BEAM Conference

March 19th – March 21st 2025

Löwengebäude Halle
Universitätsplatz 11

Handout

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Organizing Committee

Prof. Dariush Hinderberger

Prof. Rebecca Waldecker

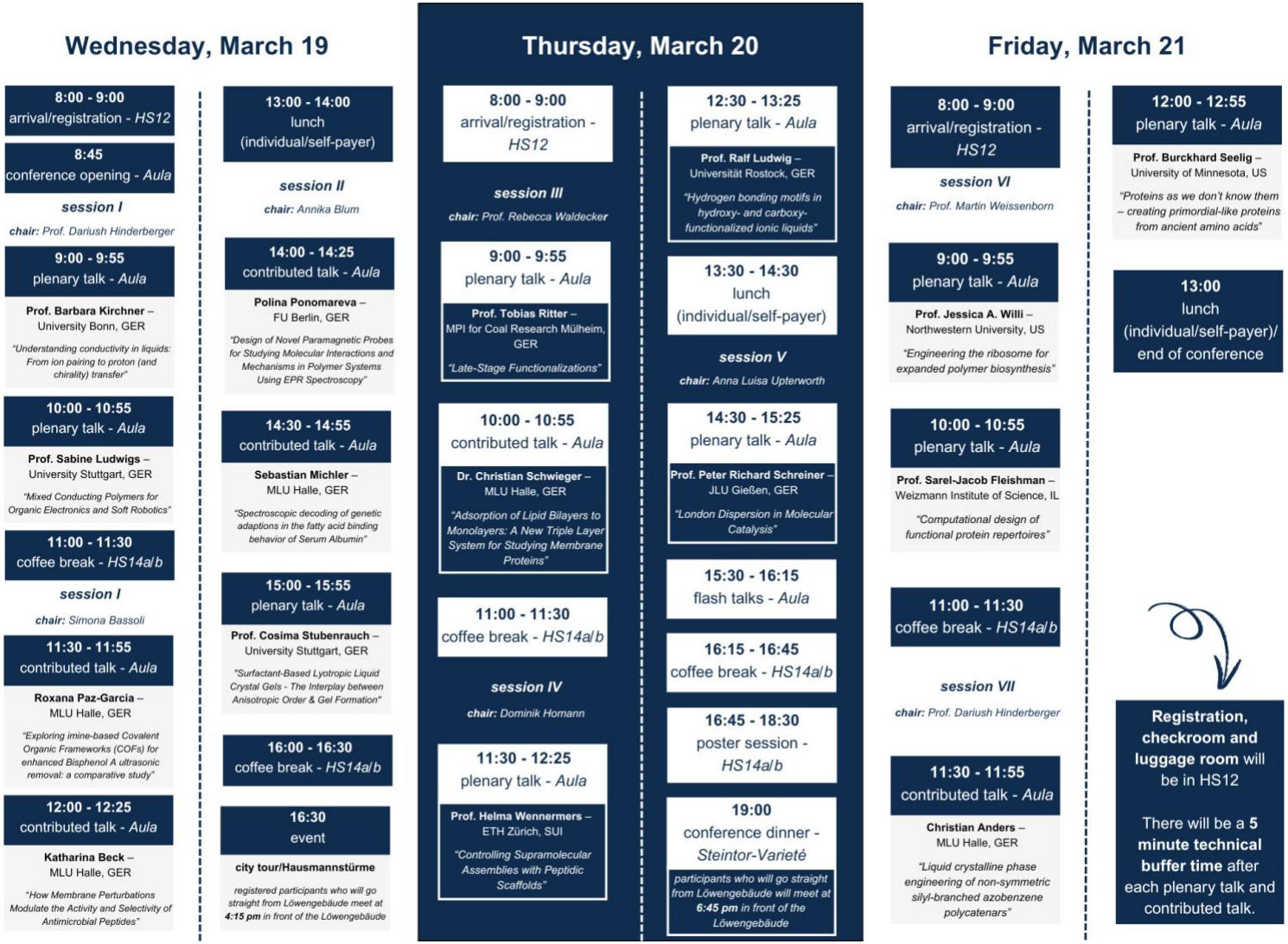
Prof. Martin Weissenborn

Dr. Imme Sakwa-Waltz

Lisa Krahnefeld

Saskia Walther

Program


Wednesday, March 19
8:00 - 9:00
arrival/registration - HS12
8:45
conference opening - Aula
session I
chair: Prof. Dariush Hinderberger
9:00 - 9:55
plenary talk - Aula
Prof. Barbara Kirchner – University Bonn, GER
"Understanding conductivity in liquids: From ion pairing to proton (and chirality) transfer"
10:00 - 10:55
plenary talk - Aula
Prof. Sabine Ludwigs – University Stuttgart, GER
"Mixed Conducting Polymers for Organic Electronics and Soft Robotics"
11:00 - 11:30
coffee break - HS14a/b
session I
chair: Simona Bassoli
11:30 - 11:55
contributed talk - Aula
Roxana Paz-Garcia – MLU Halle, GER
"Exploring imine-based Covalent Organic Frameworks (COFs) for enhanced Bisphenol A ultrasonic removal: a comparative study"
12:00 - 12:25
contributed talk - Aula
Katharina Beck – MLU Halle, GER
"How Membrane Perturbations Modulate the Activity and Selectivity of Antimicrobial Peptides"
13:00 - 14:00
lunch (individual/self-payer)
session II
chair: Annika Blum
14:00 - 14:25
contributed talk - Aula
Polina Ponomareva – FU Berlin, GER
"Design of Novel Paramagnetic Probes for Studying Molecular Interactions and Mechanisms in Polymer Systems Using EPR Spectroscopy"
14:30 - 14:55
contributed talk - Aula
Sebastian Michler – MLU Halle, GER
"Spectroscopic decoding of genetic adaptions in the fatty acid binding behavior of Serum Albumin"
15:00 - 15:55
plenary talk - Aula
Prof. Cosima Stubenrauch – University Stuttgart, GER
"Surfactant-Based Lyotropic Liquid Crystal Gels - The Interplay between Anisotropic Order & Gel Formation"
16:00 - 16:30
coffee break - HS14a/b
16:30
event
city tour/Hausmannstürme
registered participants who will go straight from Löwengebäude meet at 4:15 pm in front of the Löwengebäude
Thursday, March 20
8:00 - 9:00
arrival/registration - HS12
session III
chair: Prof. Rebecca Waldecker
9:00 - 9:55
plenary talk - Aula
Prof. Tobias Ritter – MPI for Coal Research Mülheim, GER
"Late-Stage Functionalizations"
10:00 - 10:55
contributed talk - Aula
Dr. Christian Schwieger – MLU Halle, GER
"Adsorption of Lipid Bilayers to Monolayers: A New Triple Layer System for Studying Membrane Proteins"
11:00 - 11:30
coffee break - HS14a/b
session IV
chair: Dominik Homann
11:30 - 12:25
plenary talk - Aula
Prof. Helma Wennermers – ETH Zürich, SUI
"Controlling Supramolecular Assemblies with Peptidic Scaffolds"
12:30 - 13:25
plenary talk - Aula
Prof. Ralf Ludwig – Universität Rostock, GER
"Hydrogen bonding motifs in hydroxy- and carboxy-functionalized ionic liquids"
13:30 - 14:30
lunch (individual/self-payer)
session V
chair: Anna Luisa Upterworth
14:30 - 15:25
plenary talk - Aula
Prof. Peter Richard Schreiner – JLU Gießen, GER
"London Dispersion in Molecular Catalysis"
15:30 - 16:15
flash talks - Aula
16:15 - 16:45
coffee break - HS14a/b
16:45 - 18:30
poster session - HS14a/b
19:00
conference dinner - Steintor-Varieté
participants who will go straight from Löwengebäude will meet at 6:45 pm in front of the Löwengebäude
Friday, March 21
8:00 - 9:00
arrival/registration - HS12
session VI
chair: Prof. Martin Weissenborn
9:00 - 9:55
plenary talk - Aula
Prof. Jessica A. Willi – Northwestern University, US
"Engineering the ribosome for expanded polymer biosynthesis"
10:00 - 10:55
plenary talk - Aula
Prof. Sarel-Jacob Fleishman – Weizmann Institute of Science, IL
"Computational design of functional protein repertoires"
11:00 - 11:30
coffee break - HS14a/b
session VII
chair: Prof. Dariush Hinderberger
11:30 - 11:55
contributed talk - Aula
Christian Anders – MLU Halle, GER
"Liquid crystalline phase engineering of non-symmetric silyl-branched azobenzene polycatenars"
12:00 - 12:55
plenary talk - Aula
Prof. Burckhard Seelig – University of Minnesota, US
"Proteins as we don't know them – creating primordial-like proteins from ancient amino acids"
13:00
lunch (individual/self-payer)/ end of conference
Registration, checkroom and luggage room will be in HS12
There will be a 5 minute technical buffer time after each plenary talk and contributed talk.

WIFI

SSID: event-net
Guest User Name: beam25@uni-halle.de Password: uM#7Jw/N

Instructions:
1. connect to the WLAN “event-net”.
2. After a successful connection, open the browser (accept the certificate warning if necessary).
You will be asked for your user name and password.
3. confirm entry --> done

The event network is an unencrypted conference access!

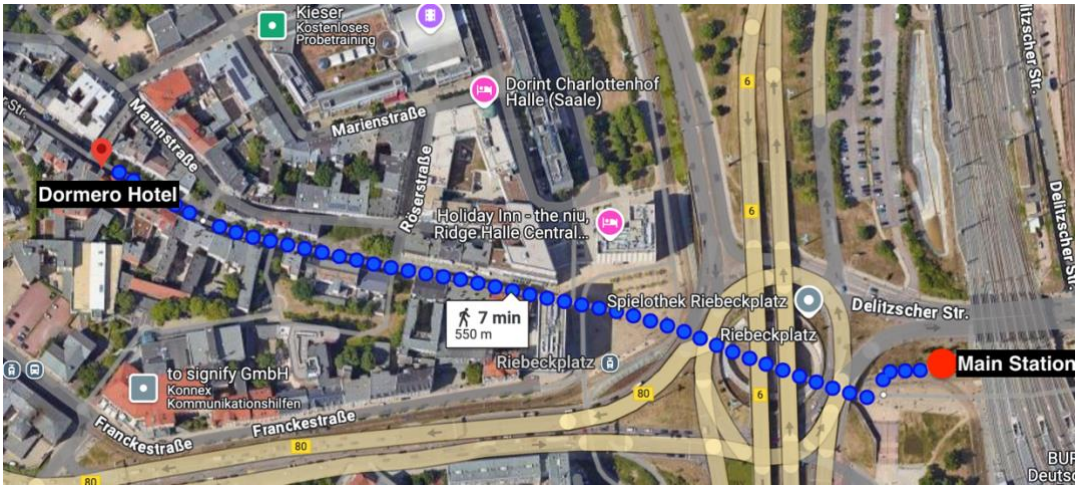
Avoid transmitting sensitive data or encrypt your access yourself (VPN).

Route Descriptions

Main Station - Dormero

From Main Station (Halle HBF) to Dormero Halle is a distance of approximately 700m (6-8 min.) across the Riebeckplatz (underneath the roads).

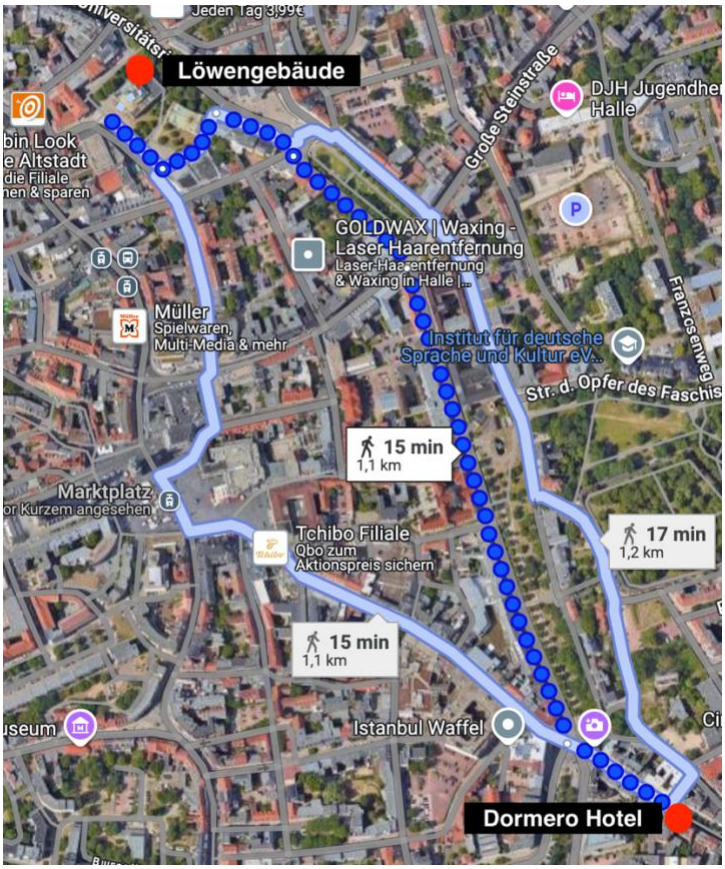
Leave main station from main entrance onto Hans-Dietrich-Genscher-Platz. Turn left towards Riebeckplatz and cross Riebeckplatz. Continue on Leipziger Straße, the destination is on the left side.



1. Leave main station from main entrance onto Hans-Dietrich-Genscher-Platz.
2. Turn left towards Riebeckplatz.
3. Cross Riebeckplatz, continue on Leipziger Str.
4. The destination is on the left side.

Dormero - Löwengebäude

From Dormero Hotel Halle to Löwengebäude is a distance of approximately 1,2m (15-17 min.).



via Hansering:

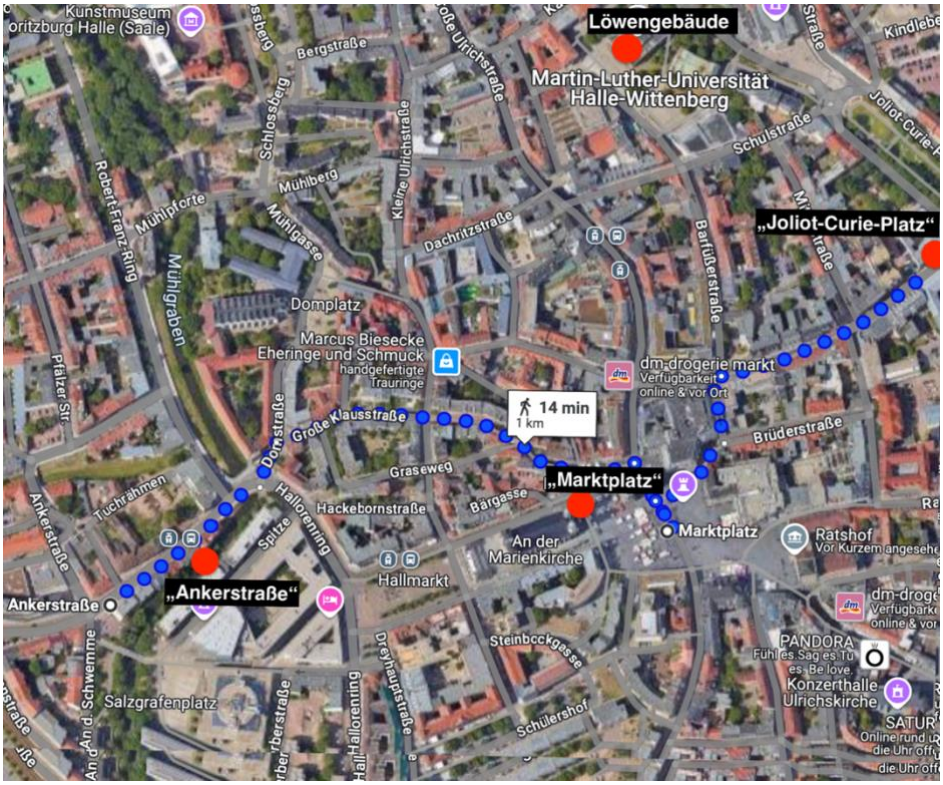
1. Leave hotel and turn left down Leipziger Straße to Leipziger Turm.
2. Turn right into Hansering and follow the street until you come to Joliot-Curie-Platz.
3. Continue straight ahead and onto Universitätsring.
4. After house number 4 on the left, turn left onto Universitätsplatz.
5. The Löwengebäude is on the left side.

via Marktplatz:

1. Leave hotel and turn left down Leipziger Straße to Leipziger Turm.
2. Go through the traffic lights and onto the lower part of Leipziger Straße.
3. Follow the pedestrian zone to Marktplatz.
4. Cross Marktplatz to the right.
5. Turn into Kleinschmieden and go straight ahead.
6. Follow Grosse Ulrichstraße to the nt-Café.
7. Turn right into Schulstraße.
8. Turn left onto Universitätsplatz. Go up the stairs.
9. The Löwengebäude is in front of you.

Ankerhof - Löwengebäude

From Hotel Ankerhof to Löwengebäude is a distance of approximately 900m (13-14 min.).

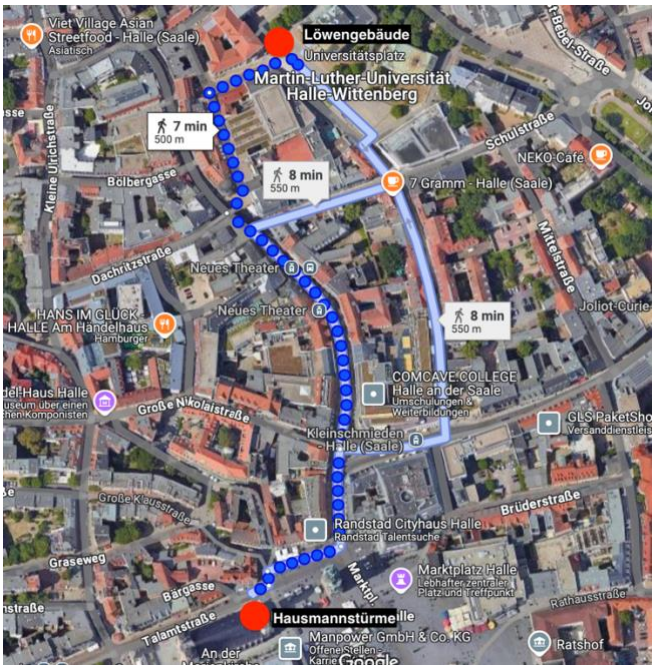


1. Leave the hotel and turn left into Ankerstraße.
2. Turn right and continue to follow Ankerstraße.
3. Turn left into Robert-Franz-Ring and follow the road.
4. Turn right into Mühlpforte.
5. Continue to follow the road when it becomes Mühlberg.
6. Continue straight ahead until you cross Kleine Ulrichstraße.
7. Continue straight ahead into Bölbergasse until you reach Große Ulrichstraße.
8. Turn right into Spiegelstraße.
9. Follow it until you turn right onto Universität-splatz. Go up the stairs.
10. The Löwen-gebäude is directly in front of you.

Löwengebäude - Marktplatz

On Wednesday afternoon some of the participants will take part in the city tour or the tour of the "Hausmannstürme". The meeting point for the city tour is the tourist information on the "Marktplatz", the participants of the other tour will meet on site at the "Marktkirche" on the "Marktplatz".

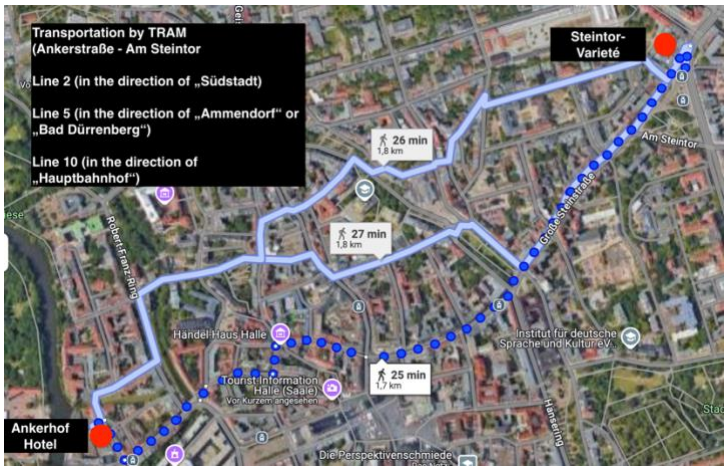
The participants who will go straight from Löwengebäude to the meeting point will meet at 4:15 pm in front of the Löwengebäude and walk together.



1. Leave the Löwengebäude and walk onto Universitätsplatz.
2. Turn left, leave Universitätsplatz and walk onto Barfüßerstraße.
3. Follow it until you come to Große Steinstraße.
4. Cross the street and turn right.
5. Turn into Kleinschmieden and walk onto the Marktplatz.
6. The tourist information center is on the right, the Marktkirche is on the other side of the street.

Ankerhof – Steintor-Varieté (conference dinner)

The conference dinner on Thursday will be at the Steintor-Varieté.
From Hotel Ankerhof to Steintor-Varieté is a distance of approximately 1,8km (25-27 min.).



via Marktplatz:

1. Leave the hotel and turn right into Ankerstraße.
2. Turn left into Mansfelder Straße and follow the road.
3. Turn right into Hallorenring and follow it until you reach Hallmarkt.
4. Go straight ahead until you reach Marktplatz
5. Go to the left into Kleinschmieden and then to the right into Große Steinstraße.
6. Follow the road until you reach Am Steintor.
7. The Steintor-Varieté is on the left.

via Löwengebäude:

1. Leave the hotel and turn left into Ankerstraße.
2. Turn right and continue to follow Ankerstraße.
3. Turn left into Robert-Franz-Ring and follow the road.
4. Turn right into Mühlpforte.
5. Continue to follow the road when it becomes Mühlberg.
6. Continue straight ahead until you cross Kleine Ulrichstraße.
7. Continue straight ahead into Bölbergasse until you reach Große Ulrichstraße.
8. Turn right into Spiegelstraße.
9. Follow it until you turn right onto Universitätsplatz. Go up the stairs.
10. Leave the Universitätsplatz on the left side of the Löwengebäude.
11. Cross the street and and go straight ahead into Unterberg.
12. Turn to the right into August-Bebel-Straße and then turn to the left into Marthastraße.
13. Follow Marthastraße until you reach Luisenstraße.
14. You can either follow Luisenstraße on the right or follow Adam-Kuckhoff-Straße and turn right onto Steintorcampus.
15. In both cases you go straight ahead.
16. You turn right into Luisenstraße and go up the stairs.
17. Go straight until you reach Am Steintor.
18. The Steintor-Varieté is on the left.

Dormero – Steintor-Varieté (conference dinner)

From Dormero Hotel to Steintor-Varieté is a distance of approximately 1,3m (18 min.).

via Magdeburger Straße:

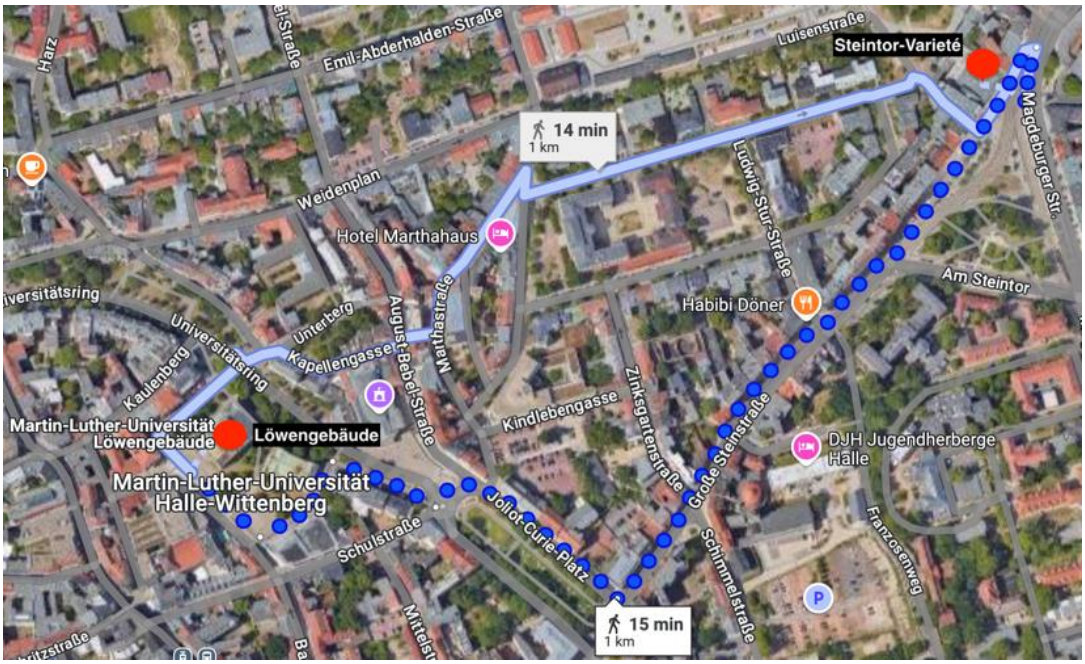
1. Leave the hotel and go straight ahead into Augustastraße.
2. Follow Augustastraße until you reach Charlottenstraße.
3. Turn left into Charlottenstraße.
4. Turn right into Anhalter Straße.
5. Follow it until you turn left into Dorotheenstraße.
6. Go through Stadtpark and follow Magdeburger Straße on the right until you reach Am Steintor.
7. The Steintor-Varieté is straight ahead.

via Joliot-Curie-Platz

1. Leave hotel and turn left down Leipziger Straße to Leipziger Turm.
2. Turn right into Hansering and follow the street until you come to Joliot-Curie-Platz.
3. Turn right into Große Steinstraße.
4. Follow the road until you reach Am Steintor.
5. The Steintor-Varieté is on the left.

Löwengebäude – Steintor-Varieté (conference dinner)

From Löwengebäude to Steintor-Varieté is a distance of approximately 1km (14-15 min.).



via Steintorcampus:

1. Leave the Löwengebäude and go to the right.
2. Leave the Universitätsplatz.
3. Cross the street and and go straight ahead into Unterberg.
4. Turn to the right into August-Bebel-Straße and then turn to the left into Marthastraße.
5. Follow Marthastraße until you reach Luisenstraße.
6. You can either follow Luisenstraße on the right or follow Adam-Kuckhoff-Straße an turn right onto Steintorcampus.
7. In both cases you go straight ahead.
8. You turn right into Luisenstraße and go up the stairs.
9. Go straight until you reach Am Steintor.
10. The Steintor-Varieté is on the left.

via Joliot-Curie-Platz:

1. Leave the Löwengebäude and walk onto Universitätsplatz.
2. Turn left and leave Universitätsplatz.
3. Turn left again and walk onto Schulstraße.
4. When you reach Joliot-Curie-Platz turn to the right and go straight ahead.
5. Turn left into Große Steinstraße.
6. Follow the road until you reach Am Steintor.
7. The Steintor-Varieté is on the left.

Abstracts - plenary talks

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Understanding conductivity in liquids: From ion pairing to proton (and chirality) transfer

Barbara Kirchner*

*Mulliken Center for Theoretical Chemistry, University of Bonn, kirchner@thch.uni-bonn.de

Ion pairing is often used to explain a reduced electrical or ionic conductivity measured by impedance spectroscopy compared to ion diffusivities measured by pulsed field gradient. In this presentation we focus on the following questions: How are ion pairs defined? Ion pair versus ion association: Are there other effects like charge transfer, polarizability, or charge screening that should be considered? Is this related to charge scaling in force fields? How do we calculate electrical conductivity? How do we control uncertainties in this and other properties? Strutural diffusion in ionic liquids can enable fast transport. Mixtures of N-methylimidazole as well as similar cations and acetic acid show an unexpected high ionic conductivity. Is water addition necessary to enable a Grotthuss-like diffusion? Furthermore, we discuss the behavior of chiral solutes in different ionic liquids where the induction of optical acitivity is observed in achiral ionic liquids. We try to understand how chirality extend to solvents. Given time, we also present ionic liquids in confinement and discuss uncertainties in modellling of ionic liquid properties.

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Mixed Conducting Polymers for Organic Electronics and Soft Robotics

Sabine Ludwigs 1*

*IPOC – Functional Polymers, Institute of Polymer Chemistry (IPOC), University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart
sabine.ludwigs@ipoc.uni-stuttgart.de

My presentation will give an overview over our recent studies on design and characterization of polymeric mixed conductors for organic electronics and switchable devices for soft robotics applications.
Self-assembly and controlled crystallization in films is a major topic in this context and different techniques to manipulate the morphology will be highlighted. A further focus is put on electrochemistry as versatile tool to control the doping level of organic semiconductors and target different redox states for, e.g., conductivity tuning in electronic devices.[1] Both, in-situ as well as ex-situ electrochemical techniques are discussed and correlations to the morphology of the films after doping are established.[2]
Beyond electronic applications, electrochemical switching can be used to induce volume swelling and deswelling. The role of mixed ionic-electronic transport[3] for switchable surfaces and soft actuators[4] will be elucidated with various in-situ techniques.

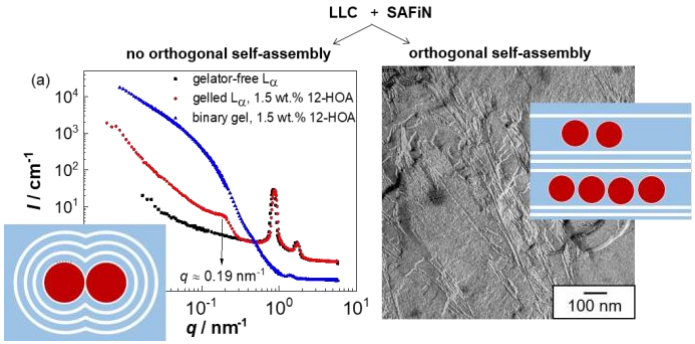
1 D. Neusser et al. *High Conductivities of Disordered P3HT films by an Electrochemical Doping Strategy*, Chemistry of Materials 2020, 32, 6003.
2 Y. M. Gross et al. *From Isotropic to Anisotropic Conductivities in P(NDI2OD-T2) by (Electro-)Chemical Doping Strategies*, Chemistry of Materials 2019, 31, 3542
3 M. Wieland et al. *Humidity-Controlled Water Uptake and Conductivities in Ion and Electron Mixed Conducting Polythiophene Films*, ACS Applied Materials & Interfaces, 2020, 12, 6742.
4 C. Dingler et al. *From Understanding Mechanical Behavior to Curvature Prediction of Humidity-Triggered Bilayer Actuators*, Advanced Materials 2021, 33, 2007982.

Surfactant-Based Lyotropic Liquid Crystal Gels

- The Interplay between Anisotropic Order & Gel Formation -

Cosima Stubenrauch, Katja Steck, Sonja Dieterich, Frank Gießelmann
Institute of Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Surfactant-based lyotropic liquid crystal gels (LLCGs) are **soft materials** which combine the **anisotropic order of a surfactant-based lyotropic liquid crystal** with the **mechanical stability of a gel**. The most prominent example of a **„natural" LLCG is the cell**. This presentation is about potential applications of LLCGs and the different strategies via which LLCGs can be obtained. The main focus is on gelation with **low molecular weight gelators (LMWG)**, which form self-assembled fibrillar networks (SAFiN). We will discuss whether or not the resulting LLCGs are **orthogonal self-assembled systems**, i.e. systems where the two coexisting structures (lyotropic liquid crystal and SAFiN) form independently.



Surfactant-Based Lyotropic Liquid Crystal Gels – the Interplay between Anisotropic Order and Gel Formation (Review), K. Steck, S. Dieterich, C. Stubenrauch, F. Giesselmann, *J. Mater. Chem. C*, **2020**, *8*, 5335-5348

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Late-Stage Functionalizations

Prof. Tobias Ritter

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ritter@mpi-muelheim.mpg.de

Late-stage functionalization reactions reliably functionalize already complex molecules to quickly access value-added molecular diversity. Late-stage functionalization is desirable in many areas of discovery such as in drug or agrochemical development, and a requirement in other areas such as the synthesis of positron-emission tomography (PET) tracers. I will describe the development of novel, modern highly selective reactions in late-stage functionalization, as well as their application in transition-metal-catalyzed and photoredox reactions, with a focus on the synthesis of 18F and 19F containing complex small molecules. In particular, I will describe the development of broadly useful C-H thianthrenation reactions, as well as the conceptual differences and advances of thianthrenium chemistry when compared to conventional reaction chemistry, with development towards applications in catalysis, drug discovery, and medicine.

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Controlling Supramolecular Assemblies with Peptidic Scaffolds

Helma Wennemers

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Self-assembly and selective recognition events involving proteins are critical in nature for the function of numerous different processes, for example, catalysis, signal transduction or the controlled formation of structural components such as bones. My group is intrigued by the question whether also peptides with significantly lower molecular weights compared to proteins can fulfill functions for which nature evolved large macromolecules. Specifically we ask whether peptides can serve as effective asymmetric catalysts, templates for the controlled formation of metal nanoparticles, hierarchical supramolecular assemblies, synthetic collagen based materials, or tumor targeting vectors.

The lecture will focus on our research in supramolecular assemblies and their application in chemical biology and supramolecular chemistry.

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Hydrogen bonding motifs in hydroxy- and carboxy-functionalized ionic liquids

Ralf Ludwig

Physical and Theoretical Chemistry, University of Rostock, 18059 Rostock, Germany
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The unique properties of ionic liquids (ILs) result from the tunable mélange of Coulomb interactions, hydrogen bonding, and dispersion interactions among the constituent ions. In hydroxy-functionalized ILs, local and directional hydrogen bonds (H-bonds) lead to the anticipated formation of ion pairs but also to the elusive formation of cationic clusters. Here, we report how hydrogen-bonding motifs in the bulk liquid and gas phase of hydroxy-functionalized ILs shed light on the general nature of hydrogen bonding. Infrared spectroscopy, nuclear magnetic resonance, neutron diffraction, and molecular dynamics simulations provide information about the structure, strength, and dynamics of cationic clusters in the bulk liquid ILs. Cryogenic ion vibrational predissociation (CIVP) spectroscopy along with density functional theory calculations has established a clear picture about the specific contacts within isolated H-bonded cationic clusters formed in the gas phase. For carboxy-functionalized ILs we provide experimental evidence for doubly H-bonded cationic dimers in the solid, liquid, and gaseous phases. This information from experiment, simulation, and theory provides a fundamental understanding of hydrogen bonding between the ions in ILs.

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London Dispersion in Molecular Catalysis[1]

Peter R. Schreiner

Institute of Organic Chemistry, Justus Liebig University Giessen, prs@uni-giessen.de

The *Gecko* can walk up a glass window because of the adhesion in hydrophobic setae on its toes that convey van der Waals (vdW) interactions with the surface. The attractive part of vdW-interactions is an electron correlation effect referred to as *London dispersion*, an interaction that has been underappreciated in molecular chemistry as being key for structures, reactivity, and catalysis. This negligence is due to the notion that dispersion is considered weak, which is only true for pairs of interacting atoms. For larger structures, the overall dispersion contribution grows rapidly and can amount to tens of kcal mol^{-1}. This presentation shows selected examples that emphasize the importance of inter- and intramolecular dispersion for molecules consisting mostly of first row atoms.[2] This forces us to re-consider our perception of steric hindrance and stereoelectronic effects, and even the transferability of chemical bond parameters from one molecule to another, both in structural chemistry[3] and, in particular, in catalysis.[4] We will also shed light on the possibilities to use machine learning approaches to improve catalytic reactions[5] and highlight the importance of optimizing for differences in activation free energies (vs. enantiomeric excess).[6]

[1] *Reviews:* a) J. P. Wagner, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2015**, *54*, 12274-12296; b) L. Rummel, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2024**, *63*, e202316364.

[2] a) S. Rösel, C. Balestrieri, P. R. Schreiner, *Chem. Sci.* **2017**, *8*, 405-410; b) P. R. Schreiner, L. V. Chernish, P. A. Gunchenko, E. Y. Tikhonchuk, H. Hausmann, M. Serafin, S. Schlecht, J. E. P. Dahl, R. M. K. Carlson, A. A. Fokin, *Nature* **2011**, *477*, 308-311; c) S. Grimme, P. R. Schreiner, *Angew. Chem. Int. Ed.* **2011**, *50*, 12639-12642; d) S. Rösel, H. Quanz, C. Logemann, J. Becker, E. Mossou, L. Cañadillas-Delgado, E. Caldeweyher, S. Grimme, P. R. Schreiner, *J. Am. Chem. Soc.* **2017**, *139*, 7428-7431;

[3] a) J. M. Schümann, J. P. Wagner, A. K. Eckhardt, H. Quanz, P. R. Schreiner, *J. Am. Chem. Soc.* **2021**, *143*, 41-45; b) J. M. Schümann, L. Ochmann, J. Becker, A. Altun, I. Harden, G. Bistoni, P. R. Schreiner, *J. Am. Chem. Soc.* **2023**, *145*, 2093-2097.

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BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Engineering the ribosome for expanded polymer biosynthesis

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The ribosome is an ancient macromolecule that performs highly accurate, efficient and programmable polymer biosynthesis. However, the ribosome is also highly conserved and resistant to changes. Advances in synthetic biology methods now allow us to use the existing machinery of the ribosome as a starting point to engineer and evolve specialized constructs capable of new and improved synthetic function. Our vision is to alter the machinery of the ribosome to expand beyond canonical protein translation and unlock entirely new modes of polymer synthesis. This talk will focus on our research driving ribosome evolution towards expressing difficult products, accepting non-canonical substrates and expanding the genetic code.

The creation of custom specialized ribosomes is a transformative technology for enhanced protein production and creating novel bioactive compounds, with future industry applications in molecular medicine, nanotech, and protein engineering.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Computational design of functional protein repertoires

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Understanding how protein sequence and structure determine function promises to unlock vast opportunities in basic and applied research. We develop strategies that combine phylogenetic analysis, atomistic calculations, and machine learning to optimise natural proteins. Thousands of protein scientists have used these strategies to generate stable therapeutic enzymes, vaccine immunogens, therapeutic antibodies, and membrane proteins for a range of needs in basic and applied research. A stabilised malaria vaccine immunogen designed in our lab has recently entered phase II clinical trials in West Africa. We now present a machine-learning strategy to design and economically synthesize millions of active-site variants that are likely to be stable, foldable, and active. We applied this strategy to design large libraries of enzymes and fluorescent proteins, and experimental screening revealed more than 10,000 functionally diverse proteins in each set. Our methods can be universally applied to optimise biologics, dramatically accelerating the development of promising proteins into useful pharmaceutical reagents and therapeutics. Furthermore, we demonstrate that these methods can be adapted to design completely new-to-nature enzymes with catalytic rates that are orders of magnitude higher than those seen to date. Thus, a unified and principled framework enables the design and optimisation of protein function.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Proteins as we don't know them – creating primordial-like proteins from ancient amino acids

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Billions of years of evolution have shaped the intricate and complex structures of proteins that facilitate most processes in modern biology. All known organisms utilize essentially the same universal genetic code, comprised of 20 amino acids, to encode the huge diversity of proteins necessary for life. Thanks to thousands of three-dimensional structures, scientists have gained a good idea of how proteins function, at least in broad strokes. However, our understanding of 'how proteins work' is likely biased by mostly looking at those proteins that are easily crystallizable and have been optimized by evolution over eons. We are speculating that polypeptides in principle may be able to take on properties and form structures that are different from what has generally been observed in biology so far.
Instead of studying modern biology, we are investigating potential scenarios of how the earliest primordial proteins could have originated. We use high throughput selection and evolution in a test tube to isolate novel proteins from vast libraries of synthetic randomized polypeptides. We have generated novel proteins from scratch – proteins that nature has never seen before. In contrast to their modern-day counterparts, these artificial proteins have not undergone natural evolution and can serve as a model for primordial-like proteins. Furthermore, we are using our in vitro selection strategy to test hypotheses on the potential predecessors of the standard genetic code. We are comparing libraries of polypeptides from different likely earlier amino acid alphabets for the ability to form structured proteins and perform simple biological functions.
While we will not be able to prove a specific history of protein-based life, these experiments are testing the feasibility of plausible evolutionary scenarios and might reveal protein properties and structures as we have not seen them before.

Abstracts - contributed talks

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Exploring imine-based Covalent Organic Frameworks (COFs) for enhanced Bisphenol A ultrasonic removal: a comparative study

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The extensive presence of endocrine-disrupting chemicals (EDCs) in water bodies, such as bisphenol A (BPA), has raised significant concerns due to their high toxicity. Even trace BPA concentrations (below 1 μg m^{-3}) can adversely affect human reproductive and endocrine systems. The present study describes the design of two imine-based covalent organic frameworks (COFs), COF-1 and COF-2, with different pore sizes for BPA adsorption. The experimental maximum adsorption capacities obtained for COF-1 and COF-2 were 2022.0 mg g^{-1} and 2074.8 mg g^{-1}, respectively. Furthermore, the experimental data were well-fitted by the PSO model, IPD, and Dubinin-Radushkevich model, indicating the superior performance of COF-2 in BPA adsorption compared to COF-1. This enhanced performance is primarily due to the higher number of aromatic rings in the structure and the larger pore size of COF-2. Additionally, the possible adsorption mechanism was analyzed using spectroscopic techniques, revealing that Van der Waals forces, π-π interactions, and hydrogen bonding involving N and O atoms from the adsorbent structure play crucial roles in the adsorption process. The regeneration of the adsorbents was evaluated over five cycles using methanol as eluent. This study underscores the synthesis of two imine-based COFs as highly efficient adsorbents for effectively removing BPA from aqueous solutions, addressing a pressing global environmental concern.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

How Membrane Perturbations Modulate the Activity and Selectivity of Antimicrobial Peptides

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Membrane-active peptides are of growing interest due to their potential antimicrobial, antifungal, and cell-penetrating properties. We investigate two cyclic antimicrobial hexapeptides, cR_3W_3 and $c(RW)_3$, composed of cationic arginine and aromatic tryptophan. Despite their similar composition and structure, their sequence differences lead to subtle but distinct amphiphilic properties that alter their induced membrane perturbation.
In order to explore their mechanism of action and selectivity, extensive biophysical analyses were conducted using model membranes containing either POPE and POPG, two lipids abundant in bacterial membranes, or POPC, a major component of mammalian membranes. We studied binding and adsorption of the peptides using monolayers and ITC experiments, observing a strong preference for negatively charged model membranes over zwitterionic ones. Both peptides altered the lipid order and packing, as determined by fluorescence spectroscopy of membrane-embedded Laurdan. Such membrane perturbations are likely to contribute to the antimicrobial killing process by initiating the dissociation of membrane proteins.
Furthermore, DSC and Laurdan fluorescence spectroscopy revealed pronounced lipid demixing and the formation of large PG-rich clusters promoted by the peptides in lipid mixtures that exhibit non-ideal mixing. Membrane permeabilization was determined by calcein release. We observed fast, all-or-none leakage for cR_3W_3, while $c(RW)_3$ exhibited only marginal leakage activity. It appears that the observed leakage is not related to the formation of large PG-rich lipid clusters, as previously described for both peptides. Instead, a significant portion of the leakage seemed to be related to vesicle fusion. Importantly, fusion is highly unlikely in microbes, but PE-containing model membranes are biased for it.

BEAM Symposium

Design of Novel Paramagnetic Probes for Studying Molecular Interactions and Mechanisms in Polymer Systems Using EPR Spectroscopy

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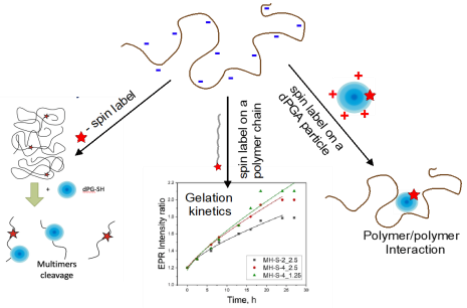
Mucus-like hydrogels are vital biological barriers that serve to shield against pathogens while enabling efficient drug delivery. In this research, electron paramagnetic resonance (EPR) spectroscopy combined with site-directed spin labeling (SDSL) is employed to probe the molecular-level interactions and dynamics within these hydrogels. The study focuses on the design of new approaches to study different mechanisms in polymer hydrogel systems.

As a first step, we investigate soft matter systems based on the synthetic high-molecular-weight sulfated polymers that mimic the rheological properties of mucus and the charge distribution along mucin chains. These polymers can be labeled with a paramagnetic probe to study the formation of multimers and their subsequent degradation upon the addition of dendritic polyglycerol (dPG) thiol particles, which are known to have a mucolytic effect in vitro. We also demonstrate by the EPR spectroscopy that positively charged dPG-amino polymers form complexes with the mucin-mimicking synthetic polymer in solution, which can help to interpret the barrier functions of mucus against viruses. Furthermore, we investigate the gelation kinetics and nanoviscosity of hydrogels by using spin labels attached to polyethylene glycol chains of varying lengths. This approach allows us to explore the dynamics of mucus self-organization with a reporter inside the hydrogel pores and provides insights into functional impairments, such as those observed in cystic fibrosis. Our findings show that the synthetic mucus-like hydrogels significantly hinder the diffusion of spin-labeled molecules, reflecting the dense network and high viscosity typical of gel matrices. These characteristics mirror the properties of native mucus, where solute transport is inherently constrained by the gel structure.

This methodology not only deepens our understanding of particle mobility and interaction mechanisms within hydrogel systems but also lays the groundwork for designing more effective pathogen barriers and drug delivery platforms.

Synthetic mucus-mimicking polymer



BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Spectroscopic decoding of genetic adaptions in the fatty acid binding behavior of Serum Albumin

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The amphiphilic transport protein Serum Albumin may carry the understanding of its evolutionary pathway within species-dependent fatty acid binding properties. In a large genetic-spectroscopic study, we applied a spin-probing approach on the seven binding pockets of Albumin and performed advanced double electron-electron resonance (DEER) and classic continuous-wave (CW) electron paramagnetic resonance (EPR) spectroscopy to investigate this protein class. By utilizing the spin-labeled fatty acids 5- and 16-DOXYL stearic acid (DSA) as model ligands, we were able to compare dynamic protein structures, internal environments of the binding pockets and the binding dynamics of fatty acids to Serum Albumins from up to seven different species. The species of interest include herbivores, carnivores, humans and crab-eating macaques. We discovered a highly complex, challenging biophysical system with various contributing components such as protein oligomers and distinct ligand binding states. The combination of different EPR experiments, frequencies and time regimes in DEER enabled an innovative deep view into the ligand binding mechanism of Albumin while we could filter the molecular distances between bound ligands depending on the desired perspective and accuracy. We found similarities but also surprising differences in the genetic-spectroscopic binding profiles of the species and correlated the EPR data with genetic and bioinformatic analyses, dynamic light scattering (DLS) and Zeta potential

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Adsorption of Lipid Bilayers to Monolayers: A New Triple Layer System for Studying Membrane Proteins

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Lipid monolayers can be used as very simple model system for one membrane leaflet. They have the advantages of being perfectly oriented, completely hydrated, and accessible through the aqueous phase. Thus, they are well suited for interaction studies with membrane binding compound, such as proteins or peptides. A variety of methods can be used in these studies, e.g., film balance measurements, fluorescence microscopy, infrared reflection-absorption spectroscopy (IRRAS) as well as X-ray reflectometry or scattering. However, no membrane spanning molecules can be studied in this system until now. Therefore, we are aiming to design a new membrane model system that makes the many advantages of established monolayer methods accessible for more complex samples.
We are exploring methods to assemble lipid bilayers underneath lipid monolayers at the air water interface. These bilayers shall host membrane spanning molecules such as integral membrane proteins or other pore forming molecules. The bilayers will be oriented, allowing to deduce molecular orientations from experiments, while still being in a well-hydrated and natural environment. We will present successful attempts in constructing such a model system, i.e., the adsorption of different lipid nanodiscs or vesicles to lipid monolayer at the air-water interface. Two different strategies, i.e., protein mediated adsorption and electrostatic adsorption lead to stable and oriented adsorption of polymer stabilized nanodiscs to the monolayer. We will show that these model systems combine the advantages of several well-established membrane models discuss further perspectives and applications.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Liquid crystalline phase engineering of non-symmetric silyl-branched azobenzene polycatenars

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Non-symmetric polycatenar liquid crystals (LC) with azobenzene moieties are known to self-assemble into a wide range of different LC phases ranging from smectic structures,[1] and columnar structures[1] to chiral bicontinuous cubic[1] as well as isotropic liquid phases[1,2]. The formation of the different phases in polycatenar molecules strongly depends on the length, type, and ratio of the terminal chains.[3]

However, it is also possible to influence the LC self-assembly by modifying the alkyl chain volume by using a bulkier silyl-branched[4,5] and nano-segregating perfluorinated chains. Additionally, the LC self-assembly could be varied by introducing different spacers connecting the branched silyl chain to the rigid core.

To this end, we report herein, the design and synthesis of non-symmetric azobenzene-based polycatenars having at one side bulky silyl-branched chains and at the other end different linear and branched alkyl or perfluoro chains. Their LC self-assembly was elucidated by optical investigations, DSC and XRD. The investigated phases range from nematic and smectic phases to different mesophases with non-cubic three-dimensional structures (M1, M2).

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Poster Abstracts – with Flash Talks

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Mixing and Demixing Dynamics in Binary Liquid Mixtures

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Phase transition such as solution processes occur in a wide variety of chemical systems and therefore also cover a broad range of time scales. An easily accessible method to study and understand them are Molecular Dynamics (MD) simulations, which allow for analysis at both microscopic and macroscopic scale. However, the simple question of how far the mixing or phase separation of the components has progressed at any given moment in a MD simulation cannot be answered by most common analysis methods, as they are limited to equilibrium states.
By computing the configurational entropy of mixing ΔS based solely on the set of atomic coordinates, we are able to gain quantitative information also from non-equilibrium states[1]. This enables a more detailed and on the fly analysis of mixing and demixing processes and their dynamics. We demonstrate the potential of our approach for the semi-automatic prediction of mixing and demixing temperatures of binary liquid mixtures. In this context, we investigate the influence of system size, temperature and chemical structure of the components with a special focus on the mixing behavior of different alkanes with (per)fluorinated compounds.

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BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Dynamic Yet Defined – Self-Assembly of Small Molecules in Solution: Colloid-Like Ionic Clusters (Ionoids).

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During the search for new polymers based on non-covalent molecular forces, a new class of colloidal ionic clusters, known as "ionoids," was discovered in 2012. These structures consist of a multicationic molecular cage, such as the "Texas-sized molecular box", combined with a dianionic salt, such as dipotassium methanedisulfonate or Fremy's salt. Ionoids are spherical, monodisperse structures with a hydrodynamic radius ranging from 6 nm to 8 nm, characterized by remarkable stability. Their self-assembly occurs spontaneously under specific solvent conditions (DMSO:glycerol:water in a 50:43:7 v/v/v ratio) after an incubation period of ten days at room temperature. This self-assembly process results from a combination of factors, including preferential solvation, viscosity, van der Waals interactions, and long-range correlated electrostatic forces. In this work we report the synthesis of "Texas-sized molecular box" and four other macrocycles, through a macrocyclization reaction combining a common heterocyclic head with five different linkers. The initial stages of the ionoids derived from macrocycles and Fremy's salt have been analyzed by means of electron paramagnetic resonance (EPR) spectroscopy. In addition, the properties of the ionoids derived from macrocycles and dipotassium methanedisulfonate (MDS) such as the forces and mechanisms governing their formation and stability have been studied using dynamic light scattering (DLS). The preparation of new linkers, heterocyclic heads, macrocycles, and ionoids is underway. Stay tuned for further results!

Poster Presentation

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Structuring Pore Space in Covalent Organic Frameworks by Cooperative Assembly of Amphiphilic Linkers

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We explore how amphiphilic linkers in Covalent Organic Frameworks (COFs) self-organize to create unique pore environments with varying polarities. By leveraging weak chemical interactions, these materials assemble spontaneously, offering new ways to control their structure and properties. Beyond simply tuning hydrophobic and hydrophilic traits, we aim to design COFs with functional groups that enable diverse molecular interactions. With their high surface area and adaptable pores, COFs hold great potential for applications in gas storage, catalysis, and sensing. Using advanced NMR techniques, we will uncover how these materials form and function at the molecular level.

Fluorinated Modification and Comprehensive Characterization of 9-Aminoacridine Dye with Fluorescence Properties

Muhammad Abu Bakar

Abstract

Fluorination of dyes can significantly increase their quantum yield and photostability, making them more useful for various imaging and sensor applications. In the current study, 9-Aminoacridine dye was modified with fluorinated ponytails of varying lengths and characterized with nuclear magnetic resonance (NMR) spectroscopy, electrospray ionization time of flight mass spectrometry (ESI-TOF-MS), ultraviolet–visible (UV-vis) spectroscopy, and fluorescence spectroscopy. ESI-TOF-MS also confirmed the successful modification of this dye with the fluorinated ponytails. The experimental molecular weights calculated with ESI-TOF-MS for these fluorinated dyes matched the calculated molecular weights. The fluorinated 9-Aminoacridine dyes showed excellent fluorescent properties compared to their parent dye. Similarly, the absorption properties of these fluorinated dyes were observed to be improved. Additionally, the partition coefficients for these fluorinated dyes will be calculated for the toluene/water system (Ln $P_{toluene/water}$), the toluene/1H,1H,2H,2H-perfluoro-1-octanol (F6H2OH) system (Ln $P_{toluene/F6H2OH}$), and the 1H,1H,2H,2H-perfluoro-1-octanol (F6H2OH)/water system (Ln $P_{F6H2OH/water}$).

Keywords: Fluorinated 9-Aminoacridine, Fluorinated ponytails and Partition coefficients.

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Synthesis of New Bifunctional Monomers for Use in Migration-Stable Polymers

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Iodonium salts, which are well established photo initiators, offer a plethora of possible structures to investigate their suitability in enhancing polymer longevity.
To achieve this, two main pathways may be followed: utilizing either covalent or non-covalent interactions. Covalent interactions can be introduced through phenyl-containing monomers which may be incorporated in the iodonium salt structure. In the case of non-covalent interactions, one or both phenyl rings can be modified with side chains that promote strong intermolecular forces, such as dipole-dipole interactions. To facilitate this, a library of Koser's salts and simple iodonium salts has been created. This collection can be used to synthesize new iodonium salts incorporating monomers or functional groups that, after dissociating, exhibit robust intermolecular interactions—such as p-stacking, fluorophilicity, dipole-dipole interactions, or halogen-halogen interactions—making diffusion out of the polymer matrix negligible. The specific type of functional group needed depends on the monomer(s) selected for polymerization and is therefore variable.

PhotUPO: Switchable UPO biocatalysis by genetically encoded photosensitizers

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Unspecific peroxygenases (UPOs) can oxyfunctionalise a broad set of substrates only requiring hydrogen peroxide as a co-substrate. High turnover numbers, stabilities and excellent selectivities render UPOs exciting enzymes for C–H activations. A major challenge for UPOs is haem-bleaching by hydrogen peroxide, lowering the catalytic efficiency. The necessity to avoid this lead to the development of different systems for the *in situ* production of hydrogen peroxide.[1] Herein we report on a new approach to avoid haem-bleaching and thus inactivation of the enzyme.

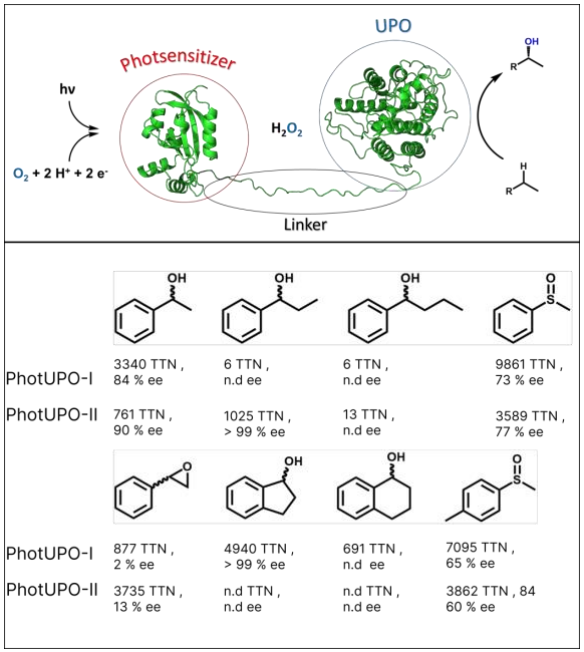

Figure 1: Principle of PhotUPO, utilizing a genetically encoded photosensitizer to fuel the UPO.

A fusion construct – photosensitizer, linker, UPO – was successfully designed and expressed in *Pichia Pastoris*. As photosensitizer a LOV photoreceptor from *D. shibae* – DsFbFP – was used. This photoreceptor can be genetically encoded and produces ROS upon excitation with the right wave length. ROS can react with the surrounding water to form hydrogen peroxide, which is then consumed by the enzyme. Photosensitizer and UPO are connected by a linker, enabling the user to express the whole construct in one run.

Photochemical as well as chemical optimisation followed and a broad substrate scope was screened. The PhotUPOs showed promising conversions with excellent ee-values (Figure 1). This system adds an easy and switchable biophotocatalytic access to oxyfunctionalised C-H bonds.

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BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Machine Learning Guided Directed Evolution of Unspecific Peroxygenases

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Epistasis, characterized by the interdependence of effects among various mutated positions, is frequently encountered in directed evolution (DE) campaigns, especially when employing multiple-site combinatorial mutagenesis libraries.[1] This phenomenon was notably observed in our prior work, which focused on engineering the unspecific peroxygenase (UPO) from *Myceliophthora thermophila* (MthUPO) for the enantiospecific hydroxylation of β-ionone.[2] To tackle the complexities introduced by epistasis and strive for a global optimum in DE campaigns, we have employed a data-driven approach, leveraging machine learning-guided directed evolution (MLDE).

A diverse library of mutants undergoes assay and sequencing to generate input data for training machine-learning models. These models are refined using various assessment metrics to accurately rank mutant activities. The most effective models guide the selection of additional mutants for assay, contributing to iterative model refinement. This process continues until predictions for untested mutants are consistently lower than those of the most active known mutants, indicating convergence. The final model's efficacy is confirmed through its accurate prediction of mutant activity levels. This approach showcases machine learning's capacity to enhance UPO engineering by effectively addressing epistasis challenges, leading to increased enzyme activity.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

How charges effect the solubilisation of artificial and native membranes by amphiphilic copolymers

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Certain amphiphilic copolymers form lipid-bilayer nanodiscs from artificial and natural membranes, thereby rendering incorporated membrane proteins optimal for structural analysis. Recent studies have shown that the amphiphilicity of a copolymer strongly determines its solubilization efficiency. This is especially true for highly negatively charged membranes, which experience pronounced Coulombic repulsion with polyanionic polymers. Here, we present a systematic study on the solubilization of artificial multicomponent lipid vesicles that mimic inner mitochondrial and fungal membranes, which harbor essential membrane-protein complexes. In particular, we compared the lipid-solubilization efficiencies of established anionic with less densely charged or zwitterionic and even cationic copolymers in low- and high-salt concentrations. The nanodiscs formed under these conditions were characterized by dynamic light scattering and negative-stain electron microscopy. Overall, our results show that some recent, zwitterionic copolymers are best suited to solubilize negatively charged membranes at high ionic strengths even at low polymer/lipid ratios [1].

As a proof of principle, we describe an efficient recovery of protein-encapsulating nanodiscs from membranes of *Chaetomium thermophilum*, a thermophilic fungus. We identified ~600 proteins by mass spectrometry and obtained two 3D reconstructions from cryo-EM for the nanodisc-containing cell extract. With this combined methodological approach, we provide a deeper understanding of eukaryotic membrane proteomes [2].

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19–21 March 2025|Halle (Saale), Germany

Effect of Multivalent Cations and Fatty Acids on the Global Dynamics of Bovine Serum Albumin at High Concentrations

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Most protein studies require dilute conditions, however, in their natural environment, most proteins are surrounded by high concentrations of various biomacromolecules. In such crowding conditions the translational and rotational mobility is reduced, which we analyze by NMR relaxometry and pulsed-field-gradient NMR experiments. Depending on the surface charge structure of the proteins a coupling or decoupling between rotation and translation can be observed. Bovine serum albumin (BSA), the most abundant protein in bovine blood shows an intermediate coupling. Through the addition of trivalent cations the interprotein intermolecular electrostatic interactions can be tuned, which leads to an interesting phase behaviour including reentrant condensation and liquid-liquid phase separation.

In commercially available BSA, naturally occurring fatty acids may or may not be removed depending on the manufacturer, which is often overlooked. We discovered that fatty-acid-free samples show a significant difference in translational diffusion coefficients and relaxation times and protein-salt-interactions which imply an additional retardation of the protein mobility.

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Targeting the endosomal membrane by biomimetic, pH-sensitive polymers

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The interaction of biomimetic polymers with membranes of various lipid compositions can cause a variety of physical-chemical membrane perturbations. These can be exploited to damage or overcome membranes in the context of drug delivery, e.g. assisting endosomal escape. The lowering of the endosomal pH, and the occurrence of the negatively charged lipid BMP during endolysosomal development, can be used to selectively permeabilize endosomal membranes.

For a rational design and selection of suitable polymers for drug delivery applications, we need to understand the underlying membrane biophysics. We investigate the principles of pH-sensitive activity and selectivity of membrane-active polycations.

The polymer pKa, pH, and lipid composition are systematically varied to reveal the network of membrane perturbation mechanisms under conditions representing cytoplasmic or early/late endosomal membranes. Membrane leakage, electrostatic lipid clustering (the local enrichment of negatively charged lipids by positively charged polycations), and membrane fusion can play important roles for membrane permeabilization. Using fluorescence and monolayer methods as well as microcalorimetry, we characterized membrane perturbations caused by the polymers. These interactions were examined using different membrane models like large and giant unilamellar vesicles, multilamellar vesicles and lipid monolayers.

We find that the pH sensitive polymers do not insert into the lipid membrane, but rather induce local heterogeneities, as well as limited membrane permeabilization. Our data indicates that the polymers interact electrostatically especially with negatively charged, i.e. endosomal-like, model membranes.

This dominance of polymer and membrane charge underlines the role of the negatively charged endosomal lipid BMP, while the pH change contributes indirectly to endosomal escape by increasing the polymer charge.

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Pathway Complexity in Supramolecular Polymerization of Peptide Amphiphiles

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In supramolecular systems, pathway complexity provides access to metastable and kinetically trapped states, offering control over material properties. Through adjustment of experimental conditions, supramolecular polymerization can yield tailored structures and diverse morphologies from identical precursors. By combining experimental and computational efforts, this study focuses on the pathway complexity in the supramolecular polymerization of peptidic, water-soluble Zn(II) porphyrins. Two peptide designs, consisting of glycine (G) and phenylalanine (F), were examined: a rigid GF_3 sequence and a more flexible G_2F_3 sequence. Both are equipped with a PEG domain for water solubility and thermoresponsive behavior. The GF_3 sequence shows rapid, spontaneous polymerization over a wide range of temperatures, while in the case of G_2F_3 an activation barrier restricts the polymerization to temperatures above 40 °C. To further characterize the supramolecular polymerization mechanisms, we developed a model with planar monomers and key parameters such as intermolecular interactions, bead size, and linker flexibility. Consistent with experimental observations, simulations demonstrated that stronger interactions promote polymerization, while increased flexibility inhibits it due to sterics. While the model indicates a power-law relationship between polymerization half-times and initial monomer concentrations, experimental results showed no concentration dependence, suggesting that more complex on- and off-pathway mechanisms exist. A minimum free energy model revealed a linear relationship between the binding free energy and the number of bonds between monomers, with stiffer monomers exhibiting higher binding energies, which implies the formation of more stable supramolecular polymers. With hybrid MD-MC simulations, we intend to map the free energy of polymers of different sizes and to generate a phase diagram to deepen our understanding of structure formation.

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19–21 March 2025|Halle (Saale), Germany

Influence of End Groups in Polymer Aggregates: A Neutron Scattering Study

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Polymer solutions have been studied in great detail in the past, however the influence of the end groups has been mostly overlooked. Recent works found the existence of polymeric micelles, when these possessed hydrophobic end groups. We investigated the solution behavior and the occurrence of micelle-like structures for (semi)-dilute systems. Using RAFT polymerization, we synthesized PNIPAM chains that are hydrophobically terminated. We also investigated these polymers after cleavage of the hydrophobic end groups. The influence of end groups regarding the solution behavior was analyzed using rheology, while the cloud points of the polymer solutions were measured via temperature dependent extinction spectroscopy. To characterize the dimensions of the polymer coils and potential aggregates dynamic light scattering was used. Small angle neutron scattering (SANS) was used, which provided insight into the internal structure of the samples. Through these, we were able to determine the ratio between individual polymer chains and the micelles. The rheological and cloud point measurements show a dependence on the end group for all polymers with molecular weights below 100 kDa. This suggest that the end groups influence not only molecular-scale interactions but also macroscopic properties of polymer solutions. SANS measurements indicate that, at low concentrations, micelles exist as individual structures. Upon increasing the concentration, micelles aggregate, leading to a distinct structure factor contribution in the scattering profile. SANS also facilitates the calculation of the size and aggregation number of these micelles. Our studies demonstrated that the terminal groups of a polymer have a substantial influence on its overall behavior in solution. This effect is especially pronounced for shorter polymers. Using SANS, we were able to gain insight into structural organization and aggregation behavior of these systems as a function of concentration and molecular weight.

BEAM Conference 2025

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On the Effects of Surface Charge of Amphiphilic Peptides on Peptide-Lipid Interactions in the Gas Phase and in Solution

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Abstract (max. 2000 characters)

The interactions between peptides and lipids are fundamental for many biological processes. Therefore, exploring the non-covalent interactions that govern these interactions has become increasingly important. Native mass spectrometry is a valuable technique for the characterisation of specific peptide-lipid interactions. However, native mass spectrometry requires the transfer of the analyte into the gas-phase and non-covalent interactions driven by the hydrophobic effect might be distorted. We, therefore, address the importance of electrostatic interactions for the formation of peptide-lipid interactions. For this, we make use of the amphipathic, antimicrobial peptide LL-37 as well as a positively and negatively charged variant thereof, and study binding of a variety of lipids by native mass spectrometry. We found that the surface charge affects the transfer of peptide-lipid interactions into the gas phase. We further compare our findings observed in the gas phase with interactions formed in solution between the peptides and lipid monolayers using a Langmuir film balance. The two approaches deliver comparable results and revealed a clear trend in the lipid preferences of all variants for those lipids with opposite charge. Notably, the unmodified wild type peptide was more flexible in the formation of peptide-lipid interactions. We conclude that native mass spectrometry is indeed well-suited to explore the interactions between peptides and lipids, and that electrostatic interactions as expressed by the surface charge of the peptides play an important role in the formation of peptide-lipid interactions.

Poster Abstracts – without Flash Talks

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

Evaluation of the Polymeric Chain Length Effect on The Solvatochromic Behavior of ESIPT Dyes

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Excited-State Intramolecular Proton Transfer (ESIPT) dyes have gathered significant interest due to their unique four-level fluorescence mechanism. This process, driven by tautomerism in the excited state, confers distinctive photophysical properties, including large Stokes shifts, high photostability and sensitivity to environmental changes. Variations in the solvation environment can alter the ratios between the enol (E*) and keto (K*) excited-state tautomers, thereby modulating dual fluorescence emission. These characteristics render ESIPT dyes highly versatile for applications spanning bioimaging to optoelectronics. However, the inherent hydrophobicity of ESIPT dyes often limits their utility in aqueous systems, where aggregation can occur. Additionally, the intramolecular proton transfer in polar protic solvents is hindered due to solvation effects and dominant intermolecular interactions. To address these challenges, this study explores the development of amphiphilic derivatives of 2-(2-hydroxyphenyl)benzoxazole to enhance the compatibility of ESIPT dyes in aqueous environments. Given their sensitivity to the microenvironment, derivatives with varying chain lengths were synthesized and evaluated. Herein, we present preliminary findings that demonstrate their synthetic accessibility and fluorescence behavior in both organic and aqueous media. Using steady-state fluorescence spectroscopy we investigated the influence of chain length on the solvatochromic properties and aggregation tendencies of the ESIPT dyes. Furthermore, the impact of varying water concentrations on fluorescence emission was examined to elucidate the driving forces leading to preferable intra- or intermolecular interactions. Understanding the photophysical behavior of amphiphilic ESIPT dyes in aqueous systems provides a promising pathway for extending their applicability to highly polar environments, thereby advancing their potential in supramolecular chemistry and biomedical material design.

BEAM Conference 2025

19–21 March 2025|Halle (Saale), Germany

High-Fidelity Understanding of Enzymes Through Integrative Computational and Experimental Data

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Understanding enzymes at the molecular level is crucial for enhancing their activity and functional specificity. A high-fidelity approach involves integrating computational methods—such as molecular dynamics simulations, quantum mechanical calculations, and machine learning techniques—with experimental data. This synergistic framework enables unprecedented insights into the structural and dynamic properties of enzymes, facilitating the rational design of improved activity and selectivity. Our work demonstrates how this integrative strategy advances the understanding of enzymatic mechanisms, paving the way for innovative approaches in enzyme engineering and biocatalysis

BEAM Conference 2025

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NMR studies of model amphiphilic polymer co-networks

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Owing to the possibility of environment-dependent property tuning, amphiphilic polymer co-networks (APCNs) have been attracting attention in recent years as possible functional materials, e.g. as media for selective transport. In order to understand the underlying mechanism of such properties, systematic studies on model systems are needed. We use well-established NMR methods to study tetra-arm PEG-PCL APCNs and their PEG-PEG analogues. These APCNs were previously shown to have near-model properties with very low inelastic defects, almost complete conversion, high fraction of ideal single links and nanoscale phase separation in selective solvents [1,2]. In this work, multiple-quantum NMR (MQNMR) is used to determine the connectivity motifs of networks with novel crosslinking chemistry aimed to improve the model nature of the APCNs. In addition, MQNMR is also used to understand the chain order in networks at isotropic as well as anisotropic swelling conditions. Pulsed field gradient NMR is used to study the diffusion of a model protein (lysozyme) in the network matrix.

Literature:

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Self-Assembly of non-covalently bonded hydrogels investigated using Molecular dynamics simulations

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I apply for a poster, in which I want to present my results and experience I gained during my first year in molecular dynamics simulation research and beginning of my PhD:

Hydrogels, with their unique physiochemical properties and versatile applications have emerged as promising materials in various fields, ranging from biomedicine to soft-matter robotics and sensors. Understanding the molecular mechanisms on the atomic level governing their behaviour is crucial for optimizing and rationalizing their functionality and design.
However, atomistic resolved structures of self-assembled hydrogels remain unknown, due to limitations of experimental approaches. Molecular dynamics simulations (MD) however, is a theoretical method that can resolve dynamic processes up to the atomistic level.
In the study I would like to present, we conduct a comprehensive investigation into the viscoelastic properties of self-organized hydrogel structures and dynamics at the atomic level using advanced molecular MD techniques to explore the knowledge gap between macroscopic properties and atomistic structures. Additionally, we present a benchmark assessing the stability of non-biased MD simulation and the determination of viscosities in Newtonian liquid systems namely methane, water, ethane and glycerol.
Our results demonstrate how viscosity estimations are feasible and self-assembly contributes to the physio-chemical properties of a gel, leading to a step towards the rationalization of hydrogel design.
The obtained results provide a summary to conduct a stable NVE simulation for any MD system and useful insights for rationalising physio-chemical characteristics of self-assembled hydrogel peptides and their structural formation and stabilization

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Cardiolipin and its Role in Ageing and Oxidative Stress on Biomimetics of the Inner Mitochondrial Membrane

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Cardiolipin (CL) represents a unique tetra-acyl phospholipid and is almost exclusively found in the inner mitochondrial membrane (IMM), comprising ~15-20 mol% of the overall phospholipid content. CL supporting the optimal function of most enzymes involved in the cellular energy metabolism (e.g. complexes I-IV in the respiratory chain). Besides its functional importance, CL modulates due to its inverse-cone shape the membrane fluidity and osmotic stability of the membrane.[1] Furthermore, it anchors signalling molecules and proteins electrostatically, playing an important role in events linked to ageing and apoptosis.[2] In cases of mitochondrial dysfunction, changes in the CL content and/or its fatty acid composition can be a dominant cause, leading to neurodegenerative and cardiac diseases.[3]
In this project, we aim to unravel the role of CL in biological membranes by mimicking the composition of the IMM in liposomes, focusing on the integrity of CL-containing membranes under oxidative stress conditions due to the presence of reactive oxygen species (ROS). One of the main emphasis lies on correlating morphology-based changes of these vesicles (e.g. size, charge, membrane fluidity) due to exposure towards various ROS such as superoxide radicals, hydrogen peroxide and hydroxyl radicals. Proof of concept is given in studies where respiratory complex I was successfully incorporated into CL-containing liposomes and changes in the enzyme's activity due to the membrane composition and presence of ROS.[4,5] Based on these promising results, we want to gain a better fundamental understanding of the importance of CL in both biomimetics as well as in biological membranes.

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Differently Charged Nanodisc-Stabilizing Copolymers Influence the Formation of Lipid Triple Layers at the Air-Water Interface

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In order to investigate the interactions of proteins with biological membranes, lipid monolayers at the air-water interface are a suitable and simplified membrane model system. Although this is a well-established model to observe interactions between various biopolymers and lipid membranes, membrane spanning proteins could not yet be studied by this system and its corresponding methods, e.g., film balance measurements, fluorescence microscopy or infrared reflection-absorption spectroscopy (IRRAS).

A new membrane model system – a well-defined lipid triple layer at the air-water interface – is our approach to solve this problem. By assembling lipid bilayers underneath a lipid monolayer, it will be possible to investigate transmembrane proteins in a fully hydrated and oriented bilayer with the aforementioned methods. To design this model system, we inject lipid bilayers, e.g., vesicles or nanodiscs, into the aqueous subphase underneath the preassembled monolayer. One promising approach to promote the triple layer assembly is electrostatic adsorption of polymer-stabilized lipid nanodiscs containing negatively charged lipids to a positively charged monolayer. The advantage of using copolymers to prepare lipid nanodiscs is to prevent possible interference with the integral membrane proteins to be analyzed. Thus, the right choice of this polymer is essential for designing a suitable triple layer model. The charges of the commonly used copolymers for nanodiscs formation, SMA and DIBMA, may interfere with the electrostatic interaction between the lipids. Furthermore, free polymers in solution may interact with the anchoring monolayer altering its desired properties.
Therefore, in this study we investigated the influence of differently charged copolymers derived from SMA on the triple layer formation. From film balance and IRRAS experiments, we conclude that although their charge has no significant influence on their interaction with the monolayer, the amount of adsorbed nanodiscs clearly depends in the charge of the used polymer.

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Archaeal diether lipids dominate membrane behavior of DPPC

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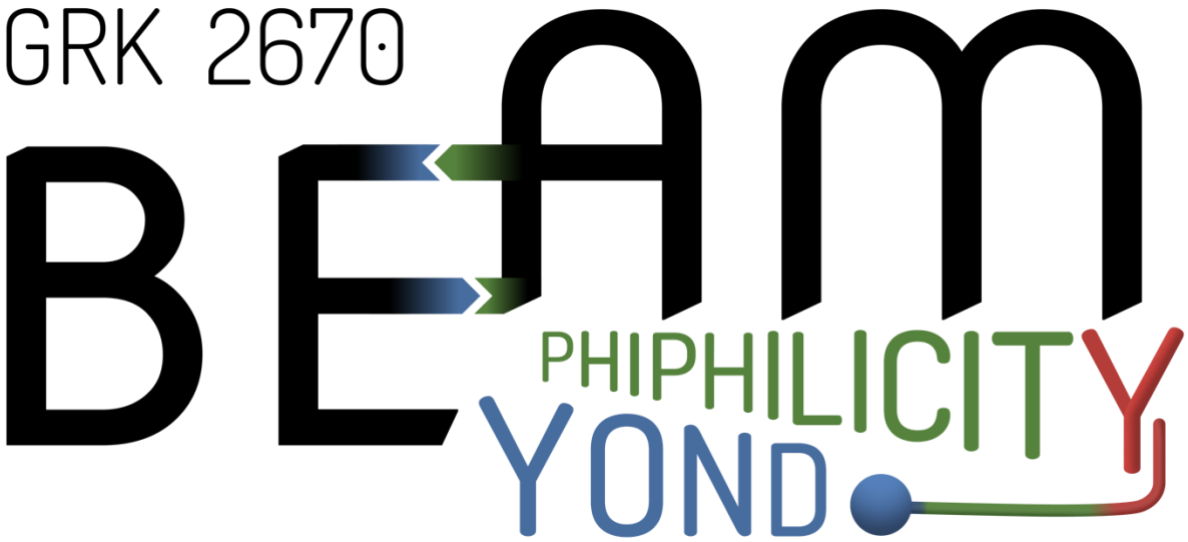
Archaeal lipids are different from bacterial lipids. Archaeal lipids are ether-linked and have isoprenoid chains instead of alkyl chains. This is supposed to make archaea and their membranes more resistant to changes in temperature or pH.

This lead to the idea to use archaeal lipids in vesicles for oral drug delivery of pH-sensitive therapeutic compounds. To quantify the influence of the archaeal diether lipids (DELs) of *H. volcanii* (Hvo) on phosphoester lipid membranes, mixtures of DELs and DPPC were characterized. Both, mixed monolayers and mixed DPPC/DEL vesicles were examined by compression film balance experiments, differential scanning calorimetry, laurdan fluorescence, and attenuated total reflection infrared spectroscopy (ATR-IR).

Unsurprisingly, we found that DEL lipid chains generally have a lower order than DPPC chains. The lipid main phase transition temperatures of DPPC and transition enthalpies decrease with increasing DEL content, even at low ratios (5-20 %). At DEL contents of approximately 30% to 50%, the liquid-expanded to liquid-condensed transition of monolayers and the main phase transition in bilayers disappear. Already at low content, DELs have a dominant influence on DPPC membrane behavior.

In summary, it could be shown that the DEL lipids of *Haloferax volcanii* are potentially suitable for oral drug delivery. Next, the membrane permeabilization shall be studied.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