Final Retreat in Wittenberg
20.4. – 21.4.2023

Thursday, 20th April 2023

Time	Event	Location
9:30	Welcome / Speaker's report	Lectorium, 3rd floor
10:00-10:20	**Wolfgang Binder** (MLU) (Chair Stephan Sydow) *Hybrid polymers as model entities in fibrillation and folding*	Lectorium, 3rd floor
10:20-10:45	Coffee break and poster exhibition (S.R. 1 & 2)	Lectorium, 3rd floor
10:45-11:30	**Matthias Hartlieb** (UniversitätPotsdam) *Tales about Antimicrobial Polymers*	Lectorium, 3rd floor
11:30-12:15	**Birgit Strodel** (Universität Düsseldorf) *Emergence of order in Aβ through molecular interactions and self-assembly*	Lectorium, 3rd floor
12:15	Group Photo	Courtyard
12:20	Lunch	Cafeteria + SR 4
14:00-14:20	**Benedikt Schwarze** (Universität Leipzig) (Chair Maria Ott) *Amyloid β40 - a research history as devious as its misfolding landscape*	Auditorium, 1st floor
14:20-15:05	**Wolfgang Hoyer** (Universität Düsseldorf) *Protofibrils vs. cross-β fibrils: Two alternative amyloid assembly types*	Auditorium, 1st floor
15:05	Coffee break	Foyer/Auditorium
15:45	PI meeting	SR 10, 1st floor
15:45	**Alycin Rhoades** (Penn State Behrend, USA) (Chair Stephan Sydow) Insights behind the CV	Auditorium, 1st floor
18:30	Dinner: Buffet	Cafeteria + SR 4
20:00	**Matthias Ullrich** (Borealis) (Chair Wolfgang Paul) *Academia & industry: Two career paths, less divergent than one may think*	Auditorium, 1st floor

Evening in the Library

Final Retreat in Wittenberg
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Friday, 21st April 2023

Time	Event	Location
9:00-9:20	**Kay Saalwächter** (MLU) (Chair Oleksandr Dolynchuk) *Our progress in understanding polymer crystallization*	Auditorium, 1st floor
9:20-10:05	**Kostas Daoulas** (MPI Mainz) *Ultra coarse-grained modelling of near-crystalline functional polymers: what can we learn?*	Auditorium, 1st floor
10:05	Coffee break	Foyer, Auditorium
10:45-11:45	**Michael Büker** (Science journalist) (Chair Jonas Warneke) *Science Communication: From the Lab Out Into the World*	Auditorium, 1st floor
11:45-12:30	**Peter Seeberger** (MPI KG Potsdam) *Synthetic Polysaccharides as Basis for Material Science Applications* + some information on the CTC	Auditorium, 1st floor
12:30	**Lunch**	Cafeteria + SR 4
13:45-14:30	**Alicyn Rhoades** (Penn State Behrend, USA) (Chair Friedrich Kremer) *Flow-Induced Crystallization Polymers Across the Spectrum of Backbone Rigidity*	Auditorium
14:30-15:00	Conclusion, farewell reception	Foyer/Auditorium

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Poster exhibition (SR 1 & 2, 1st floor)

1. Yu Qiang, Mohd Afiq Bin Anuar, Albrecht Petzold, Kay Saalwächter, Thomas Thurn-Albrecht (A01)
   Semicrystalline morphology and intracrystalline chain dynamics in different polyesters

2. Tonghua Liu, Albrecht Petzold, Kay Saalwächter, Thomas Thurn-Albrecht (A01)
   The effect of entanglement density of semi-crystalline polymer on the stress-strain curve

3. Matthias Rohmer, Yue Cai, Özgün Ucak, Wolfgang H. Binder (A03)
   Secondary structure, assembly and cooperativity in dynamic supramolecular polymers

4. Alexander Korn, Holger A. Scheidt, Daniel Huster (A06)
   The conformation of pyroglutamated amyloid ß fibrils: Extended or Hairpin?

5. Timur Shakirov, Wolfgang Paul (A07)
   Intra- and intermolecular strucutre formation in the presence of specific interactions

6. Christian Lauer, Wolfgang Paul (A07)
   Dimerization of Polyglutamine using PRIME20 and SAMC

7. Malte Neudorf, Maria Ott, Jochen Balbach, Kay Saalwächter (A08)
   Organization and Interactions of eye-lens crystallins proteins

8. Thomas Kunze, Christoph Dressler, Svetlana Pylaeva, Daniel Sebastiani (A09)
   Primary Nucleation Mechanism of Short Amyloid Peptides from Computer Simulation

9. André Paschold, Niclas Starke, Wolfgang H. Binder (A12)
   Assembly of modified peptides and polymer hybrid molecules

10. Bruno Voigt, Julia Hesselbarth, Carla Schmidt, Jochen Balbach (A12)
    The Pre-Nucleation Equilibrium of the Parathyroid Hormone

11. Christian Laube, Torsten John, Lisandra L. Martin, Herre Jelger Risselada, Bernd Abel (B01)
    Aggregation and Self-Assembly of Amyloidogenic Peptides at Functionalized and Nanostructured Interfaces"

12. Marthinus van Niekerk, Muhammad Tariq, Oleksandr Dolynchuk, Thomas Thurn-Albrecht (B03)
    Effect of substrate interaction on crystallization kinetics and crystal orientation

13. Stefan Schnabel, Maximilian Conradi, and Wolfhard Janke (B04)
    Scaling of theta polymers and collapse dynamics of (Ala)_N

14. Nazmul Hasan, Karsten Busse and Jörg Kreßler (B07)
    Crystallization of i-PMAA at the air-water interface and in thin films

15. Wycliffe Kipnusu, Evgeny Zhuravlev, Christoph Schick, Friedrich Kremer (B08)
    The Initial Molecular Interactions in the Course of Enthalpy Relaxation and Nucleation in Polyethylene terephthalate (PET) as Monitored by Combined Nanocalorimetry and FTIR Spectroscopy

16. Stephan Sydow, Tobias Thalheim, Jörg Schnauß and Frank Cichos (B10)
    F-Actin Photo-Fragmentation as an Artificial Secondary Nucleation Model

17. Twinkle Bhatia, Jana Wägele, Silvia De Sio, Maria Ott (B12)
    Fibrillation in macromolecular crowded environment

18. Rene Sattler, Varun Danke, Heiko Huth, Mario Beiner (B14)
    Polyamides with long methylene sequences: Influence of sequence length on structure and crystallization kinetics

19. Wing Kit Or, Martin Tress (B15)
    Polymer Crystallization in Nanoscopic Sample Sizes by Dielectric Spectroscopy

20. Alaa Hassan, Martin Tress (B15)
    Towards Conductivity Measurements of Individualized Macromolecules

21. Anika Wurl, Tiago Mendes Ferreira (B16)
    Crystallization of polymer chains under anisotropic confinement in liquid crystals

22. Anna-Maria Tsirigoni, Zeynep Atris, Melis Göktas, Ana Vila Verde, Kerstin G. Blank (B17)
    Force-induced α-β transitions in coiled coil (CC) structures

23. Sebastian Kawa, Markus Rohdenburg, Ziyan Warneke, Jonas Warneke (B18)
    Ion Soft-landing of Permanent Cations: Polymerization and Beyond

Abstracts (invited speakers)

Science Communication: From the Lab Out Into the World

Michael Büker
Science Communiation

"So what is it you do, really?" – it's a tricky question scientists hear from friends and relatives. Can you explain your work to outsiders? Yes, it can be done. And even beyond friends and family, it can help inform society. We'll look at some techniques and results from real-life experience. A discussion about the risks and benefits of science communication is very welcome.

Ultra coarse-grained modelling of near-crystalline functional polymers: what can we learn?

Kostas Daoulas
Max Planck Institute für Polymer Research, Mainz

Inevitably, large-scale computational studies of structure-property relationships in polymers require simplified models, which achieve the necessary efficiency by mapping large groups of actual atoms on single interaction centers. However, the implementation of ultra coarse-grained models can be also very challenging: the significant simplification of the molecular structure can eliminate features that are, in fact, crucial for structure formation. One important class of materials, where such problems are expected, are functional polymers with backbones comprising aromatic rings and small side chains – conjugated polymers are a typical case.
Nevertheless – and this is one of the main ideas we plan to convey – the perspectives of simplified models in studies of such "board-like" polymers are better than one might initially expect. One reason is that these polymers commonly exhibit pronounced structural disorder [1]. Even their crystalline phases can have large para-crystallinity, whereas one often observes [1,2] only small-scale molecular aggregation and liquid-crystalline mesophases. This structural "noise", combined with the collective nature of the ordering processes, might mitigate the reduction of microscopic details, rendering simplified models useful for addressing certain questions.
First, we will summarize some simplified models used in generic studies of polymer order, crystallization in particular. We will argue why these approaches are insufficient for board-like functional polymers and highlight some simplified models that have been developed for these materials. Next, we will focus on an approach [3,4] where near crystalline, sanidic, mesophases are described by combining a minimalistic representation of polymer architecture with generic anisotropic potentials. As an application, we will present new simulation results related to studies of texture of P3HT films [5] where face-on and edge-on orientation of crystalline lamellae is favored at the bottom and top surface, respectively. These results highlight the need for understanding the elastic properties of highly ordered, almost crystalline, mesophases.

[1] Noriega et al, *Nature Mat.* 2013, **12**, 1038-1044.
[2] Stingelin N., *Polym. Int*. 2012, **61**, 866-873.
[3] Greco C., Melnyk A., Kremer K., Andrienko D., Daoulas K. Ch. *Macromolecules* 2019, **52**, 968-981.
[4] Wood E. L., Greco C., Ivanov D. A., Kremer K., Daoulas K. Ch. *J. Phys. Chem. B.* 2022, **126**, 2285-2298.
[5] Dolynchuk O., Schmode P., Fischer M., Thelakkat M., Thurn-Albrecht T. *Macromolecules* 2021, **54**, 5429-5439.

Tales about Antimicrobial Polymers

Matthias Hartlieb
Universität Potsdam
Fraunhofer Institute for Applied Polymer Research (IAP), Potsdam

With steadily increasing levels of antimicrobial resistance (AMR), mankind is slipping into a post antibiotic era, in which the advances of modern medicine are in jeopardy. As the antibiotic pipeline is running dry, the need for new antimicrobial drugs is increasing. Antimicrobial polymers (APs) offer a promising solution, as their mechanism of action – the permeabilization of bacterial membranes – is unsusceptible toward AMR.[1] However, their selectivity between eukaryotic and prokaryotic cells is still insufficient for clinical applications.
To guide APs and direct their activity against prokaryotic cells, a plethora of parameters can be altered. The amphiphilic balance, molecular weight, or the type of charged unit are among them. One additional important aspect in this context is the polymer architecture, as it fundamentally changes the physico-chemical properties of APs.[2] Using bottle brush copolymers as a platform for APs, we could show that confinement and multivalence in such structures has profound impact on their biological activity.[3-4] Indeed, optimizing structural parameters yields highly selective APs featuring increased antimicrobial activity and markedly different membrane interaction.[5]
Compared to polymer morphology, the amphiphilicity of APs is a more fundamental property and virtually all polymers used in this context contain cationic, as well as hydrophobic subunits. In our recent work we questioned whether hydrophobicity is an essential property in APs and found that it can be replaced by hydrogen bonding as an alternative attractive interaction entirely. As hydrophobicity is a major driving force behind unspecific toxicity, this finding enables the design of Aps featuring tremendous selectivity. Combined, these aspects open new ways to APs with increased activity and lowered unspecific toxicity paving the way to APs in biomedical applications.

[1] M. Hartlieb, E. G. L. Williams, A. Kuroki, S. Perrier, K. E. S. Locock, *Curr. Med. Chem.* **2017**, *24*, 2115-2140.
[2] A. Kuroki, P. Sangwan, Y. Qu, R. Peltier, C. Sanchez-Cano, J. Moat, C. G. Dowson, E. G. L. Williams, K. E. S. Locock, M. Hartlieb, et al., *ACS Appl. Mater. Interfaces* **2017**, *9*, 40117-40126.
[3] S. Laroque, M. Reifarth, M. Sperling, S. Kersting, S. Klöpzig, P. Budach, J. Storsberg, M. Hartlieb, *ACS Appl. Mater. Interfaces* **2020**, *12*, 30052-30065.
[4] A.-C. Lehnen, A. M. Bapolisi, M. Krass, A. AlSawaf, J. Kurki, S. Kersting, H. Fuchs, M. Hartlieb, *Biomacromolecules* **2022**, *23*, 5350-5360.
[5] A. M. Bapolisi, P. Kielb, M. Bekir, A.-C. Lehnen, C. Radon, S. Laroque, P. Wendler, H. M. Müller-Werkmeister, M. Hartlieb, *Macromol. Rapid Commun.* **2022**, *43*, 2200288.

Protofibrils vs. cross-β fibrils: Two alternative amyloid assembly types

Wolfgang Hoyer
Universität Düsseldorf

Amyloid fibrils, in which multiple copies of a protein molecule are stacked along the fibril axis in a highly regular cross-β structure, are a characteristic feature of many diseases. The spreading of these protein aggregates over the affected organ has been linked to disease progression. Under the same conditions that favor cross-β fibril formation, a second amyloid assembly type is formed which is often referred to as protofibril. Protofibrils are also rich in β-structure, but are shorter, less rigid, curvilinear assemblies of oligomeric subunits. Protofibrils formed from amyloid-β peptide (Aβ) may represent the main toxic species in Alzheimer's disease, as they are more effective than cross-β fibrils at inducing synaptic dysfunction and triggering inflammation. In November 2022, phase III clinical trial data for an anti-

protofibril monoclonal antibody reported it to be the first drug to slow mental decline in a robust clinical trial. Here we elucidate the mechanism of protofibril formation, identify physiological conditions that promote protofibril assembly, and identify the interplay between protofibrils and cross-β fibrils. We find that protofibrils form comparatively fast and antagonize their replacement by cross-β fibrils both by competing for monomers and by blocking secondary nucleation sites for cross-β fibril formation. The critical protein concentration required for protofibril formation can be reached in acidic conditions as present in endosomes/lysosomes.

Flow-Induced Crystallization Polymers Across the Spectrum of Backbone Rigidity

Alicyn Rhoades
Penn State Behrend, USA

Processing of thermoplastics during injection molding and blow molding usually includes melt flow followed by rapid cooling at rates up to 103 K/s and solidification at high supercooling. Fast scanning calorimetry (FSC) is able to cover high processing rates and wide temperature windows by just using a few nanograms of the sample. In reality, polymers of all types are subject to melt processing and the resulting conditions oftentimes result in Flow Induced Crystallization (FIC). This presentation will systematically consider FIC in a series of polymers with increasing backbone stiffness and inter/intramolecular interactions. Coupling FSC with other techniques, including micro-IR spectroscopy, atomic force microscopy, polarized optical microscopy, and X-ray computed tomography the kinetics, polymorphism, and morphology transition associated with FIC will be discussed for polyolefins, polyamides, poly (ether ether) ketone and its composites. In addition, the role of the nematic phase on FIC in rigid backbone polymers will also be discussed.

Synthetic Polysaccharides as Basis for Material Science Applications

Peter Seeberger
Max-Planck Institute for Colloids and Interfaces Potsdam

Rapid preparation of polysaccharides is by automated glycan assembly (AGA)[1] using a synthesizer[2] provides access to diverse glycans as large as 151-mers.[3] Accelerated synthesis methods4 are now used to synthesize ever more complex glycans including challenging cislinked polysaccharides[5] are enabling fundamental investigations into the structure and function of polysaccharides.
Synthetic glycans are key in combination with single molecule imaging,[6] molecular modelling and other physical methods to characterize carbohydrate structure. [7-9] We use synthetic polysaccharides to address fundamental questions of carbohydrate structure, folding and material science. [10, 11]
Recently, we described the design, synthesis, and characterization of the first stapled oligosaccharides. Automated assembly of β-(1,6)-glucans equipped with two alkenyl side chains was followed by on-resin Grubbs metathesis for efficient ring closure with a variety of cross-linkers of different sizes. Oligosaccharide stapling increases enzymatic stability and cell penetration. [12]

Finally, I will briefly introduce the Center for the Translation of Chemistry (CTC) a new large research center aiming to help move from a chemical industry based on fossil resources to recycling and renewable feedstocks.

1. Guberman, M.; Seeberger, P.H.; J. Am. Chem. Soc., 2019, 141, 5581.
2. Hahm, H.S.; Schlegel, M.K.; Hurevich, M.; Eller, S.; Schuhmacher, F.; Hofmann, J.; Pagel, K.; Seeberger, P.H.; Proc Nat Acad Sci USA, 2017, 114, E3385.
3. Joseph, A.; Pardo-Vargas, A.; Seeberger, P.H.; J. Am. Chem. Soc., 2020, 142, 8561.
4. Danglad-Flores, J.; Leichnitz, S.; Sletten, E.T.; Joseph, A.A.; Bienert, K.; Le Mai Hoang, K.; Seeberger, P.H.; J. Am. Chem. Soc., 2021, 143, 8893.
5. Zhu, Y.; Delbianco, M.; Seeberger, P.H.; J. Am. Chem. Soc., 2021, 143, 9758.
6. Wu, X. Delbianco, M.; Anggara, K.; Michnowicz, T.; Pardo-Vargas, A.; Bharate, P.; Sen, S.; Pristl, M.; Rauschenbach, S.; Schlickum, U.; Abb, S.; Seeberger, P.H.; Kern, K.; Nature 2020, 582, 375
7. Delbianco, M.; ... Seeberger; J.Am.Chem.Soc. 2018, 140, 5421.
8. Yu, Y.; … Seeberger, P.H.; Delbianco, M.; J Am. Chem. Soc. 2019, 141, 4833.
9. Yu, Y.; Tyrikos-Ergas, T.; Zhu, Y.; Fittolani, G.; Bordoni, V.; Singhal, A.; Fair, R.J.; Grafmüller, A.; Seeberger, P.H.; Delbianco, M.; Angew.Chem.Int.Ed. 2019, 58, 13127.
10. Anggara, A.; Zhu, Y.; Delbianco, M.; Rauschenbach, S.; Abb, S.; Seeberger, P.H.; Kern, K.; J. Am. Chem. Soc., 2020, 142, 21420.
11. Anggara, K.; Zhu, Y.; …Seeberger, P.H.; Kern, K.; Proc Nat Acad Sci USA, 2021, 118, e2102168118
12. Ricardo, M.G.; Reuber, E.E.; Yao, L.; Danglad-Flores, J.; Delbianco, M.; Seeberger, P.H.; J. Am. Chem. Soc., 2022, 144, 18429.

Emergence of order in Aβ through molecular interactions and self-assembly

Birgit Strodel

Universität Düsseldorf / Foschungszentrum Jülich

Amyloid-β peptide (Aβ) is an aggregation-prone peptide associated with neurodegeneration in Alzheimer's disease. Aβ accumulates spontaneously and forms aggregates of varying sizes, with smaller prefibrillar oligomeric aggregates being particularly neurotoxic. However, such small oligomers are difficult to study by experimental means because they are transient, present in small amounts, and heterogeneous. We use molecular dynamics (MD) simulations to systematically investigate the structure and assembly mechanisms of Aβ oligomers. Based on Markov state modeling applied to sub-millisecond MD data for Aβ dimers, tetramers, and hexamers, we succeeded in identifying the metastable oligomer structures and the transition kinetics between them. In addition, we analyzed how different internal conditions, such as peptide length or sequence modifications, and environmental changes, such as the presence of a neuronal membrane, small lipid clusters, or glycosaminoglycans, affect petide structure and aggregation. The main findings are that i) Aβ is able to undergo a transition from disorder to order through interactions with other molecules, including other Aβ peptides, and ii) the amyloid oligomerization process requires a β-hairpin motif, which is present in wild-type Aβ but not in truncated or scrambled peptide variants.

Academia & industry. Two career paths. Less divergent than one may think.

Matthias Ullrich

Borealis Polymere GmbH, Burghausen

This open evening discussion will revolve around career options in academia and industry. It is geared towards scientists who are in the final stage of working on their higher academic degrees and/or in research positions. Matthias will give a testimonial of his own career. Particularly, he will share the factors that governed the decisionmaking of “where to go” during his time as a post-doc, and the thinking and emotions that were part of that evolution process.
The intention is to provide fruit for thought, as a basis for an open discussion around career, life, and happiness.