventionally, pyrazoles and pyrazolines can be accessed via [3+2] dipolar cycloaddition of nitril imines and dipolarophiles, requiring hydrazonoyl halo-genides as starting material, which are synthesized from hydrazones using hazardous chemicals like hypochlorite or NCS. [2] The electrochemical generation of 1,3-dipoles was established in our group for oxidation of aldoximes to the corresponding nitrile oxides, recently even for highly lipophilic betulin aldoxime. [3,4] We now developed a sustainable protocol for the electro-organic synthesis of 1,3,5-substituted pyrazoles and pyrazolines from readily available hydrazones and alkenes or alkynes. The reaction employs inexpensive sodium iodide as electrolyte as well as mediator, allowing for in situ formation of nitrile imines. Operating the reaction in a biphasic system using environmentally benign solvents allows for application of even highly sensitive alkenes such as styrene as dipolarophiles that would usually undergo side reactions or polymerization under electrolytic conditions. Thus, we herein present a protocol allowing for synthesis of pyrazolines from lab scale to 15-fold scale-up >10 g without any loss in yield.

References:
Zeolites and zeosils are interesting materials for the application as molecular sieves or catalysts in organic reactions. The catalytic activity of zeolites is often generated by metal atoms that are incorporated into the zeolite framework. To adapt a zeolite with characteristic properties for individual applications it is possible to modify the structure by using different structure-directing agents (SDA) in the synthesis. Most SDAs are organic amines or alkylammonium salts, but it is also possible to use metal complexes. In this research, a zeosil with a structure similar to chabazite is synthesized by using the tricationic Co$^{III}$(tacn)$_2$ ($1,4,7$-triaacacyclononane = tacn) complex as SDA. The resulting yellow solid is called LMU-2 (Ludwig-Maximilian-University-2). The cobalt complex is located in the cages of an interrupted porous silica framework (-CHA) similar to the chabazite (CHA) topology, but featuring [Si–O···H···O–Si]$^-$ hydrogen bonds.[1] Careful calcination of LMU-2 yields a material with CHA topology. The colour of the material changes from yellow to blue, showing that cobalt has remained in the sample. The oxidation and the coordination state of the cobalt is analysed using different spectroscopic methods. Co-containing zeotypes are interesting catalysts for various reactions.

![Figure 1: Schematic presentation of the transformation of LMU-2 (a) to CHA (b) during calcination, accompanied by a colour change from yellow (c) to blue (d).](image)

References:
The JungChemikerForum Würzburg consists of approximately 11 members enrolled in the master or doctorate program in Chemistry, Pharmacy or a teaching profession in chemistry. Among other activities such as organizing a scientific presentation given by a guest professor every semester, which attracts about 200 students (Figure 1), the “ChemSyStM” is held every other year. The ChemSyStM (Chemistry Symposium for Students of Mainfranken) is a symposium which gives master students and students in their doctorate studies a chance to present their work with a poster or a presentation. There are approximately 100 active participants, who get evaluated by professors of the University Würzburg, selecting the best posters for a prize. In cooperation with the JCF Erlangen-Nürnberg and the JCF Bayreuth, excursions to CERN in Geneva and BASF SE in Ludwigshafen took place. In cooperation with the jDPG (youth group of the German Physical Society) we fought in a “Science Battle” between the Faculty of Chemistry and the Faculty of Physics. About 600 students listened to and evaluated entertaining scientific talks given by physics and chemistry professors, declaring the final winners by the volume of applause.

Figure 1: Selection of past lectures organized by the JCF Würzburg.
Theoretical studies investigating the mechanism of methanol formation over Cu/ZnO(Al) based catalysts

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Cu/ZnO-based catalysts have been used to synthesize MeOH from syngas (CO/CO2/H2) for almost 60 years. Methanol production is a major industrial process, reaching 311 million tons per year in 2030 and growing. However, the mechanism of MeOH formation via CO2 hydrogenation remains under discussion. Key areas of debate are the role of O defects/vacancies on the ZnO surface, Cu-Zn synergism at the interface, the formation of Cu/Zn alloys, the role of ZnO (i.e. SMSI), etc.[1,2] Here, we present a computational study of all of the possible intermediates relevant to MeOH synthesis on a realistic model catalyst surface (a Cu cluster on a reconstructed polar ZnO surface with Al-doping).[3] We provide a detailed analysis of the different surface sites, stabilities, activation of the intermediates on the surface and activation barriers for relevant elementary processes.

References:
Sustainability is a timely topic of immense societal relevance in which chemistry has a key role to play. JCF’s Sustainability Team is built around the central question: “How can we as young chemists contribute to a sustainable future and inspire others to take action?” In the team, we discuss ideas and initiate projects to raise awareness and promote sustainability through practical approaches. Our current projects include a sustainability guide, the design of sustainable JCF giveaways, a survey to assess the appropriateness of sustainability in education, and a white paper that presents young chemists’ views on this topic in the context of the UN Sustainable Development Goals (SDGs). With these initiatives, we want to promote sustainability on different levels, by making the work of the JCF itself more sustainable, promoting the aspiration and initiative of young chemists on a national and international stage and giving young chemists a voice in shaping a more sustainable future. We are always looking for new creative ideas and welcome motivated team members who would like to participate in their realization.

References:
Large refractive index changes in Metal-organic frameworks

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Optical systems are important for devices in industry and our daily lives. Refractive index modulation can be an important tool for the fabrication of miniaturized low-cost optoelectronics. Metal-organic frameworks (MOFs) are promising materials for many typical applications of porous materials, like storage and separation of gases, catalysis and sensing. In our recent work, we focus on the preparation of MOF thin films with optical quality, that can be used as refractive index modulators. For this application, MOF thin films need to be homogeneous, crack-free and crystalline. Changes in the refractive index ($n$) of a MOF can for example be initiated by adsorption of guest molecules in the porous network.\textsuperscript{[1]} To date refractive index changes have been limited to $\Delta n \approx 0.1$.\textsuperscript{[2]}

An interesting preparation method for MOF thin films is the cycled direct growth.\textsuperscript{[1]} In this method, MOF films are crystallized from a methanolic mixed solution of the precursors with short reaction times at room temperature. This process can be repeated several times when thicker films are needed. We modified this method and obtained crack-free and homogeneous ZIF-8 films with enhanced optical quality.

In this research, MOF thin films were fabricated on different substrates such as glass and silicon wafers and characterized with respect to their crystallinity and optical properties. Refractive indices were measured by ellipsometry but were also investigated via UV/Vis spectroscopy. The refractive index was successfully modulated in a large range of up to $\Delta n \approx 0.2$ by the adsorption of different substances like alcohols or aromatic compounds. Fast refractive index changes could also be obtained by switching via the gas phase.

![Figure 1: Transmission spectra of ZIF-8 thin films after 3, 5 and 8 deposition cycles compared to glass.](image)

References
Performing click reactions of acetylene-substituted phthalocyanine molecules of new kinds of azide-derived insecticide carbamates

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Antibiotics containing oxazolidinone, sulfamate and carbamate functional groups are included in the category of new generation antibiotics. After the various biological activities, antibacterial, anti-inflammatory and antiviral properties of carbamate and oxazolidinone-derived molecules have been discovered, they can be used to synthesize some natural compounds, since most of these antibiotics are effective against gram-positive bacteria and tuberculosis (TB). The synthesis of new antibiotic derivatives formed by these groups has increased in recent years and many drugs obtained have attracted great interest [1].

Macrocyclic compounds including porphyrins and phthalocyanines have shown to be efficient electrocatalysts and optical limiting materials, due to their redox activity, strong electron donating character and extended π-system [2]. In this study, firstly, azide derivative carbamate compound was synthesized. Then, as a result of click reaction with acetylene substituted phthalonitrile molecules, a new ligand containing triazole groups was obtained. Synthesis of new zinc metal phthalocyanine (ZnPc) compounds was carried out under suitable reaction conditions of these carbamate-triazole containing phthalonitrile ligands [3]. The new products was successfully designed and prepared, and was characterized by FTIR, UV-Vis, and Maldi-TOFF Mass spectroscopic techniques.

References:

Figure 1: The synthesizing of new carbamate-triazole containing zinc phthalocyanine
Production of high energy capacity hybrid material containing Reduced Graphene Oxide-Quinoline Zinc Phthalocyanine (rGO/KZnPc)

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Phthalocyanines (Pcs) are macroheterocyclic compounds consisting of four isoindole units bonded to each other by nitrogen atoms at meso positions and can be obtained by changing the central metal ion and peripheral substituents and are used as pigments and have many applications such as energy conversion, gas sensor and liquid crystal. Quinoline is a heterocyclic aromatic organic compound that has various pharmacologically active synthetic and natural compounds of its derivatives are common [¹]. The graphene family includes reduced graphene oxide (rGO), graphene oxide (GO), graphene sheets, and several-layer graphene members. GO has unique physical and chemical properties [²]. In this project, graphene oxide were obtained first, starting from graphite. Then, new rGO-metallic quinoline-zinc substituted phthalocyanine nanohybrid materials (RGO-KZnPc) have been obtained as a result of the hydrothermal reduction reaction of GO with the zinc metal quinoline-substituted phthalocyanines (KZnPc) we have also synthesized [³]. After the necessary characterizations are made, new anode materials have been prepared and investigated energy density by electrochemical methods after these materials and other electrode additives were coated on Ni-foam (NiF) as a substrate.

![Figure 1: Schematic illustration of preparation for the KZnPc-rGO/AB electrode](image)

References:
Microwave-based substitution reactions on silicon compounds

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Si–N-functionalized compounds represent central intermediates in silicon chemistry, which are of great importance in the modification of silicon surfaces. Substitutions to alkoxy silanes (Si–O) likely represent the most important functionalization of aminosilanes.[1]

A well-known silylating agent is hexamethyldisilazane, which reacts with various alcohols. In contrast, aminosilanes with sterically more demanding substituents often lead to low yields in these reactions, which is due to the high kinetic barrier. Substitutions on (rac)-1-[methyl(naphthalen-1-yl)(phenyl)silyl]piperidine (1) with phenols as well as silanols show and confirm those low yields after long reaction times; other alcohols, like ethanol, do not show any conversion.

The synthetical access of various alkoxy silanes could be extended with the help of a new reaction method using microwave radiation. Amine functionalities on Si–N-functionalized silanes were selectively substituted with numerous alcohols.

Figure: 1: Selective transformation of Si–N-functionalized silane 1 performed by microwave radiation reactors.

The long reaction time Figure 1 can be explained by the decreased reactivity due to the large substituents at the silicon center, which could be improved by using more reactive Si–NH-functionalized compounds. [2] In addition, investigations are currently being carried out to transfer this new synthesis method to chiral systems. Moreover, the stereospecificity of microwave-based substitution reactions should be researched in detail in future experiments.

References:
Colloidal 2D Nanoplatelets with Tuneable Optical Properties and Efficient Emission from the Visible to the Infrared

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Colloidal two-dimensional (2D) semiconductor nanocrystals, so called nanoplatelets (NPLs) and nanosheets (NSs), provide optoelectronic properties notably different from their solid-state material and 0D (dot) and 1D (rod) nanocrystal counterparts. The 2D structure leads to decreased dielectric screening of charge carriers and results in a strong quantum-confined thickness and increased exciton binding energies. 1 For example, this strong thickness confinement leads to suppressed Auger recombination in UV-Vis active cadmium selenide (CdSe) NPLs and enables their application in lasing.2

In the visible range of the electromagnetic spectrum, cadmium chalcogenide NPLs provide a powerful material class for the above-mentioned applications. Their distinct optical absorption and emission features as well as their close to unity photoluminescence quantum yield make them ideal systems for (directed) light sources, e.g. by an encapsulation in polymeric matrices or in waveguides. 3

2D lead chalcogenide NPLs on the other hand are excellent materials for near-infrared applications, with optical properties tailored to the spectral windows necessary for biological imaging and glass fiber optics. 4,5 For example, we tune the absorption and photoluminescence (PL) of PbSe NPLs over a broad energy range (PL: 900 – 1550 nm) by controlling their lateral size, and by treating the NPL surface with metal halides (PL quantum yield increase to >50 %).

Our colloidal chemistry routes and integration opens up new pathways for direct syntheses and straightforward incorporation of colloidal NPLs as efficient emitters at UV-Vis and technologically relevant telecommunication wavelengths.

References:
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The Effect of Thermal Treatment on Carbon Felt Electrodes for Vanadium Redox Flow Batteries

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Our society still relies heavily on fossil fuels to cover the worldwide energy demand. However, it is necessary to invest in renewable energy sources for the problems arising from greenhouse gas emissions. Since these sources produce a fluctuating power output, one major challenge in the future will be the availability of suitable energy storage devices. Vanadium Redox Flow Batteries (VRFBs) represent a promising large-scale stationary energy storage approach. They are generally operated with porous electrodes based on carbon fibers, such as carbon felts or papers, whose properties significantly influence battery efficiency and lifetime. Due to their hydrophobic nature, the pristine electrode materials show relatively low electrochemical activity and poor wettability.  

One solution to improve the properties of the electrode materials is a heat treatment before application, which is known to introduce oxygen-containing functional groups at the material’s surface and to enhance the electrochemical activity. On this basis, the presented study aims to improve the understanding of the relationship between electrode and performance in VRFBs by investigating the effect of thermal treatment on the electrode properties.

Figure 1: Schematic illustration of the aim of the presented study – investigating the influence of thermal treatment on the properties of carbon felt electrodes.

References:
Palladium carbonyl carboxylate complexes of aromatic acids

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Palladium carbonyl carboxylate (PCC) complexes attract attention due to some specific properties. PCC contain palladium in rather unstable formal oxidation state (+1). Having 4- and 6-nuclear metal cores PCC are able effectively delocalize both an excess and a lack of electron density, which makes them potentially versatile catalysts or/and catalysts precursors. Properties of PCC containing carboxylate anions of alkyl and alkyne carboxylic acids have been studied earlier.[1,2] Herein we report synthesis, spectral properties and theoretical study of relative stability of possible isomers for PCC containing carboxylate anions of benzoic acid and its CF3-substituted derivatives.

A series of PCC with general formula of Pdₙ(CO)ₙ(RCO₂)ₙ (R = Ph (1), CF₃-2-C₆H₄ (2), CF₃-3-C₆H₄ (3) and CF₃-4-C₆H₄ (4)) have been prepared via substitution of acetate groups in palladium carbonyl acetate according to the following scheme:

\[
Pd₄(CO)₄(CH₃CO₂)₄ \xrightarrow{PhH, r.t., 1h} Pdₙ(CO)ₙ(RCO₂)ₙ
\]

According to EA all the complexes have the same Pd:CO:RCO₂ ratio 1:1:1. IRS data confirm bridging coordination mode of both CO- and RCO₂-groups. Considering the early observed dependence of PCC structure on electronic properties of substitute R we supposed 4-nuclear structure for complexes 1–4 (see fig. 1a). We also carried out DFT study of possible isomers of complex 1 with different positions of CO- and RCO₂-groups around the metal core (fig. 1b). Calculations results showed that isomer 1-I has the lowest relative energy – at least 20 kcal/mole below all the rest isomers.

References:
1,2-Diaminoalkynes (diaminoacetylenes, DAAs) represent an electron rich and highly reactive class of alkynes, which have found growing interest in last years and show versatile reactivity either in analogy to conventional alkynes or driven by its “hidden” diaminodicarbene character. Herein we present Dimorpholinoacetylene, a new derivative of this interesting kind of species through our reliable synthetic protocol that proceeds over a Fritsch-Buttenberg-Wiechell rearrangement. The DAA undergoes a dimerization at elevated temperatures to cleanly produce the corresponding enyne which was used to synthesize four membered cyclic bent allene (CBA) complexes. Furthermore cyclopentadienone (CPD) iron complexes were obtained which are currently studied as catalyst precursors for several (de-)hydrogenation reactions. Finally, the synthesis of a tetramorpholino cyclobutadiene (CBD) dication as one of the first known and fully characterized Hückel aromatic four membered ring dicaticonic systems is shown herein. The crystal structure of this compound shows nearly perfect planarity of the four membered ring and theoretical calculations of the Nucleus Independent Chemical Shift (NICS) as an aromaticity index indicate this species to exhibit an aromatic diatropic ring current.

Scheme 1: Versatile dimerization reactions of Dimorpholinoacetylene to create CBA complexes, iron CPD tricarbonyl or the Hückel aromatic CBD dication.

References:
Microstructural and thermoelectric characterization of electrospun \( \text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta} \) ceramics from nanofiber mats

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Calcium cobaltite \( \text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta} \) is among oxides a promising \( p \)-type thermoelectric material with good functional properties and high thermal stability in air. To improve the performance of this thermoelectric ceramic for energy harvesting, it is necessary to increase the power factor \( \sigma \alpha^2 \), which includes the electrical conductivity \( \sigma \) and the Seebeck coefficient \( \alpha \). The improvement of the thermoelectric performance can be accomplished via nanostructuring and texturing of the oxide-based ceramics by means of electrospinning. In this work, polycrystalline \( \text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta} \) nanofiber mats with hollow and porous structure have been fabricated by sol-gel based electrospinning and subsequent calcination at medium temperatures to obtain small particle sizes. Examination on the influence of the thermal treatment on the microstructural and thermoelectric properties of these electrospun nanofibers was performed. Microstructural characterization of the nanofibers by transmission electron microscopy showed an anisotropic particle growth along the increase of the calcination temperature from nanoparticles to platelets, which are expected due to the layered crystal structure of \( \text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta} \). These findings are also consistent with the evident formation of calcium cobaltite at 873 K from the X-ray diffraction pattern. Determination of the thermoelectric properties of the calcined and sintered ceramic nanofibers perpendicular to the pressing direction were also carried out and compared to a commercial \( \text{Ca}_3\text{Co}_{4-x}\text{O}_{9+\delta} \) reference powder. The Seebeck coefficient and the electrical conductivity reveal a dependence on the closed porosity and relative density of the ceramics.
Applications of Suzuki-Miyaura Coupling/Cross Metathesis Reactions for the Total Synthesis of Prenylated Isoflavone Natural Products

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The first total syntheses of 3'-prenylbiochanin A (1), neobavaisoflavone (2) and 7-methoxyneobavaisoflavone (3) are described. Compound 1 was first isolated from Erythrina sacleuxii. [1] Compounds 2 and 3 were first isolated from Psoralea corylifolia. [2] 2 was later isolated from E. sigmoidea and it showed activity against Staphylococcus aureus. [3] The key steps involved Suzuki-Miyaura coupling of the appropriately substituted 3-iodochromones and 4-hydroxyphenylboronic acid for the construction of the isoflavone core [4] and regioselective prenylation via oxy-allylation followed by Claisen rearrangement and olefin cross metathesis. [5] This route overcomes limitations identified for a previously investigated 2,3-oxidative rearrangement approach. [6,7]

Figure 1: Structures of Compounds 1, 2 and 3

References:
Development of a suitable experiment design for in situ Electrochemical Raman spectroscopy

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Spectroelectrochemical measurements can give insight into electrochemical reactions and information on processes on the molecular scale. One of them, the in situ Raman spectroscopy, contributes data regarding surface species, their orientation, and binding situation. Additionally, it is possible to see changes over time ascribed to changes in the reaction environment, e.g., potential. Necessary considerations for a successful setup design (Figure 1) and an experiment procedure as optical concerns, surface enhancement procedures, and laser choice in conjunction with an electrode material give a wide range of opportunities for a setup realization. This work will overview common pitfalls and potential outcomes of Raman spectroscopic measurements of the electrode/electrolyte interface and show ways to improve the spectroelectrochemical measurements.

Figure 1: a) Scheme of the components of an in situ electrochemical Raman spectroscopic set up with (1) laser beam and scattered light, (2) water immersion objective, (3) sapphire window, (4) Pt counter electrode (5) reference electrode, (6) Cu working electrode, (7) electrochemical cell. b) photographic image of the spectroelectrochemical cell under experimental conditions.

References:
The spotlight of current research is on the synthesis of nanoparticles with various shapes, sizes, and properties as well as on their assembly into three-dimensional functional nanostructures commonly known as aerogels. Nowadays, the assembly of nanoparticles (NPs) into meso- or macrostructures is of high interest since the assembly process helps to overcome the disadvantages of the colloidally dispersed particles and provides a platform for self-supported gel structures. In these functional nanostructures, the structure and properties can be controlled and fine-tuned to the smallest details, which is why there is a wide variety of applications in different fields, e.g. photocatalysis, catalysis and sensing.

The production of functional nanostructures includes the wet-chemical synthesis of stable nanoparticle colloids followed by their controlled destabilization to enable the arrangement of the nanoparticles into highly porous, voluminous and interconnected networks. Since the synthesis of the building blocks is isolated from the assembly process, the optical properties, electronic structure, and structural morphology can be tailored by countless synthesis strategies developed in colloidal nanocrystals chemistry. Due to the different nanoparticle building blocks, e.g. semiconductor, metal, metal oxide, and their surface chemistry, there are many different assembly strategies developed yet offering control over the network structure, porosity as well as the individual nanocrystal building block connection. [1]

Figure 1: Photographs and SEM images of different functional nanostructures. a) and b) Aerogel of CdSe/CdS nanorods, c) Cryoaerogel of Pt NPs, d) printed CdSe/CdS aerogel-based QR code, e) SEM images of cryoaerogel, d) SEM images of CdSe/CdS nanorod aerogel.

References:
Lithium, Sodium, or Potassium precursors? Alkali Metal Based Triimidosulfite Cages as Versatile Precursors for Single-Molecule Magnets

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Based on the sodium \([S(tBuN)₃(thf)₃Na₃SNa₃(thf)₃(NtBu)₃S]\) (II)\(^{[1]}\) and potassium precursor \([S(tBuN)₂(tBuNH)₂K₃(thf)₅K₃{[(HNtBu)(NtBu)₂S]₂}]\) (III) the syntheses and magnetic properties of two mixed metal triimidosulfite based alkali-lanthanide metal cages \([{(tBuNH)Dy{K(0.5tmeda)}₂{(NtBu)₃S}₂}]\) (1) and \([{ClDy(Na(thf))₂{(NtBu)₃S}₃}]\) (2) are reported. Preventing lithium chloride co-complexation led to a significant increase of single-molecule magnet (SMM) performance to previously reported sulfur-nitrogen ligands\(^{[2,3]}\). The Dy\(^{III}\)-complexes 1 and 2 display slow relaxation of magnetization at zero field, with relaxation barriers \(U = 70.3\) cm\(^{-1}\) for 1, 512.9 and 316.3 cm\(^{-1}\) for 2, respectively. Significantly, the latter complex 2 also exhibits a butterfly-shaped hysteresis up to 7 K\(^{[4]}\).

Figure 1: The sodium based triimidosulfite \([S(tBuN)₃(thf)₃Na₃SNa₃(thf)₃(NtBu)₃S]\) (II) leads to a promising Dy(III) SMM \([{ClDy(Na(thf))₂{(NtBu)₃S}₃}]\) (2)\(^{[4]}\).

References:

CO$_2$ as a tuning parameter for the head group properties of non-ionic EO-surfactants

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Investigation of carbon dioxide (CO$_2$) as sustainable resource is of fundamental interest for research and industrial applications. It can be used as a building block in chemical compounds such as polymers or surfactants.[1] Substituting ethylene oxide (EO) units in abundantly produced non-ionic EO-surfactants by CO$_2$ can increase the sustainability and save natural and fossil resources. Similarly interesting, introducing CO$_2$ gives a new tuning parameter for non-ionic surfactants, allowing to better match particular application requirements and thereby a more economical consumption and potentially even opening up pathways for novel formulations.[2]

The solubilization potential of CO$_2$ towards industrial relevant oils (decane, isopropylpalmitate, bis(2-ethylhexyl)carbonate) with different polarity has been characterized by small-angle neutron scattering (SANS) and compared with data from static and dynamic light scattering (SLS, DLS), interfacial tension measurements (IFT) and quantitative NMR (qNMR). At a given surfactant concentration, the use of CO$_2$-containing surfactants can greatly increase the solubilization capacity for oils compared to that of conventional EO-surfactants, as the incorporation of CO$_2$ into the head group renders the surfactant more effective with respect to their interfacial activity.

![Figure 1: Interfacial tension of EO surfactants with varying amount of incorporated CO$_2$ units for 25°C and 35°C. With increasing CO$_2$ amount the interfacial tension against isopropylpalmitate is decreasing.](image)

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**References:**


C–H Bond Activation via Series of Small Molecule Manganese Catalysts

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Current synthetic methods for oxidizing unactivated hydrocarbons are quite limited and often lack selectivity. Due to the lack of efficient and selective synthetic approaches, our lab has previously investigated an Fe(II) complex that is capable of oxidizing an array of hydrocarbon substrates. [1] Recently, an analogous Mn(II) catalyst series has been developed in our lab, in which the manganese center is coordinated by a ligand bearing two nitrogen atoms and 1–3 oxygen atoms, and is denoted as MnII(N2Ox), where x = 1–3. Each of these complexes is capable of oxidizing methanol to formaldehyde (C–H BDE = 96 kcal/mol) in the presence of oxygen atom donor molecules. Of these complexes, the MnII(N2O1) is capable of oxidizing hydrocarbon substrates. The substrate reactivity scope and characterization of the active catalyst of this complex is explored. We report the ability of MnII(N2O1) to epoxidize cyclooctene and cyclohexene (Figure 1), as well as form allylic oxidation products with cyclo-

Figure 1: Formation of MnIV(N2O1)(O) complex with oxygen atom donor (OAD) in situ, and subsequent epoxidation of alkene substrates; L denotes a halide or solvent molecule.

References:
[1] Cappillino, P, J.; Caradonna, J, P. Studies of iron(ii) and iron(iii) complexes with fac-N2O, cis-N2O2 and N2O3 donor ligands: models for the 2-His 1-carboxylate motif of non-heme iron monooxygenases. Dalton Trans. 2012, 41, 5662-5677
Casein as Release System and Blocking Layer for Implant Coatings

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In situ tissue engineering requires to functionalize the surfaces of implants, to achieve better biocompatibility or to release pharmaceuticals. Often a burst release of such pharmaceuticals takes place, and the surface functionality is gone rapidly. Casein-micelles (M-Cas) offer unique release capabilities for hydrophobic and hydrophilic substances. The direct use of casein-micelles is often not possible because of the requirement of separation and cleaning steps. In this work, M-Cas were reconstructed with a dialysis method and used as release system for curcumin as a model drug. [1] Modified electrospun polycaprolactone (PCL)-fiber mats were coated with chitosan / tripolyphosphate nanoparticles (CS/TPP-NP) and functionalized with the reconstructed M-Cas. [2] CS/TPP-NPs and Na-caseinate (Cas) were used as blocking layer to slow down the release of curcumin loaded micelles, shown in Figure 1.

Figure 1: Relative release of curcumin from fiber mats functionalized with reconstructed casein micelles at 37 °C in a Na2CO3 (pH 11), a) without blocking layers and b) with blocking layers (2 x (CS/TPP(1 mg/mL)-Cas(0,1 mg/mL))). The additional blocking layers showed a change in the release kinetics for curcumin.

The layers were investigated by surface zeta-potential (ZP) measurements, indicating that the layers are separated. The layer separation could provide different phases, which must be penetrated by the released substance. Indeed, the release of the curcumin from surfaces was possible and the blocking layers had a significant influence on the kinetics.

References:
Optimization of a cinnoline scaffold against *Plasmodium falciparum*

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Malaria is a prevalent and dangerous infectious disease, affecting millions every year. The current recommended therapeutic treatment of Artemisinin Combination Therapy (ACT) consists of artemisinin paired with other antimalarial drugs like lumefantrine or piperaquine. However, ACT has shown increased instances of resistance to *Plasmodium falciparum* necessitating the need for continued drug discovery efforts. The target product profile for malaria calls for the development of a single dose, orally efficacious drug, with an excellent selectivity profile.

Sequencing the *Plasmodium falciparum* parasite genome has revealed that kinases are expressed throughout every stage of the life cycle. Given this, a lead repurposing strategy starting with the clinically approved human EGFR inhibitor, Lapatinib, will be utilized. A scaffold hop led to the identification of the 4-aminocinnolines which were potent against *P. falciparum*. Previous work focused on the optimization of this chemotype for *Trypanosoma brucei*, the causative agent of human African trypanosomiasis. Building on this, we are working to further optimize potency against *P. falciparum*. Additionally, we will describe our efforts to combine potent activity with improved physicochemical and ADME parameters. Further, we will describe our efforts to understand the molecular mechanism of action of this series.
Formylation as key step for new tandem reactions – Towards BODIPY dyes

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4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) dyes experience an increasing demand due to their excellent photo- and thermo-, as well as their chemical stability. Therefore, they are utilized in a number of future-oriented applications such as organic lasers, OLEDs, fluorescent sensors, photosensitizers, solar cells etc.[1]

Conventional BODIPY syntheses show low overall yields. Therefore, an one-pot reaction to BODIPY dyes was developed involving literature known hydroformylation[2] or formylation[3] reaction conditions and subsequent substitution reaction with pyrrole nucleophiles under organo-catalytic conditions to obtain dipyrromethanes which are then straight-forward transformed to BODIPYs.

Figure 1: One pot synthesis scheme of BODIPY dyes from available precursors.

References:
Convergent Total Synthesis of Streptothricin Analogs

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Streptothricin F is a member of the streptothricin natural products class and is highly active against Gram-positive and Gram-negative pathogens of resistance-concern and many members of the so-called ESKAPE pathogens. Despite this potent activity, the streptothricins have not been systematically pursued in drug discovery efforts due to toxicity and resistance concerns. Recently, through cryo-EM characterization we have identified a novel binding site of streptothricin F within the ribosome of Gram-negative Acinetobacter baumannii. Additionally, our in vitro pathogen screening and eukaryotic cell cytotoxicity data on streptothricin F indicates significant toxicity reduction with only modest potency loss when compared to other steptothricins. Accordingly, we have completed a convergent, diversity-enabling total synthesis of streptothricin F consisting of 35 total steps and an overall yield of 0.40%. With this fully developed streptothricin F synthesis, we are pursuing the synthesis of both previously reported and novel analogs of the streptothricin class.
Community Involvement within NFDI4Chem towards Digitalisation of all Key Steps in Chemical Research

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NFDI4Chem is an initiative to build an open and FAIR infrastructure for research data management in chemistry. Since its launch in 2018 as a grass root movement, there has been enormous support from different partners within the chemistry community. The main fundamental aim of NFDI4Chem is to promote Open Science and Research Data Management (RDM) in accordance with the FAIR data principles. Thus, to create a holistic concept for access to and (re-)usability of research data. As project partner within the NFDI4Chem consortium the German Chemical Society (GDCh) has its main task in engaging with the chemistry community worldwide to create awareness for and foster the adoption of FAIR data management as well as to initiate processes to integrate RDM and data science into the chemistry curricula. Through its profound national and international network with chemical societies, publishers, and through its 27 divisions, GDCh strives to collect and analyse related communities’ requirements. Likewise, dissemination and training are intended for all career levels starting from undergraduates, in addition discipline-specific training material is developed. In collaboration with other partners, NFDI4Chem intends to also offer incentives for innovations. NFDI4Chem is supported by the German Research Foundation (DFG) under project number 441958208.
Studies towards the Total Synthesis of Natural Product Mumbaistatin

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Mumbaistatin (1), a polyketide natural product isolated from Streptomyces sp. DSM 11641, is the strongest natural inhibitor of glucose-6-phosphate translocase 1 (G6P-T1) known so far. [1] This enzyme plays a crucial role in hepatic glucose release as well as in angiogenic processes associated with brain tumour development. Its inhibition offers new perspectives in the treatment of type-2 diabetes mellitus and in chemotherapy. [2]

Despite its enormous pharmacological relevance, no total synthesis of Mumbaistatin has been concluded 20 years after its discovery. This is mainly due to the structural complexity of the unique tetra-substituted benzophenone core motif. In this project, a new synthetic strategy avoiding impracticable late-stage oxidation is envisaged (scheme 1).

Scheme 1: Retrosynthetic analysis of Mumbaistatin (1).

Key step is the construction of the fully functionalized carbon skeleton via carbonylative Suzuki coupling of anthraquinone triflate 2 with aryl boronate 3. Triflate 2 can be prepared from known 2-bromo-8-methoxy-1,4-naphthoquinone via regioselective Diels-Alder reaction and is employed with various model substrates of 3 to probe the generality of this approach. Besides verification and completion of the structural elucidation, further biological tests and SAR studies are planned in case of a successful synthesis.

References:
The influence of unsymmetrical homoleptic tris(siloxy) molybdenum alkylidyne complexes on the activity of alkyne metathesis

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Alkyne metathesis catalysts carrying siloxide ligands and especially the tuning of those ligands have become a strong field of interest. Mo(VI) alkylidyne complexes with siloxide ligands of the type "OSiR₃" (R = Ph, OtBu) are highly active catalysts with great functional group tolerance. Moreover, the geometry of the Mo–O–Si angle shows different effects on the Lewis acidity of the molybdenum centre. [1] Mo(VI) alkylidyne complexes bearing bent siloxide ligands therefore hold an increasing electrophilicity at the metal centre, which can be represented, upon other terms, by the chemical shift of the ¹³C alkylidyne signal. HABERLAG [2] and THOMPSON [3] synthesized symmetrical substituted homoleptic 2,4,6-trimethylbenzylidyne Mo(VI) complexes therefore our group had a rising interest in the trend of the activity on alkyne metathesis, including terminal alkynes, of unsymmetrical substituted tris(siloxy) molybdenum alkylidyne complexes (Figure 1).

Figure 1: Overview of (un-)symmetrical substituted homoleptic tris(siloxy) 2,4,6-trimethylbenzylidyne molybdenum complexes. [2,3]

References:
Molecular systems harvest diffusive sunlight on large areas and funnel it onto high-efficiency solar cells. They have a great potential to meet the increasing energy demand.

Here, we present a biomimetic concept that reduces the intrinsic losses of a Luminescent Solar Concentrator (LSC). An excess of randomly oriented pigments collect light from any direction. These donors transfer the energy to aligned acceptor chromophores through FRET.\[1\]

We discovered important structural principles of molecules which are responsible for the alignability. The pigments are embedded in a polyvinyl alcohol matrix which is then stretched. It was found that some molecules align and others stay randomly oriented. On closer inspection, it was found that the alignment is highest when the number of groups pointing out (black) of this planar band (red) is smallest. Solvent Green 7 is the donor and Rhodamine 123 the acceptor of the new two dye system.\[2\]

References:

Figure 1: Donor and acceptor molecule of the new ultrafast funneling material. The planar band is drawn in red and the groups which are pointing out are drawn in black. On the left is a schematic graphic of a LSC. Randomly oriented green donor pigments absorb sun light and transfer the energy to the aligned red molecules which emit almost all photons towards a photovoltaic cell.
Using Open SPR to Elucidate a Lead for Drug like Molecule to Inhibit the PPARγ/FABP4 Complex as a Potential Treatment of Metabolic Syndrome.

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Aberrant protein-protein interactions (PPIs) are the underlying cause of many diseases, and their inhibition could potentially lead to new therapeutics. For example, overexpression of Fatty Acid Binding Protein-4 (FABP4) mediates the down-regulation of Peroxisome Proliferator-Activated Receptor-γ (PPARγ), a phenomenon implicated in the development of obesity-linked diabetes and heart disease[2]. We hypothesize that inhibiting this protein-protein interaction (PPI) could prevent development of the above diseases, while sparing other essential functions of these two proteins, thereby reducing the likelihood of on-target toxicity compared to current treatments, which can have serious side-effects. Thus, we seek to characterize the binding interface of FABP4/PPARγ, to (1) identify the binding site on each protein, (2) determine which site is most druggable and therefore most suitable to target with a small molecule inhibitor, and (3) from this information, elucidate the type of molecule needed to effectively inhibit formation of the complex. Specifically, we will perform alanine scanning mutagenesis using an Open SPR instrument to identify which regions on each protein form the binding interface, and which specific amino acids provide most of the binding energy. These results, supported by a computational evaluation of the druggability of the two interface sites using FTMap, will reveal which of the two proteins FABP4 or PPARγ has the best chance of being drugged, and will provide guidance as to which approaches for inhibiting this PPI are most appropriate (e.g. conventional inhibitor versus a beyond Rule-of-Five compound versus a covalent inhibitor).

References:
Functionalization strategies to facilitate multi-depth, multi-molecule modification of nanostructured oxides for triggered release applications.

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The ability to achieve multi-molecule and depth specific functionalization of nanostructured material has continued to attract interest because of its potential applications, e.g., in drug-releasing implant materials. In this work, we described a simple approach to achieving this multilayer functionalization by exploiting the functionalization strategies.

This model multi-functionalized system was obtained by surface modification of Zirconia nanotubes (ZrNT) with functional phosphonic acid based molecules. The extent of achievable molecular density on the ZrNTs was evaluated as a function of the functionalization techniques, bulk immersion (BI) and micro-contact printing (µCP), qualitatively and quantitatively via water-contact angle measurements, via the surface analytical techniques XPS and Tof-SIMS depth profiling and drug release properties were monitored via dye release studies. Our research, as summed up in the schematic below (Figure 1), indicates that sequential functionalization via BI and µCP can be used to achieve multi-molecule/depth functionalization of nanostructured oxide materials and that such systems can potentially be triggered to release the loaded molecules by external factors.

Reference:
Hydrodefluorination via Bi(I)/Bi(III) Redox Catalysis

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Three elementary organometallic steps, oxidative addition (OA), ligand metathesis (LM) and reductive elimination (RE), define the innate capacity of transition-metal centers to revolve between different oxidation states in numerous catalytic processes. However, such catalytic cycle remains elusive for all low-valent main-group compounds. Herein, we demonstrate this possibility in the Bi(I)/Bi(III)-catalyzed hydrodefluorination (HDF) of polyfluoroarene feedstocks, yielding partially fluorinated building blocks. [1] The rationally designed bismuthinidenes, based on Phebox scaffold, exhibit dramatically higher catalytic reactivity compared to the state-of-the-art bismuthinidenes. Oxidative addition step was confirmed by NMR studies and a well-defined Phebox-Bi(III)(4-tetrafluoropyridyl) triflate. Spectroscopic studies of a transient bismuth hydride during catalysis provided solid evidence for a rare C–H reductive elimination from a main-group center.

Figure 1: HDF via Bi(I)/Bi(III) catalysis: elementary organometallic steps at low-valent main-group centers.

References:
Copper mediated intramolecular vs. intermolecular oxygenations: The spacer makes the difference!

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Copper complexes in combination with dioxygen are important as potential catalytic systems for regio- and stereoselective aerobic oxygenations of aromatic and aliphatic C-H bonds at ambient temperatures. In that context I investigated a copper(I) complex with an imine ligand derived from (+)-camphor and 2-(2-aminoethyl)pyridine that forms a bis(µ-hydroxido) dicopper complex upon reaction with dioxygen at room temperature. It is detectable by UV-vis for several hours up to a few days, depending on the solvent and could be structurally characterized. [1]

Figure 1: (a) copper(I) complex in acetone, (b) after leading O₂ through the solution for 4 min, (c) after leaving (b) for 1 d at room temperature, and the molecular structures from complexes crystallized from the according solutions. [1]

In contrast to previous observations with a similar aminomethyl derived ligand, this complex rather oxygenates acetone or thioanisole as external substrates with conversions up to 94% instead of undergoing an intramolecular ligand hydroxylation. I could demonstrate that dioxygen gas is activated and introduced into the substrate during oxygenation, through kinetic investigations and ¹⁸O₂ isotope labeling.

References:
The effect of trans-resveratrol on the molecular organization of lipid membranes

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The main goal of studies was to investigate the effect of trans-resveratrol on cell membrane models of eukaryotic organisms. Trans-resveratrol has an effect on the cardiovascular system and it is also one of the substances with anti-cancer activity. [1,2] The literature presents that pharmacological effect of trans-resveratrol is associated with its incorporation into cell membrane and membrane-lipid composition modification. [3]

The investigations were performed for different model systems containing sphingomyelin (SM), 2-oleoyl-1-pallmitoyl-sn-glycero-3-phosphocholine (POPC) and cholesterol (Chol) which are the main components of the mammalian cell membranes. The POPC and SM ratios were 1:1 and cholesterol content was 5, 15 and 33.3%. In the research Langmuir monolayer technique with Brewster Angle Microscopy support and liposomes were applied. [4]

The obtained results show a significant effect of trans-resveratrol on model biomembranes. It was found that the addition of this substance leads to the changes of membrane fluidity and reduces the order of hydrophobic chains.

References:
Visible Light Initiated Hydrooxygenation of Unactivated Alkenes — A Strategy for Anti-Markovnikov Hydrofunctionalization

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Hydrofunctionalization of unactivated alkenes is an indispensable mean in synthetic chemistry. Given that addition of electrophilic species into alkenes intrinsically follows the Markovnikov rule, a regioselectivity switch presents a major challenge. Herein, we present a visible light promoted strategy for the selective anti-Markovnikov hydrooxy-genation of unactivated alkenes. Therefore, an innovative reagent was carefully designed to release a highly reactive and strongly underdeveloped alkoxy carbonyloxyl radical upon reduction, which selectively adds into alkenes. Hydrogen atom abstraction from 2-phenyl malononitrile is the key to form the product. We believe that this protocol is a significant addition to existing hydrofunctionalization reactions and further highlights the importance of rational reagent design towards the development of methods to tackle challenging synthetic transformations.¹

We are convinced that such radical approaches will find broad application in the future.

Figure 1: Anti-Markovnikov selective hydrooxygenation of unactivated alkenes utilizing an innovative pyridinium salt and 2-phenyl malononitrile as H atom donor.¹

References:
The use of an easily accessible azahelicene as a strongly reducing photoredox catalyst as a metal-free alternative to the commonly used precious metal based photoredox catalysts is demonstrated. An improved two-step synthesis for the recently published helical compound [1] is described and its photophysical properties with respect to its use as a photoredox catalyst are evaluated. Its viability as a visible light photoredox catalyst is proven by application in two multicomponent reactions, a one pot sulfonylation/arylation [2] of styrenes under basic conditions and a one pot sulfonylation/aminalkylation [3] of styrenes under acidic conditions.

**Figure 1:** Synthesis of quinolino[2"',1''':2'',3'']imidazo[4'',5'':3',4']benzo[1',2':4,5]-imidazo[1,2-a]quinoline (Azahelicene) and application as a catalyst in two multicomponent photoredox reactions.

**References:**
Effects of passivation on perovskite solar cells

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To fight climate change, we need renewable energy sources in large quantities. One solution is photovoltaics (PV). New PV materials need to be cheap, highly efficient, and stable in order to succeed. Perovskite solar cells (PSC) have developed as a good competitor to silicon based solar cells. [¹] Nevertheless, defects in the perovskite crystal structures limit the efficiency due to non-radiative charge recombination losses.

One strategy to minimize recombination losses is to passivate the perovskite structure with Phenylethylammoniumchloride (PEACl). This improves the efficiency from 20.4% to 22.7%, by forming a 2D Ruddlesden-Popper (RP) phase ((PEA)₂(Cs₁-x FA x)n₋₁Pbₙ(1₋ₙCly)₃ₙ₊₁). [²] The occurrence of these defects is coupled to the nanoscale structure, e.g., to grain boundaries (GB) and crystal facets. A good method to investigate the local effect of such passivation on the nanoscale is an Atomic Force Microscope (AFM). Combined with Kelvin-Probe detection (KPFM) makes it possible to locally map the effect of defects in terms of changes in work function and photopotential of the material simultaneously.

Here, we studied the photopotential dynamics of the passivated perovskite using time-resolved approach of KPFM. By comparing to unpassivated surfaces, we could show that the effect of defect passivation occurred homogeneously over the sample. We were able to identify areas on the unpassivated sample with an unfavourable higher defect state density compared to the passivated one.

KPFM is able to show the advantages of a passivation strategies. The passivation improves the efficiency and stability of PSCs and make them even more competitive to others.

References:
**B1CTcu5 peptide derivatives as potential antimicrobial agents: design and discovery of new drugs**

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*Mycobacterium tuberculosis* (MTB) is the leading cause of death in the world and is considered a critical priority according to the WHO [1]. At present, advances in drugs discovery against this pathogen are scarce, and a drastic increase is expected after the COVID-19 pandemic [2]. Antimicrobial peptides (AMPs) or also known as host's own peptides, are biomolecules that have high antibacterial activity and even with multidrug-resistant bacteria [3]. Within this group of AMPs, we have B1CTcu5, isolated from the secretion of frog skin (*Clinotarsus curtipes*), and it showed activity against MTB [4]. In this way, the aim of this research was to study an *in vitro* library of B1CTcu5 AMP analogs, modifying its structure by incorporating tryptophan for fluorescence emission and replacing cysteine with lysine and serine residues from the original sequence. Peptide analogs were obtained by the solid phase peptide synthesis method, using the Fmoc strategy, using Rink-amide resin and Fmoc-amino acids coupled with HOBt and DIC, cleaved at 2.5:2.5:95% TIS/H2O/TFA, then purified by HPLC and characterized/identified by mass spectrometry. For the study of antimycobacterial (MTB strain H37Rv), antifungal (*Candida Albicans*) and antibacterial (*Escherichia coli, Pseudomonas Aeruginosa, Staphylococcus aureus, Salmonella Typhimurium*) activity microplate method were used and evaluated after 7, 3 and 1 days, respectively. Preliminary results show potential antimicrobial activity (2 – 64 µg/mL or > 80% inhibition, depending on the McFarland or REMA quantification method) and demonstrate possible new peptide sequences in the challenge of new drug discovery.


References:


Imaging of fuel cell components by atomic force microscopy

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For the refinement of fuel cell electrodes, the investigation of the ionomer distribution inside the catalyst layer of the electrodes is crucial. [1,2] In proton exchange membrane fuel cells, ionomers like Nafion® are used as binder and serve as solid electrolytes.[1] A homogenous ionomer distribution inside the catalyst layer was related with high fuel cell performances and a higher catalyst utilisation, allowing the reduction of scarce and expensive catalyst material in fuel cell applications.[1,2] Previously, the feasibility of material-sensitive atomic force microscopy (AFM) of single cell cross sections was demonstrated under close to operando conditions.[3] In this work, material-sensitive AFM was applied to study the structure of Nafion®-containing catalyst layers, resulting in a material contrast of the Nafion® and the Pt catalyst supported on Vulcan® carbon due to different adhesion forces between sample and AFM probe (Fig. 1). The material contrast as well as potential artefacts are discussed. An outlook on future applications of AFM to investigate fuel cell components and catalyst materials will be given.

Figure 1: a) Schematic of the catalyst layer structure with low adhesive supported catalyst and high adhesive Nafion®; b) False color representation AFM image of the adhesion force measured on a fuel cell catalyst layer cross section containing supported catalyst and Nafion®.

References:
Ion incidence angle dependent pattern formation at AZ® 4562 photo resist by Ar⁺ ion beam erosion

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Polymers are part of our daily life and have many applications that may require certain surface properties, i.e. food packaging or healthcare products.¹² A powerful method for influencing the surface properties of polymers without altering the properties of the bulk material is the use of ion beams.² A multitude of nanopatterns was observed by utilizing a wide range of ion incidence angles (0° – 75°) for the erosion of commercially available photoresist AZ® 4562. The observed sequence of angle-dependent patterns (nanoholes, ripples, facets) (see Figure 1) is already known from inorganic materials. The variation of the erosion time (5 min – 60 min) showed a temporal evolution of the nanopatterns. Additionally, a changed composition of the polymer surface could be detected by means of X-ray photoelectron spectroscopy.²

Figure 1: Ion beam incidence angle influences the formation of nanopatterns on the surface of AZ® 4562.

References:
(2) Rüdiger, T.; Mitzschke, M.; Prager, A.; Liu, Y.; Abel, B.; Schulze, A.; Frost, F. Ion incidence angle dependent pattern formation at AZ 4562® photo resist by Ar⁺ ion beam erosion. Applied Surface Science 2022, 574, 151682.
Developing a Lab-based Chemistry Escape Room Game for High School Students

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In recent years the number of beginning student in natural sciences is in decline.¹ To encourage more high school graduates to take up studies in this field, it is crucial to get young students excited about this field. For this purpose, suitable offers must be developed. Hence, we designed a lab-based escape room for high school students, which is conceptualized for 90 minutes and can therefore be played during a regular school lesson. During the escape room game, the students need to use their basic knowledge from school chemistry classes to solve different puzzles. All puzzles are implemented in a background story about an environmental pollution crime to raise awareness about this major issue for society and highlight the solutions chemistry can provide. The escape room can be supervised by a single teacher and all necessary materials are assembled in a suitcase which is provided free of charge for educational institutions by the youth organisation JCF of the German Chemical Society.

Figure 1: Schematic display of two experiments implemented in the escape room game.

Development of a battery seminar for pupils

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It is important to get young pupils excited about the field of natural sciences to inspire them to take up studies in the STEM field including mathematics, information science, natural sciences, and technology and engineering after school. Thus, extracurricular offers for pupils must be established. Therefore, we developed a seminar for pupils in grades 8 to 10 or 11 to 13 about the topic “battery research and the everyday work of a battery researcher”. During this three-hour seminar, the pupils deepen their knowledge about the basics of electrochemistry, which are required to understand the working principle of a battery. Furthermore, the concepts of everyday used batteries including Li-ion batteries and future battery concepts based on Na, Ca, and Cl will be introduced. To highlight battery research and the importance of research and practical experiments, the pupils will be supervised while performing basic electrochemistry experiments including building a lemon battery. The seminar will be held in schools by Monja Schilling and will be provided free of charge by the German Network of Young Scientists juFORUM e. V.
Distribution of Relaxation Times (DRT) Study on the Positive Half Cell of a Vanadium Redox Flow Battery

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Due to the increasing energy demand worldwide and the urgency of action because of climate change, new energy storage devices are needed to balance the fluctuations of renewable energy sources. The vanadium redox flow battery is a promising technology for large-scale energy storage but still needs to overcome significant lifetime and efficiency challenges, which are decreased by polarization losses during operation. It is essential to conduct experiments in a setup that closely mimics the cell’s operating conditions to gain new insights into the reaction and transport processes in a vanadium redox flow battery. Therefore, a unique 3D-printed flow cell was designed to ensure steady-state conditions during the measurements. The processes of the positive half-cell were characterized by electrochemical impedance spectroscopy, and the recorded data were analyzed using the distribution of relaxation times method, which is a frequently used method in research for lithium-ion batteries or in our group for fuel cell characterization. [1,2] We could assign the peaks in the DRT spectrum to the electrochemical reaction, the transport through the electrode structure, and the diffusion processes of the vanadium species. Thus, we could identify the individual processes in the positive half-cell of the VRFB and their contributions to the overall impedance. This information is vital in search of optimized operating conditions with reduced polarization losses.

Figure 1: Schematic illustration of measurement including cell setup, EIS spectra, and DRT spectra.

References:
Combining coordination chemistry and carbolithiation

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Living anionic polymerization initiated by lithium alkyls is a well-known pathway to highly defined polymers. Especially, styrene and its derivatives can be polymerized successfully with high control of the polymeric features. By using functionalized initiators, it can be ensured that each polymer chain carries the functionalization, which represents an advantage over ω-functionalization. 2-(Dimethylaminomethyl)pyridine (1) showed promising applicability as an anionic initiator in the model carbolithiation reaction, as it was successfully lithiated and subsequently added to 1,1-diphenylethylene. Moreover, 1 provides a further characteristic as a bidentate ligand. Due to its chelating properties, transition metal complexes of rhenium, ruthenium, silver, and palladium were successfully synthesized with ligand 1.

The possibility to combine both characteristics of compound 1 allows an access to defined polymers as ligands for transition metal complexes. Thereby, compound 1 offers a wide variety of promising applications, which aim to be discovered in future research.

Figure 1: Compound 1 can be used as a ligand for transition metals like rhenium or can be carbolithiated to 1,1-diphenylethylene.

References:
Application of mixed-acidic cation-exchange resins in IC-ESI-MS for the determination of free amino acids in beer

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The separation and quantification of multifunctional, ionic compounds in complex sample matrices is a challenging issue in disciplines as environmental or food science. This study demonstrates the prospects of ion chromatography coupled to ESI-MS for such applications.

Besides its popularity as a beverage, beer is a complex sample matrix as it contains water, ethanol, carbohydrates as major compounds and many minor compounds like amino acids. The monitoring of these substances allows to control the fermentation process and guarantees consistency in product quality and flavour. [1]

Recently, mixed-acidic cation-exchange resins (MCX) with both strongly and weakly acidic functional groups attached to the polymeric substrate were developed and optimized for the analysis of standard amino acids. [2] The separation method using this novel stationary phase chemistry provides a derivatization-free analysis (both pre- and post-column) and offers precise and accurate results with LODs in the nmol/L order of magnitude. Superior separation results compared to existing methods are obtained due to the tailored selectivity of the column for the multifunctional analytes under investigation. The unique selectivity in combination with highly symmetrical peaks and efficiencies up to 37000 N·m⁻¹ allows the separation of 20 standard amino acids in 30 min using an isocratic elution program.

Herein, the trace level free amino acid composition of different types of beer was successfully analysed using MCX columns operated with ESI-MS detection. The method proofed to be robust when applied to the different, complex samples matrices and is expected to be a valuable tool for further analytical challenges.

References:
Luminescence Encoding of Polymer Microbeads during Polymerization

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Luminescent polymer microbeads, encoded either with organic dyes or semiconductor quantum dots (QDs), are applied in screening platforms for biomolecule binding interactions. [1] The encoding of these beads is important for the realization of optically distinguishable barcodes that can be read e.g., by a flow cytometer or a fluorescence microscope. Dye encoded beads often suffer from photobleaching and can introduce difficulties due to spectral crosstalk in emission. Ideal for color multiplexing are QDs that absorb in a very broad wavelength range and reveal narrow emission bands, which enables simultaneous excitation of differently colored QDs. [1,2] There are several challenges to be overcome for QD encoding of polymer beads. Swelling procedures in combination with premanufactured beads often suffer from inhomogeneous QD loading, and encoding by QD addition during polymerization reactions can result in several problems like the separation of QDs from the monomer phase, a broad size distribution of the polymer particles, or loss of QD fluorescence. This encouraged us to explore simple and effective approaches to QD encoding of polystyrene microbeads and identify suitable polymerization reactions and QD surface ligands that tackle these challenges. The best results were obtained using QDs bearing a polymerizable surface ligand dispersed in hydrophobic monomer droplets that were subsequently polymerized. [3] Moreover, we systematically investigated the resulting fluorescence properties like emission and photoluminescence quantum yield of the resulting QD-encoded beads using fluorescence spectroscopy, integrating sphere spectroscopy, and fluorescence & electron microscopy.

References:
Metal-free electrochemical fluorodecarboxylation of aryloxyacetic acids to fluoromethyl aryl ethers

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Introducing a fluorine moiety into organic molecules is of high interest for various applications in agrochemical and pharmaceutical chemistry. The use of fluorine as a bioisostere for hydrogen in drugs can alter parameters like the metabolic stability or membrane permeability and therefore improve the drugs potency. [1] Since the publication of methods for the mediated fluorocyclization of N-allylcarboxamides [2] and N-propargylamides [3] to the corresponding oxazolines/oxazoles by the Waldvogel lab, a new method for the direct electrochemical fluorodecarboxylation of aryloxyacetic acids to fluoromethyl aryl ethers has been established. [4] Similar to the previously published synthesis of aryl methoxymethyl ethers [5] the formation of KOLBE-products cannot be observed. This method utilizes a simple to execute metal-free protocol in undivided cells with constant current to convert a number of different aromatic and heteroaromatic substrates in yields of up to 85%. Furthermore, it also benefits from the general advantages of an electrochemical reaction protocol: The use of electric current as a traceless oxidant, easy scalability, inherent safety, prevention of reagent waste and the possibility to tune the redox potential. [6]

Scheme 1: Electrochemical fluorodecarboxylation of aryloxyacetic acids to fluoromethyl aryl ethers.

References:
Selective depolymerization of Kraft lignin and black liquor using electrolyzed carbonate

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Figure 1: Overview of the process of obtaining fine chemicals and biofuels from lignin.

After cellulose and hemicellulose, lignin represents a major part of plant biomass. Due to the large waste stream originating from pulping processes, Kraft lignin and lignosulfonates, to name two examples, are of technical interest. Because of the polyphenolic structure, the biopolymer lignin is qualified as a potential renewable feedstock to produce bio-based aromatic fine chemicals such as vanillin and acetovanillone. Furthermore, lignin, but also black liquor, a by-product from the Kraft process, could also be suitable as a potential sustainable feedstock for the production of biofuels. However, the complexity and degradation stability of the molecular structure make the depolymerization highly challenging but also worthwhile. We developed an electrochemically supported method for the highly selective degradation of Kraft lignin to water-soluble degradation products such as the fine chemicals vanillin and acetovanillone, but also polymer fragments that may function as feedstocks for biofuels. Therefore, the electrically ex-situ generated high-performance oxidant peroxodicarbonate (PODIC) was employed as a lignin depolymerization. PODIC is simply produced through continuous electrolysis of an aqueous carbonate solution using a boron-doped diamond anode, which makes it an especially sustained oxidizing agent. Addition of the oxidant to a solution of lignin, or even black liquor itself, gives an oxidized polymer that subsequently undergoes thermally induced depolymerization. In summary, the developed method relying on electrolyzed carbonate as sustainable oxidizing agent allows for selective degradation of Kraft lignin to vanillin and acetovanillone as well as water-soluble degradation products, which could be implemented into biofuels.
Synthesis of Aza[10]CPPs towards a Charge Shuttling Rotaxane

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[n]Cycloparaphenylenes are rigid macrocycles consisting of n para linked phenylenes. A special feature of [10]CPP is the formation of highly stable inclusion complexes with C60 through a perfect size and shape match. This unique interaction was used by our group to synthesize a rotaxane based on a central [10]CPP⊃C60 complex.[1] Physicochemical studies revealed the dynamic nature of the CPP-fullerene interaction which demonstrated the potential of [10]CPP to act as mediator for charge transfer in combination with electron-donor stoppers. Such an architecture could be a “supramolecular solution” to premature charge recombination that is a major impediment in the areas of photocatalysis and OPV.

Figure 1: C60 association constants (Ka) of Aza[10]CPP (bright blue), N-Me-Aza[10]CPP (green) and [10]CPP (dark blue).

To lower the LUMO level of [10]CPP we incorporated nitrogen into the CPP scaffold and thus synthesized Aza[10]CPP and N-Me-Aza[10]CPP. We studied their C60 binding affinities in solution and in the gas-phase and investigated photo-induced charge transfer processes in the [10]CPP⊃C60 complexes by transient absorption spectroscopy to investigate the potential of the synthesized CPPs as charge mediators.

References:
Preparation and Characterization of Molybdenum Disulfide-Reduced Graphene Oxide (MoS2/RGO) Nanomaterials for energy application

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Transition metal dichalcogenides (TMDCs) are a major class of 2D graphene cognate and possible to synthesize by mechanical cleavage, chemical vapor deposition, epitaxial growth, and chemical method the same as graphene 2D materials. Molybdenum disulfide (MoS2) nanostructures, which are a member of TMDCs, are gaining increasing popularity with potential application potentials in various fields due to their unique physicochemical properties [1]. Nowadays, MoS2 has attracted plenty of recognition in electrochemical energy storage devices attributed to its innate ionic conductivity and higher theoretical capacity than graphite, owing to its graphene analogous structure. The above intrinsic properties of model material 2D MoS2 clearly depicts the material advantages of 2D-TMDs towards electrocatalytic applications such as (1) water splitting hydrogen fuel generation, (2) metal ion batteries, and (3) super capacitors were discussed in recent works [2].

In this study, MoS2/RGO nanohybrid materials will be obtained as a result of mixing 2D nanostructured MoS2 and synthesized GO with different ratios (such as 90/10, 80/20) [3]. For the characterization of these obtained 2D structured nanocomposite materials, their morphology and structures will be elucidated by analysing them with spectroscopic methods such as FTIR, Raman, XRD, SEM, EDX, UV-Vis.

References:
Synthesis of $\beta$-SiAlONs $\text{Si}_{6-z}\text{Al}_z\text{O}_z\text{N}_{8-z}$ in a wide range of $z$

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$\beta$-SiAlONs are $\beta$-$\text{Si}_3\text{N}_4$ derivatives of general formula $\text{Si}_{6-z}\text{Al}_z\text{O}_z\text{N}_{8-z}$, $z = 0$-4.2. Properties of $\beta$-SiAlON are closely related to $z$ value. Density, hardness, fracture toughness, bending strength, thermal diffusivity, heat capacity and thermal conductivity of $\beta$-SiAlON decreased with an increase in the $z$ value. Although a lot of studies are dealt with synthesis and properties of $\beta$-SiAlON, however, there is no systematic studies of $\beta$-SiAlON in wide ranges of Si/Al ratio and temperature under the same conditions. We studied the synthesis of $\beta$-SiAlON in almost full range of $z$ values ($z = 1, 2, 3$ and 4) starting from the mixtures of AlN, $\alpha$-$\text{Si}_3\text{N}_4$ and $\text{Al}_2\text{O}_3$ powders, the latter one was prepared by sol-gel technique to increase a surface area and reactivity. All four target $\beta$-SiAlONs were obtained with the yields of 77-93% (considering the content of target phase in the product) by annealing for 1.5-3 h at 1550-1750°C under $\text{N}_2$ flow (at 1 bar). For $z = 1$ and 2 the highest content of target $\beta$-SiAlON was observed after annealing at 1650°C (90% and 84%) and for $z = 3$ and 4 the temperature of 1550°C was enough to get $\text{Si}_3\text{Al}_3\text{O}_3\text{N}_5$ and $\text{Si}_2\text{Al}_4\text{O}_4\text{N}_4$ with the yields of 93% and 77%. What is also quite interesting is that $\beta$-SiAlONs with higher content of AlN compared to starting compositions are readily formed at 1550°C. Thus, for $z = 1$ the $\text{Si}_4\text{Al}_2\text{O}_2\text{N}_6$ formed at 1550°C with the yield up to ~59% and $\text{Si}_3\text{Al}_3\text{O}_3\text{N}_5$ was found to be the major product (~74% yield) for $z = 2$ under the same conditions. Formation of 15$R$, 21$R$ and 12$H$ polytypoids also has to be mentioned as well as $\zeta$-SiAlON ($\text{Si}_3\text{Al}_7\text{O}_3\text{N}_9$) and $\theta$-SiAlON ($\text{Si}_3\text{Al}_12\text{O}_9\text{N}_{10}$).

Figure 1: Left: XRD patterns for the samples $1\text{S3-16}$ (a, ca. 90% of $\text{Si}_6\text{Al}_4\text{O}_4\text{N}_{8-}$); $2\text{S1.5-16}$ (b, ca. 84% of $\text{Si}_3\text{Al}_2\text{O}_2\text{N}_3$); $3\text{S3-15}$ (c, ca. 93% of $\text{Si}_3\text{Al}_3\text{O}_3\text{N}_5$) and $4\text{S3-15}$ (d, ca. 77% of $\text{Si}_2\text{Al}_4\text{O}_2\text{N}_4$). Right: SEM image of sample $3\text{S3-15}$.

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Au NRs modified regenerated cellulose fibers for SERS applications

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Surface-enhanced Raman scattering (SERS) is recently of keen interest due to its high sensitivity and specificity in the detection of a wide range of organic compounds. However, one should bear in mind, that this technique owes its great potential to the use of suitable substrates that are responsible for enhancing the Raman scattering signal through different mechanism. [1,2] Lately, cellulose has emerged as one of the interesting platforms for making SERS substrates, because it shows weak SERS response, hence providing low interference and background signals during the measurements. [2,3] Other, also important merits of cellulose, are its high availability, low price, susceptibility to chemical functionalization and, above all, flexibility. [2,3] Because cellulose by itself does not enhance the Raman signal, it is necessary to modify it (or its derivatives, i.e., fibers or paper) using plasmonic nanoparticles. [2,3]

Herein we show development of the SERS substrate based on the regenerated cellulose fibers, that owes its SERS activity to the presence of gold nanorods (Au NRs) in its internal structure, and not only on the surface, as it is shown elsewhere, thus ensuring superior stability of the obtained material. [3] This flexible cellulose-based substrate exhibiting plasmonic activity, enable easy and reproducible detection of different analytes via SERS technique. Furthermore, the presented substrate shows superior stability, thus proving it good reusability and the long shelf life.

References:
Investigation and Antioxidant Properties of Transition-metal dichalcogenides (TMDs) Molybdenum Disulfide-Reduced Graphene Oxide (MoS2/RGO) Nanohybrid Materials

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Transition metal dicalcogenides (TMDCs) are a family of two-dimensional layered materials with interesting physical, electronic and chemical properties [1]. The atoms in the layers are held together by strong covalent interactions and the layers stack through van der Waals forces. TMDCs have been extensively investigated in energy storage, sensors, catalysis, and biomedicine. Molybdenum disulfide (MoS2) has been investigated as a drug delivery carrier in many studies [2]. In particular, it has been suggested to be used in photothermal therapy (PTT) treatments for cancer due to its high photothermal conversion efficiency in the near infrared (NIR) region. Despite these pioneering studies, research using MoS2 for its biological properties and targeted drug delivery is still limited [3]. GO-doped MoS2/RGO nanohybrid structures will contribute to current research in areas such as photodynamic therapy of cancer (PDT), revealing antioxidant properties such as DPPH radical capture.

References:

Figure 1: GO-doped MoS2/RGO nanohybrid structures
Synthesis of D$_6$-$^{13}$C-vinyl pyruvate as a precursor for hyperpolarised magnetic resonance imaging

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During the last decades, magnetic resonance imaging (MRI) developed into one of the most relevant clinical imaging methods. It is non-invasive, does not rely on ionizing radiation, and has good temporal, as well as spatial resolution. Currently, $^{1}$H is by far the most observed nucleus because other MR-active nuclei, like $^{13}$C, occur in comparatively low abundances, resulting in low intensities. The solution to this problem is hyperpolarisation (HP), which allows the signal intensity to potentially be increased over 105-fold. The HP of nuclear spins has shown its ubiquitous applications in chemistry, biophysics and medicine. Dynamic nuclear polarization (DNP) allows for such polarization and has already shown promising results for metabolic investigations of endogenous biomolecules, like pyruvate, which can indicate certain diseases like cancer. HP via para-hydrogen induced polarization (PHIP) is a fast and cost efficient alternative to DNP and takes advantage of the high spin order of para-hydrogen (pH2). PHIP-sidearm hydrogenation (PHIP-SAH) relies on the hydrogenation of an unsaturated sidearm in a suitable precursor with pH2 (Fig. 1). The high spin order of pH2 can be transferred to a specific carbon nucleus via spin order transfer (SOT) to yield high polarizations of the desired nucleus. One of the previous shortcomings of PHIP-SAH was the lack of suitable precursors.

We were able to establish a novel synthesis for the vinylation of $\alpha$-carbonyl carboxylic acids, yielding their highly sensitive vinyl esters. Using our synthesis, enabled us to vinylate pyruvic acid via its chloride to vinyl pyruvate with appreciable yields. Thus, the synthesis with the fully deuterated D4-pyruvic acid was carried out. This method also allows the introduction of a fully deuterated sidearm, further increasing the polarization. This rendered it possible to synthesize the D6-$^{13}$C-vinyl pyruvate, which subsequently was successfully hyperpolarized to P = 40 % (extrapolated for 100 % pH2) at MOIN CC by Dr. Pravdivtsev (Fig. 1).

Figure 1: Hyperpolarization of D$_6$-$^{13}$C-vinyl pyruvate via hydrogenation with pH$_2$ and spin order transfer.
Improving performance of luminescent nanothermometers based on non-thermally and thermally coupled levels of lanthanides by modulating laser

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Optical sensors based on lanthanide ions usually enable temperature control based on the analysis of changes in the intensity ratios of the bands associated with their thermally and nonthermally coupled levels. The optimal nanothermometer should show a high relative sensitivity and good temperature resolution. [1,2,3]

An up-converting, inorganic nanoluminophore, YVO₄:Yb³⁺, Er³⁺ was synthesized using the hydrothermal method and a subsequent calcination. Its emission spectrum consists of four Er³⁺ bands in range 500–850 nm and one Yb³⁺ band located around >900 nm (λex = 975 nm). The obtained compound exhibits temperature-dependent luminescence properties, hence it is used as an optical nanosensor of temperature. The determined band intensity ratios of the non-thermally coupled levels of Yb³⁺/Er³⁺ and thermally coupled levels of Er³⁺ are correlated with temperature, and they are used for ratiometric sensing of temperature. The effects of the pump (NIR laser) power on the luminescence properties of the material, including band intensity ratios, absolute and relative sensitivities and temperature resolution are analysed. [3]

Research shows that in the case of luminescent thermometers exhibiting non-linear phenomena (e.g. up-conversion emission), and using the luminescence intensity ratio of the bands originating from the transitions with a different number of photons participating in the relevant radiative processes, change of the laser power may significantly affect the determined thermometric parameter values, and performance of the sensor. [3]

References:
[3] Stopikowska N.; Runowski M.; Skwierczyńska M.; Lis S. Improving performance of luminescent nanothermometers based on non-thermally and thermally coupled levels of lanthanides by modulating laser power. Nanoscale 2021, 13, 14139-14146
Enantioselective Nickel-Catalyzed Hydrocyanation Employing TADDOL-derived Phosphine-Phosphite Ligands

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Nitriles are very valuable synthetic intermediates as they give access to a broad variety of functional groups via single-step conversions. As an atom-economic approach to nitriles, the transition metal-catalyzed hydrocyanation of alkenes (or alkynes) involving the formal addition of HCN remains a challenging task.¹ The modular TADDOL-derived phosphine-phosphite ligands of type 1 developed by the Schmalz group proved to be successful in several asymmetric metal-catalyzed transformations.² These chiral ligands are accessible in only 4 synthetic steps and gave superior results in the enantioselective Ni-catalyzed hydrocyanation of vinylarenes 3.³,⁴

Scheme 1: a) Modular phosphine-phosphite ligands; b) Enantioselective hydrocyanation of vinylarenes; c) Hydrocyanation of phenyl alkenes; d) Hydrocyanation of homostilbenes; e) Potential application.

In the search for novel atom-economic methodologies we are further investigating possible applications of this protocol. With ω-phenyl-1-alkenes 5 Ni-chain-walking leads to the formation of benzylic nitriles 6. This phenomenon was also studied with homostilbenes 7. Attempts to apply the Ni-catalyzed hydrocyanation in the synthesis of new allocolchicine derivatives are underway.

References:
Total Synthesis of Ageladine A and Photoageladine

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The fluorescent alkaloid ageladine A (1) was isolated from the marine sponge Agelas nakamurai by the Fusetani group.[1] Interestingly, pH-dependent fluorescence of 1 was observed with a maximum at pH 3–4.[2] In the light of the chemoselective photoreactivity of 2-azidobenzimidazole derivatives towards amino acids and peptides, we wondered whether it is possible to design an azido analog of ageladine A (1) that would become fluorescent on binding to target molecules. In the first phase of the project, a synthesis of ageladine A (1) was to be developed that would also provide a “photoageladine” 2 carrying an azido instead of an amino group in the 2-position of the imidazopyridine core.

Figure 1: Structures of ageladine A (1), photoageladine 2, tricyclic imidazolone 3, and BODIPY-inspired boron complex 4.

Differing from the existing total syntheses for ageladine A (1)[3], we started with a pyridine derivative instead of building up the pyridine ring. The biaryl axis of tricycle 3 was assembled in satisfactory yield only when a Pd-precatalyst was employed. As in other syntheses of the pyrrole-imidazole alkaloids, the regio- and chemoselective dibromination of the pyrrole section proved to be challenging. We solved that problem by synthesizing the BODIPY-like boron complex 4 that underwent smooth dibromination. Decomplexation to photoageladine 2 was accomplished with ZrCl4 in MeCN/MeOH. Reduction of the azide to the amine succeeded with Na2S and provided ageladine A (1, 7.9% over 9 steps). Encouragingly, the fluorescence of the azido compounds is much weaker than of the amino compounds.

References:
Evonik Preisverleihung des JCF Münster

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Since around ten years the JCF Münster organizes a special yearly prize, honouring exceptional accomplishments during the doctoral or master thesis. The prize is sponsored by Evonik and always accompanied by a small lecture by Evonik and a guest lecture organized by the JCF. The event is followed by an open get-together afterwards with drinks and pretzels as an opportunity for a friendly exchange between recipients, professors, Evonik and guest lecturers.

The prize is a joint project of JCF, Evonik and the professors of the chemistry faculty. Professors and students can propose candidates and a jury consisting of professors from each institute ranks the applicants based on different criteria.

The event is one of the longest standing ones of the JCF Münster and one of our biggest opportunities that is used for the solicitation of new members. We are thankful to Evonik for the longstanding cooperation and sponsorship of this special event and we hope this can inspire other JCFs for similar projects!
Melt-processable Polyacrylonitrile Precursor for FDM-printing

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Due to their tuneable surface area and high electric conductivity, porous carbon represents a suitable material for electrodes in double-layer capacitors. Today, carbon electrodes are often produced from active carbon that comes as a powder. The required structural integrity of the electrode can only be achieved by mixing the active material powder with binder materials.¹,² However, these binders are often electrochemically inactive, decreasing the overall performance of the electrode by blocking of the surface and porosity of the active material. A widely employed precursor for carbon materials in mechanical and structural applications is polyacrylonitrile (PAN). PAN can be converted into carbon in a thermal conversion process. Unfortunately, PAN is typically manufactured as a fiber in solvent intensive wet- and dry-spinning processes, limiting the shape of the electrodes to fabrics and non-wovens with limited conductivity between fibers. Moreover, the spinning process is costly, as large amounts of solvent are required, which need to be recovered when transferring the process to industrial scales.

Here, we present the realization of a melt-processable PAN as a carbon precursor. We copolymerize a plasticizer, which is produced from inexpensive substrates. The internally plasticized melt-PAN copolymer exhibits a $T_g$ as low as 60 °C, enabling melt-processing well below the stabilization/oxidation temperature. The melt-PAN can be processed by fused deposition modelling without solvents, resulting in monolithic and binder-free carbon structures after thermal conversion.

I will present the synthesis and subsequent processing steps and the electrochemical properties of this new class of materials. 3D-printed electrodes from this material exhibit specific capacities of up to 39 mF/cm².

References:

Azo bond formation on metal surfaces

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On Surface Chemistry has attracted extensive attention as a bottom up strategy for the synthesis of two dimensional materials with interesting properties and functions. Various organic reactions have been realized on metal surfaces. [1,2,3,4]

N based functional groups such as azo groups show valuable properties in photo switching. [5] They are obtained through azo coupling using diazonium salts in solution phase chemistry, but the cross coupling of nitro and amino compounds is still challenging. In on surface chemistry, the redox cross coupling of nitroarenes and arylamines was realized on a silver surface (Figure 1). In comparison with nitro nitro and amio amino homocoupling, this is the most efficient reaction on the surface.

![Figure 1: Brutto reaction equation of the Redox Coupling of a bifunctional monomer to linear azo polymers and STM images of the nanostructures on Ag(111) before and after the reaction.](image)

XPS measurements and theoretically and experimentally analyzed model compounds further support the correct structural assignment. It was found, that the metal type and the surface orientation have a significant influence on the reaction outcome. Based on DFT calculations a step-wise formation of partially oxidized/reduced precursors from the starting material along with N–N bond formation is suggested as the most likely reaction pathway.

References:
Carbodiimide-driven dimerization and self-assembly of artificial, ribose-based amphiphiles


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Dissipative reaction cycles can give rise to chemical systems with life-like properties. [1,2] Although ribonucleotide-based amphiphiles have been reported previously, [3] the generation of a dissipative reaction network based on the aggregation of these building blocks is still elusive. [4] Herein, we report the synthesis, self-assembly, and dimerization of novel ribonucleotide-based amphiphiles. Notably, we observed that the addition of 1 ethyl-3-(3-dimethylaminopropyl)-carbodiimide (EDC) leads to rapid and selective dimerization of the amphiphiles into pyrophosphates, which decreases the critical aggregation concentration (CAC) by a factor of 25 when compared to the monomers, leading to the in-situ formation of large aggregates (Figure 1). [5] Even though our efforts to complete the dissipative reaction cycle were unsuccessful, this work contains valuable lessons for those who seek to address a crucial weakness of the RNA world hypothesis by combining fuel-driven oligomerization with compartmentalization.

Figure 1: The EDC-driven dimerization of ribose-based amphiphiles leads to an in-situ reduction of the critical aggregation concentration (CAC) and formation of large aggregates.

References:
Influence of the PEO-\textit{b}-PHA Block Lengths on the Mesopore Size

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Mesoporous materials are evoking increasing interest due to the large and readily accessible interface area they possess. Consequently, porosity can be found in various applications, such as heterogeneous catalysis, photocatalysis, coatings, and capacitors\textsuperscript{[1]}. Both pore size and wall thickness are crucial parameters governing electrical, optical, and mechanical properties of thin film devices, as well as determining heat and mass transport in porous catalysts. In this regard, it is highly desirable to tailor mesoporosity by suitable soft templates. Especially, in a medium pore size regime of about 50 nm comprising a balance between a still high surface area and an unrestricted mass flow within the pore structure, the choice of proper soft templates, however, is limited. Here, a library of poly(ethylene oxide)-block-poly(hexyl acrylate) copolymers was synthesized by means of a supplemental activator reducing agent atom transfer radical polymerization (SARA ATRP)\textsuperscript{[1]} enabling an adjustment of the PHA block length. In addition, the choice of the PEO macroinitiator offered a variation in PEO block length. Hence, a relationship between block length and porosity was deduced after soft templating of silica and subsequent argon physisorption experiments. The pore size turned out to be highly sensitive to the PHA block length but almost not to the PEO micelle corona. The set of accessible and reproducibly tunable pore sizes in a regime around 50 nm paths the way to systematic studies concerning the ideal porosity for e.g., electrocatalytic applications in regard to maximizing stability and activity.

Figure 1: Synthesis of PEO-\textit{b}-PHA block copolymers as templates for mesoporous materials.

References:
Studies towards the total synthesis of Camporidine A

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Camporidine A belongs to the class of polyketide alkaloids and was isolated and characterized by Hong and coworkers from gut bacteria of the genus Streptomyces of the carpenter ant Camponotus kiusiuensis in 2019. [1] It bears several interesting structural motifs condensed on a small molecule. Especially the central piperidine-cyclopentene-epoxide 6/5/3 tricyclic core structure containing four stereocenters and a huge variety of different functionalities is an interesting challenge for synthetic chemists. Furthermore, the antimetastatic and anti-inflammatory activities render Camporidine A an interesting and challenging target molecule for enantioselective total synthesis. [1]

Scheme 1: Short retrosynthesis of Camporidine A including a central substrate controlled imino-Diels-Alder reaction.

The core idea is to build the tetrahydropyridine core structure with two of the needed stereocenters in a substrate controlled imino-Diels-Alder reaction. An intermolecular as well as an intramolecular imino-Diels-Alder approach were examined upon its feasibility. While the diene can be obtained in an enantioselective fashion starting from cyclopentenone and 1-octine via an enantioselective CBS-reduction and a Suzuki cross-coupling.

References:
Luminescent properties of the FeS$_2$@YF$_3$:Yb$^{3+}$,Er$^{3+}$ nanocomposite

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Nanocomposites are nanomaterials consisting of multiphase solid materials with at least one dimension in the nanoscale. The choice of FeS$_2$ as a plasmonic material is important due to both magnetic and plasmonic properties, and low cost of its precursors. [1] The FeS$_2$@YF$_3$:Yb$^{3+}$/Er$^{3+}$ core@shell materials with luminescent-plasmonic properties were synthesized with the use of the hydrothermal method. Properties of the obtained composite materials were analyzed. Both materials i.e. FeS$_2$@YF$_3$:Yb$^{3+}$/Er$^{3+}$ and YF$_3$:Yb$^{3+}$/Er$^{3+}$ exhibit visible-green up-conversion luminescence. Different ratio between emission bands (i.e. color tuning) was observed in synthesized core/shell nanomaterials due to interaction between the core and the shell. [2] These innovative, multifunctional materials can be used in optoelectronics, detection and security systems, and as novel sensors.

Figure 1: Emission spectra of YF$_3$:Yb$^{3+}$,Er$^{3+}$ and FeS$_2$@YF$_3$:Yb$^{3+}$,Er$^{3+}$ materials. Inset: Emission spectra of FeS$_2$@YF$_3$:Yb$^{3+}$,Er$^{3+}$ in function of the increasing laser power.

References:

[1] Li, B.; Huang, L.; Zhong, M.; Wei, Z.; Li, J. Electrical and magnetic properties of FeS$_2$ and CuFeS$_2$ nanoplates. RSC Advances 2015, 5, 91103–91107

Comparison of the impact of a fully fused and a covalently attached naphthaloylenebenzene moiety on the spectroscopic properties of Cu(I) photosensitizers

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The systematic study and improvement of photosensitizers is the prerequisite to bring solar energy conversion into practice. To this end, the integration of donor-acceptor units like naphthalene imide or diimide derivatives allows to adapt the photophysical and electrochemical properties of a chromophore in a wide range.\[1\] In our research, a novel rylene type diimine ligand (named biipo) with a fully rigid and extended π-system in its backbone was prepared by directly fusing a 1,10-phenanthroline building block with 1,8-naphthalimide.\[2,3\] For comparison, also the NIphen ligand and its heteroleptic Cu(I) complex [(xant)Cu(NIphen)]PF$_6$ (CuNIphen, with xant = xantphos) was synthesized by covalently attaching 1,8-naphthalimide to 1,10-phenanthroline.

It is of great interest to compare the spectroscopic and electrochemical properties of the fully fused and the covalently attached systems. Therefore, a combination of single crystal X-ray diffraction (XRD), cyclic and differential pulse voltammetry, time-resolved emission and transient absorption spectroscopy as well as (TD)-DFT calculations was used to analyze the redox behavior and excited state properties in detail.

References:


Harnessing ynamide activation to access deuterated carbonyls

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In modern organic and medical chemistry, isotopic labelling has proven a powerful tool for the elucidation of mechanisms and metabolic pathways,[1,2] by enabling the precise monitoring of specific atoms. Recent discoveries have showcased that, due to altered cytochrome P₄₅₀ metabolism, drugs with selectively incorporated deuterium atoms can possess improved pharmacokinetic properties and reduced toxicity.[3] Given the vast utility and potential of deuterium labelling, easy and efficient access to isotopically enriched building blocks is of paramount importance.

Based on our expertise in the handling of keteniminium ions, we envisioned to harness their reactivity for the generation of deuterium-enriched carbonyls.[4] In this work, we present the activation of ynamides using a deuterated Brønsted acid (Scheme 1), followed by trapping with D₂O, to generate the α-bisdeuterated carbonyls in high yields and with excellent levels of isotope incorporation.[5] The synthetic utility of this transformation is further highlighted by gram scale reaction and further functionalisations, without deuterium erosion.

Scheme 1: Formation of α-bisdeuterated imides by activation of ynamides.

References:
MXene-assisted preparation of well-intergrown ZIF-67 membrane for helium separation

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While many efforts have been made in improving the hydrogen separation performance of MOF membranes (metal-organic frameworks) over the last decades, attention about helium separation has been rarely raised despite the soar of helium price. As a member of MOF family, ZIF-67 has a suitable pore size for helium separation. However, it prefers homogenous nucleation, hindering the preparation of continuous membranes.

MXene is a new family of 2D materials with the general formula $M_{n+1}X_nT_x$, where M is one or more early transition metals, X is carbon and/or nitrogen, T_x stands for the surface terminations (e.g. –OH), and n = 1 – 4. By the assistance of laminarly stacked Ti$_3$C$_2$T$_x$ films, well-intergrown ZIF-67 membranes were prepared. Several analytic methods, including time-dependent in-situ XRD, HRTEM, and EELS, have found that the MXene films, despite being as thin as 90 nm, could host a high amount of Co (II) ions.

Figure 1: SEM images of (a) MXene-assisted ZIF-67 membrane, (b) rim of the same disk without MXene coverage, and (c) cross-section of the MXene-assisted ZIF-67 membrane.

As shown in Figure 1, well-intergrown ZIF-67 membranes (4.1 μm thick) were formed on Co (II)-MXene modified α-Al$_2$O$_3$ disks, while only a few discrete ZIF-67 grains were present in the MXene-free area after solvothermal synthesis. Single-gas and mixed-gas permeation experiments showed that the ZIF-67 membranes exhibited excellent gas separation performance and long-term thermal stability for the gas mixtures He/N$_2$ and He/CH$_4$, superior to the state-of-the-art MOF membranes.
Responsive Polymer Morphologies through Arylazopyrazole Photoswitches

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Supramolecular structures, which can be reversibly switched in shape, are extremely interesting for the development of intelligent materials. In this project we created light-responsive polymers, which can build different aggregates in aqueous solution. Amphiphilic block copolymers with varying block length were synthesized via reversible-addition-fragmentation-chain-transfer (RAFT) polymerization. Our polymers can self-assemble in water and build different supramolecular morphologies as micellar or wormlike structures. The hydrophilic block consists of water-soluble poly(oligo(ethylene glycol) methacrylate (POEGMA), while the hydrophobic part contains an arylazopyrazole (AAP) derivative as a photoswitch. With the implementation of the light-responsive AAP into the block copolymer the hydrophobicity of the block chain can be changed via irradiation with green light (520 nm, E-Isomer) and UV light (365 nm, Z-Isomer). The AAP in the polymer could be switched from E- to Z-state reversible over various cycles. The configuration of the AAP also has an influence to the aggregation behavior of the polymers. With different self-assembly methods different morphologies depending on the isomerization state of the AAP in the block copolymer could be achieved. So, the polymer containing the E-Isomer can form micelles, while with the one containing the Z-Isomer wormlike structures could be obtained.

Figure 1: Light-responsive polymer system, building different supramolecular structures dependent on configuration of the AAP in the hydrophobic block of the amphiphilic polymer.
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