SupraChem 2024

Ulm University | February 25-27

Book of Abstracts

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Organic Materials

SupraChem 2024 is the seventh conference of this biannual series that brings together supramolecular chemists and scientists from related fields for three days. The meeting will allow us to share and discuss cutting-edge research and recent developments in areas ranging from supramolecular polymers, metal-organic structures, molecular cages, supramolecular machinery and dynamic systems, life-like assemblies, and biomimetic materials.

We are looking forward to your participation in this stimulating meeting and welcome you to Ulm in February 2024!

Yours sincerely,

Job Boekhoven, Max von Delius, and Birgit Esser

Conference Chairs

Schedule

Day 1 – Sunday, February 25, 2024

3.30 – 4.30 PM	**Registration**
4.30 – 6.00 PM	**Session 1**: *Non-equilibrium systems*
4.30 – 4.45 PM	**Kick-off for SupraChem2024**
	Job Boekhoven, Max von Delius, Birgit Esser
4.45 – 5.30 PM	**Keynote Speaker – David Leigh**
5.30 – 5.45 PM	**Guillermo Monreal Santiago**
5.45 – 6.00 PM	**Lukas Zeininger**
6.00 – 8.00 PM	**Welcome Party at Foyer N27**

Day 2 – Monday, February 26, 2024

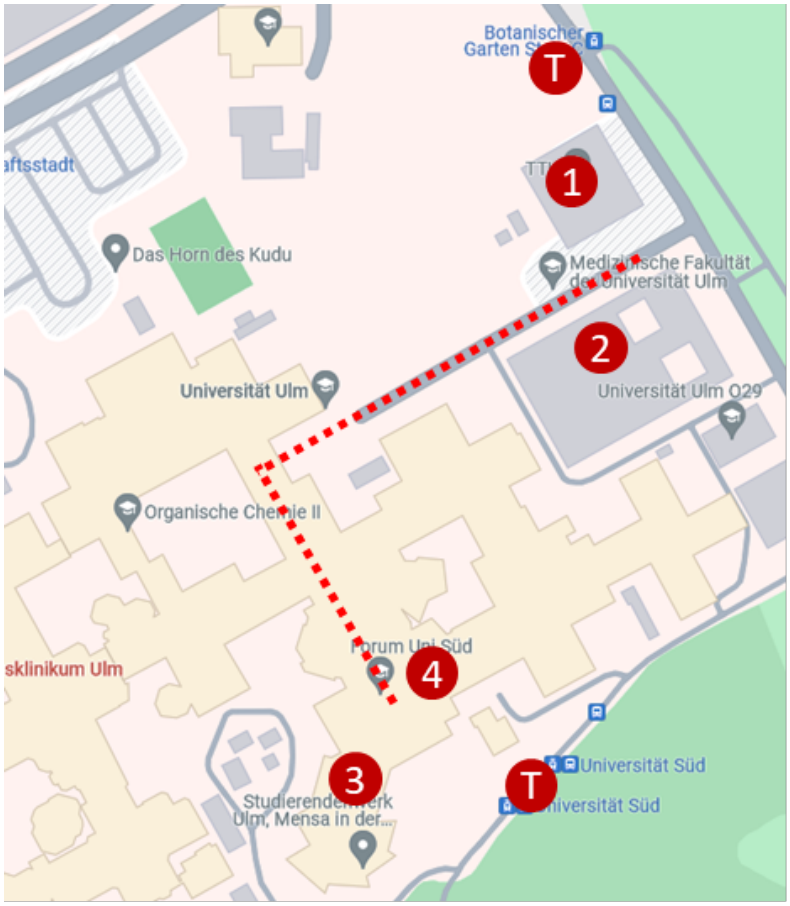
9.00 – 10.30 AM	**Session 2**: *Engineering of* de Novo *Life*
9.00 – 9.45 AM	**Keynote Speaker – Sijbren Otto**
9.45 – 10.00 AM	**Laura Heinen**
10.00 – 10.30 AM	**Kerstin Göpfrich**
10.30 – 11.15 AM	**Coffee Break at Foyer N27 (2)**
11.15 – 12.30 PM	**Session 3:** *Supramolecular Catalysis*
11.15 – 11.30 AM	**Bartosz Lewandowski**
11.30 – 12.00 PM	**Jochen Niemeyer**
12.00 – 12.30 PM	**Konrad Tiefenbacher**
12.30 – 1.45 PM	**Lunch Break**
1.45 – 3.20 PM	**Session 4**: *Hosts & Materials I*
1.45 – 2.15 PM	**Invited Speaker for the Cram-Lehn-Pedersen Prize lecture**
	Niveen Khashab
2.15 – 2.45 PM	**Angela Casini**
2.45 – 3.00 PM	**Tomáš Solomek**
3.00 – 3.15 PM	**Larissa von Krbek**
3.15 – 3.20 PM	**Conference group photo**

3.20 – 4.00 PM	**Coffee Break at Foyer N27**
4.00 – 5.45 PM	**Session 5**: *Hosts & Materials II*
4.00 – 4.30 PM	**Claudia Caltagirone**
4.30 – 4.45 PM	**Mariana Kozlowska**
4.45 – 5.15 PM	**Michael Mastalerz**
5.15 – 5.30 PM	**Shikha Dhiman**
5.30 – 5.45 PM	**Poster Pitches**
5.45 – 8.00 PM	**Poster Session, Drinks and Snacks in the Mensa**

Day 3 – Tuesday, February 27, 2024

9.00 – 10.30 AM	**Session 6**: *Nucleic Acid Nanotechnology*
9.00 – 9.45 AM	**Keynote Speaker – Hanadi Sleiman**
9.45 – 10.00 AM	**Elisha Krieg**
10.00 – 10.30 AM	**Ivan Huc**
10.30 – 11.00 AM	**Coffee Break at Foyer N27**
11.00 – 13.00 PM	**Session 7**: *Cages, Knots and Switches*
11.00 – 11.30 AM	**Invited Speaker – Rafal Klajn**
11.30 – 12.00 PM	**Fabien Cougnon**
12.00 – 12.15 PM	**Brigitta Duzs**
12.15 – 12.45 PM	**Guido Clever**
12.45 – 13.00 PM	**Closing remarks and poster prize announcement**
	Job Boekhoven, Max von Delius, Birgit Esser

Important locations



1. **TTU** – lecture hall
2. **N27** – coffee breaks and welcome reception
3. **Mensa** – lunch and poster session
4. **Cafeteria Southside** with Burger Bar

T **Tram Stations**

Lunch menu: https://studierendenwerk-ulm.de/en/food-and-drink/mensa-lunchrooms-and-cafeterias-2/

In case you get lost, the address of the TTU lecture hall

Meyerhofstrasse 1, 89081 Ulm

Speakers abstracts

Keynote Speaker 1

David Leigh (University of Manchester), Sunday, February 25, 4.30 PM

Giving Chemistry Direction

In recent years examples of synthetic molecular machines and motors[1] have been developed,[2] all be they primitive by biological standards. Such molecules are best designed to work through statistical mechanisms. In a manner reminiscent of Maxwell's Demon,[3] random thermal motion is rectified through ratchet mechanisms,[3-8] giving chemistry direction.

It is increasingly being recognised that similar concepts can be applied to other chemical exchange processes.[9] Ratchet mechanisms—effectively chemical engines[10] in which catalysis[4,6,7] of 'fuel' to 'waste' is used to drive another chemical process—can cause directional impetus in what are otherwise stochastic systems, including reversible chemical reactions. This is ushering in a new era of non-equilibrium chemistry, providing fundamental advances in functional molecule design and the first examples of molecular robotics,[11,12] overturning existing dogma and offering fresh insights into biology and molecular nanotechnology.

For a musical introduction, see 'Nanobot': https://bit.ly/2M5Zwdl

[1] The Nobel Prize in Chemistry 2016–Advanced Information. Nobelprize.org. Nobel Media AB 2014. Web. 6 Oct, 2016, http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2016/advanced.html.
[2] "Rise of the molecular machines", Angew. Chem. Int. Ed. 54, 10080 (2015).
[3] "A molecular information ratchet", Nature 445, 523 (2007).
[4] "An autonomous chemically fuelled small-molecule motor", Nature 534, 235 (2016).
[5] "Rotary and linear molecular motors driven by pulses of a chemical fuel", Science 358, 340 (2017).
[6] "A catalysis-driven artificial molecular pump", Nature 594, 529 (2021).
[7] "Autonomous fuelled directional rotation about a covalent single bond", Nature 604, 80 (2022).
[8] "A tape-reading molecular ratchet", Nature 612, 78 (2022).
[9] "Design, synthesis and operation of small molecules that walk along tracks", J. Am. Chem. Soc. 132, 16134 (2010).
[10] "Chemical engines: Driving systems away from equilibrium through catalyst reaction cycles", Nat. Nanotechnol. 16, 1057 (2021).
[11] "Sequence-specific peptide synthesis by an artificial small-molecule machine", Science 339, 189 (2013).
[12] "Stereodivergent synthesis with a programmable molecular machine", Nature 549, 374 (2017).

Keynote Speaker 2

Sijbren Otto (University of Groningen), Monday, February 26, 9.00 AM

Mechanism of Emergence in the Approach Toward De-Novo Life

How the immense complexity of living organisms has arisen is one of the most intriguing questions in contemporary science. We have started to explore experimentally how organization and function can emerge from complex molecular networks in aqueous solution.[1] We focus on networks of molecules that can interconvert, to give mixtures that can change their composition in response to external or internal stimuli. Noncovalent interactions within molecules in such mixtures can lead to the formation of foldamers.[2,3] In contrast, molecular recognition between molecules in such mixtures leads to their mutual stabilization, which drives the synthesis of more of the privileged structures. As the assembly process drives the synthesis of the very molecules that assemble, the resulting materials can be considered to be self-synthesizing. Intriguingly, in this process the assembling molecules are replicating themselves, where replication is driven by self-recognition of these molecules in the dynamic network.[4] The selection rules that dictate which (if any) replicator will emerge from such networks are starting to become clear.[5] We have also witnessed spontaneous differentiation (a process akin to speciation as it occurs in biology) in a system made from a mixture of two building blocks.[6] When such systems are operated under far-from-equilibrium flow conditions, adaptation of the replicators to a changing environment can occur.

Replicators that are able to catalyse reactions other than their own formation have also been obtained, representing a first step towards metabolism.[7,8] Rudimentary Darwinian evolution of purely synthetic molecules has also been achieved [9] and the prospect of synthesizing life de-novo is becoming increasingly realistic.[10]

[1] Li, J.; Nowak, P.; Otto, S. J. Am. Chem. Soc. 2013, 135, 25, 9222-9239.
[2] Liu, B.; Pappas, C. G.; Zangrando, E.; Demitri, N.; Chmielewski, P. J.; Otto, S. J. Am. Chem. Soc. 2019, 141, 1685-1689.
[3] Pappas, C. G.; Mandal, P. K. Liu, B.; Kauffmann, B.; Miao,X.; Komáromy, D.; Hoffmann, W.; Manz, C.; Chang, R.; Liu, K.; Pagel, K.; Huc, I.; Otto, S. Nature Chem. 2020, 12, 1180–1186.
[4] Carnall, J. M. A.; Waudby, C. A.; Belenguer, A. M.; Stuart, M. C. A.; Peyralans, J. J.-P.; Otto, S. Science 2010, 327, 1502-1506.
[5] Malakoutikhah, M.; Peyralans, J.J-P.; Colomb-Delsuc, M.; Fanlo-Virgos, H.; Stuart, M. C. A.; Otto, S, J. Am. Chem. Soc. 2013, 135, 49, 18406-18417.
[6] Sadownik, J. W.; Mattia, E.; Nowak, P.; Otto, S. Nature Chem. 2016, 8, 264–269.
[7] Monreal Santiago, G.; Liu, K.; Browne, W. R.; Otto, S. Nature Chem. 2020, 12, 603-607.
[8] Ottelé, J.; Hussain, A. S.; Mayer, C.; Otto, S. Nature Catal. 2020, 3, 547-553.
[9] K. Liu, A. Blokhuis, C. van Ewijk, A. Kiani, J. Wu, .W.H. Roos, S. Otto Nature Chem. 2023, in press.
[10] Adamski, P.; Eleveld, M.; Sood, A,; Kun, A.; Szilágyi, A.; Czárán, T.; Szathmáry, E.; Otto, S. Nature Rev. Chem. 2020, 4, 386–403.

Keynote Speaker 3

Hanadi Sleiman (McGill University), Tuesday, February 27, 9.00 AM

DNA Self-Assembly: From Pathway Complexity to Drug Delivery

DNA nanotechnology can assemble materials on the nanoscale with exceptional predictability and programmability. In a sense, this field has reduced the self-assembly space into a simple ‘alphabet’ composed of four letters (A, T, G, C). Nature, on the other hand, relies on many more interactions to build its functional structures and supramolecular chemistry has taken advantage of these interactions to assemble materials with highly diverse structures and functions.

This talk will describe our efforts to merge the field of supramolecular chemistry with DNA nanotechnology. This approach results in new motifs and functionalities that are unavailable with base pairing alone. Starting from a minimum number of DNA components and combining them with organic molecules and polymers, we create 3D-DNA host structures, such as cages, nanotubes, and spherical, cylindrical, or lamellar nucleic acids. These nanostructures are fascinating in their self-assembly behaviour and promising for targeted drug delivery. They can encapsulate and selectively release drugs and nucleic acid therapeutics. We find that they resist nuclease degradation, and silence gene expression in vitro and in vivo, in tissues and cell types that are difficult to access with other constructs.

We will also discuss the ability of small molecules to reprogram the assembly of DNA, away from Watson-Crick base-pairing into new motifs. This is a fundamental shift in the field, as it expands the DNA ‘alphabet’ without complex synthesis. The resulting DNA structures can be applied to gene delivery, tissue regeneration and materials science.

[1] N. Seeman, H. Sleiman, DNA Nanotechnology, Nat. Rev. Mat., 2017, 17068.
[2] F. Rizzuto, C. Platnich, X. Luo, M. Dore, C. Lachance-Brais, G. Cosa, H. Sleiman, A dissipative pathway for the structural evolution of DNA fibers, Nat. Chem., 2021, 13, 843–849.
[3] M. Dore, T. Trinh, D. de Rochambeau, P. Xu, J. Li, H. F. Sleiman, Thermosetting supramolecular polymerization of compartmentalized DNA fibers with stereo sequence and length control, Chem, 2021, 7, 2395-2414.
[4] K. E. Bujold, J. C. C. Hsu and H. F. Sleiman; Optimized DNA “Nanosuitcases” for Encapsulation and Conditional Release of siRNA, J. Am. Chem. Soc. 2016, 138, 14030–14038.

Invited Speaker for the Cram-Lehn-Pedersen Prize lecture

Niveen Khashab (King Abdullah University of Science and Technology)
Monday, February 26, 1.45 PM

Supramolecular Hosts: From Energy Intensive Separations to Sensors and Soft Robotics

Host-guest based mechanisms have been heavily exploited for molecular recognition and eventual separation/ entrapment of a guest molecule. Choosing the right host has in most of the cases depended on complimentary size and charge thus, focusing mainly on the intrinsic interactions of the guest in the cavity of a macrocycle or a cage. Interestingly, expanding host-guest interactions to the extrinsic environment of the host afforded an intriguing set of molecular descriptors that ultimately led to unexplored host-guest interactions. In this talk, a set of supramolecular hosts ranging from 2D macrocycles to 3D cages are presented with intriguing intrinsic and extrinsic host-guest interactions that enabled them to be used for hydrocarbon and isomers separation from crude oil as well as smart recognition units in polymer composites for sensors and soft robotics. Understanding the full range of supramolecular interactions will ultimately promote a better integration of molecular building blocks to design and fabricate the “next -generation” sustainable and smart materials.

Invited Speaker

Rafal Klajn (Institute of Science and Technology, Austria), Tuesday, February 27, 11.00 AM

Supramolecular machinery for disequilibrating azobenzenes

DisEquilibration by Sensitization under Confinement (DESC) is a supramolecular approach to isomerize photoswitchable molecules from the stable state to the metastable state using visible light of the desired wavelength (including red light). I will show that a combination of a coordination cage and a visible-light sensitizer can act together to selectively bind and sensitize the E isomer of various azobenzenes and other azo switches. Upon switching to the metastable Z isomer, the azoarene loses its affinity to—and is expelled from—the cage, which can then convert additional copies of E into Z. In this way, the cage·sensitizer complex acts as a light-driven supramolecular machine, converting light energy into chemical energy in the form of out-of-equilibrium photostationary states that cannot be accessed directly using visible light.

Selected Speakers

Guillermo Monreal Santiago (University of Strasbourg), Sunday, February 25, 5.30 PM

Responsive coacervates as a tool for controlling supramolecular structures

We propose complex coacervates as a platform to control supramolecular structures by proxy. Coacervates are micron-sized droplets that form in water due to interactions between polyelectrolytes. They spontaneously sequester supramolecular monomers from solution, localizing them and acting as a new responsive environment for their self-assembly. This allows us to localize supramolecular structures, and make them sensitive to stimuli that target the coacervate, rather than the structures themselves.
In this talk, I will discuss how the combination of salt-responsive coacervates with light-responsive monomers allows us to access a broad range of supramolecular structures from a single molecule.

Furthermore, I will introduce how my group is developing new stimuli to interact with complex coacervates.

Lukas Zeininger (Max Planck Institute of Colloids & Interfaces)
Sunday, February 25, 5.45 PM

Dissipative Supramolecular Equilibrium-Balanced Actuation and Motion of Messenger Droplets

In this contribution, the design of a synthetically minimal complex emulsion platform that, controlled by supramolecular recognition events at the interface, is able to adapt autonomously and reversibly to its chemical environment, will be presented. The droplets can serve as a messenger colloid to quantitatively visualize, measure and report force gradients in temperature, chemistry and concentration with up to femtomolar sensitivity and we will disclose how multiple independent dissipative responsive modalities in the system can collaborate to balance novel reversible tactile responses of all liquid matter, which has significant implications for future soft robotic and sensing technologies.

Laura Heinen (DWI - Leibniz-Institute for Interactive Materials)
Monday, February 26, 9.45 AM

Minimal metabolism for synthetic life-like vesicle systems

Engineering artificial metabolism in synthetic systems is a challenging task. Inspired by endosymbionts, that rely on the energy supply from their host cell, we developed synthetic vesicles that can exchange ATP across their membrane. Here, I will demonstrate an example of ATP cross-feeding synthetic vesicles. One population of vesicles produces and exports ATP, while a second population of vesicles takes up the ATP and uses this chemical energy to fuel ATP-consuming reactions. The vesicles are a future platform technology to fuel energy-dependent processes in a sustained fashion such as in synthetic cells, as biological nanoreactors and as the building blocks of life-like systems materials.

Kerstin Göpfrich (Heidelberg University) Monday, February 26, 10.00 AM

RNA origami hardware for synthetic cells

Today's living cells emerge from the complex interplay of thousands of molecular constituents. Our vision is to create a simpler model of a cell that consists of a lipid vesicle and operates based on our own custom-engineered and genetically encoded molecular hardware made from DNA and RNA nanotechnology. Recently, we demonstrated the power of two-photon 3D laser printing for synthetic biology, realized mechanisms for vesicle division and build functional DNA and RNA-based mimics of cytoskeletons, capable of cargo transport and signal transduction. Ultimately, by coupling GUV division to their informational content and their function, we aim for a prototype of a synthetic cell capable of evolution.

Bartosz Lewandowski (ETH Zürich) Monday, February 26, 11.15 AM

Catalytic Length-Controlled Oligomerization with Synthetic Programmable Templates

Templated synthesis is a powerful strategy to access oligomers from monomeric building blocks in a length-controlled manner. These reactions require, however, the use of stoichiometric amounts of the template with respect to the product formed. Herein, we present catalytic macrocyclic templates that promote the formation of oligomers of a small molecule substrate with a remarkable degree of length-control. The templates consist of rigid oligoproline moieties that are decorated with catalytic sites at defined distances on both sides of the macrocyclic cavity. The dimensions of the macrocycles and the number of catalytic moieties thereon determine the number of monomers that are incorporated into the growing oligomer, thus allowing access to specific products with lengths pre-programmed by the template.

Jochen Niemeyer (University of Duisburg-Essen) Monday, February 26, 11.30 AM

Rotaxanes, catenanes and macrocycles: Using the supramolecular toolbox for the design of novel catalysts

The development of highly efficient organocatalysts has revolutionized chemical catalysis in the last decades. Especially the use of chiral Brønsted-acids, such as 1,1´-binaphthyl-phosphoric acids, has enabled a plethora of highly useful stereoselective transformations.

Our group has recently developed chiral [2]rotaxanes, [2]catenanes and non-interlocked macrocycles3 based on 1,1´-binaphthyl-phosphoric acids. These were successfully applied as catalysts for various transformations, such as enantioselective transfer-hydrogenations, Michael-additions and fluorinations.

In our research, we are investigating how the special nature of the mechanical bond influences the application in catalysis. In this context, we develop novel methods for the synthesis of the desired interlocked catalysts, we investigate the special nature of bifunctional catalysts and we try to approach catalyst structures with mechanical chirality.

Konrad Tiefenbach (University of Basel) Monday, February 26, 12.00 PM

How does a supramolecular capsule enable catalytic β-selective glycosylations for diverse substrates?

My group is interested in exploring catalysis inside supramolecular containers. We recently found that the hexameric resorcin[4]arene capsule is able to catalyze the beta-selective glycosylation of a wide range of electrophiles and nucleophiles. This general scope is very unusual. Evidence was found that a proton wire mechanism observed in some enzymes is likely at work.

Angela Casini (Technical University Munich) Monday, February 26, 2.15 PM

Supramolecules for Targeted Therapy and Imaging

The biomedical application of discrete SCCs, specifically self-assembled 3D-metallacages, is an emergent field of study. In this lecture, I aim at summarising the key concepts and challenges in this fascinating research area, starting with the main synthetic and design principles and illustrating representative examples from our group. Thus, the case of "lantern-shaped" cationic $[M_2L_4]^{n+}$ cages (M = Pd(II), Pt(II), L = bitopic monodentate N-donor ligand) will be presented, as well as their use either as targeted drug delivery systems or as new (radio-)theranostic agents.

Tomáš Solomek (University of Amsterdam) Monday, February 26, 2.45 PM

Organic Cages with Aromatic Diimides: Porosity, Photochemistry, and Heteroleptic Architectures

I will discuss my group's effort to incorporate chromophores into covalent organic cages. Thereby, we create materials that are not only porous, but display intriguing photochemistry that emerges from the high-symmetry spatial arrangement of these chromophores and from the presence of internal voids that can nanoconfine solvent. I will further show that the shape of covalent organic cages allows for unexpected supramolecular solid-state assemblies. Finally, I will briefly discuss our recent effort to beat the dynamic self-sorting in these structures and to synthesize heteroleptic covalent organic cages with high selectivity.

Larissa von Krbek (University of Bonn) Monday, February 26, 3.00 PM

Switchable macrocycles

Photoswitchable molecules can reversibly interconvert between two different isomers. With new applications for photoswitches constantly emerging, the necessity arises to continue to develop photoswitches with different properties than the already established ones. We have developed a versatile synthesis for macrocyclic azobenzenes, which allows for facile modification of these photoswitches. One example shows high chemical stability, long half-life of its Z-isomer, quantitative ZàE conversion under white light, and excellent separation of the excitation bands to address either the E or Z-state selectively. Almost quantitative ZàE conversion, even under white light, is a unique feature with an important impact on applications, in which the configuration under ambient light needs to be close to 100%.

Claudia Caltagirone (University of Cagliari) Monday, February 26, 4.00 PM

Indole-based receptors for anion binding, sensing and transport

Since when the first papers on indole-based receptors for anion binding were published at the end of 2000s, this heterocycle has become quite popular in the design of anion receptors. Indole, like pyrrole, contains a single hydrogen-bond donor group, but is slightly more acidic, and is employed in biological systems to bind anions such as chloride and sulfate. During the presentation it will be shown that when indole is used to functionalize different scaffolds, interesting receptors for various applications such as anion and small molecules sensing, anion transport or development of novel self-assembled supramolecular materials can be obtained.

Acknowledgements
Financial support from MUR (PRIN_PNRR P2022XHLTX), and NextGeneration EU, Return project (PE0000005 CUP:F53C22000730002) is gratefully acknowledged.

Mariana Kozlowska (Karlsruhe Institute of Technology) Monday, February 26, 4.30 PM

Automated design of supramolecular aromatic metal-organic assemblies

Fabrication of materials comprising optimized assemblies and functional chromophore molecules enables efficient tailoring of material properties. However, the verification of molecular structure and materials morphology, dynamics and property relationships is experimentally cumbersome. In addition, a number of properties and their change in time are of a multiscale character that have to be considered to tackle the proper material responses.

Based on decade-long method development, virtual design strategies have become ever more important. Such design with multiscale methods profit from the availability of automated tools, enabling the screening of huge libraries of organic molecules in their in silico models of supramolecular assemblies. As an example, the controlled arrangement of molecules in a material can be modulated using the metal-organic framework (MOF) approach. In my talk, I will demonstrate the application of automated workflow tools to design MOF materials with the simultaneous prediction of their properties from quantum mechanics and molecular mechanics.

Michael Mastalerz (Heidelberg University) Monday, February 26, 4.45 PM

Controlling π-Stacking – Towards New and Reliable Crystal Engineering Synthons for Materials Chemistry

Crystal Engineering is a subtopic of supramolecular chemistry dealing with the controlled crystallization of molecules and thus controlling the materials properties of a compound, which is in the solid state strongly depending on the geometric arrangement of the molecular units to each other. This is especially important in the field of organic electronics, where charge-transport between molecules is largely dominated by the spatial arrangement of the aromatic molecules. However, a crystal engineering synthon is a reliable unit that if placed to a molecule will dominate the crystal-packing and mainly those motifs with relatively strong directing interactions such as hydrogen or halogen bonding have been used as crystal engineering synthons. π-Stacking is in comparison to other supramolecular interactions very weak and usually non- or less directional and therefore arrangement of aromatic molecules is difficult to be controlled. Nevertheless, exactly this is demanded for organic electronics.

In the talk, strategies of reliably controlling arrangement of π-systems without the aid of further supramolecular tools (e.g. hydrogen or halogen bonding, coordination chemistry) will be introduced.

Shikha Dhiman (University of Mainz) Monday, February 26, 4.45 PM

Supramolecular Polymers to Liquid Droplets Using Competitive Interactions

The discovery of phase-separated organelles has reignited interest in phase separation in molecules and materials. Despite the challenges posed by low propensity and unfavorable entropy, modulating the energy landscape with competing supramolecular interactions presents promising strategies. Our work demonstrates that benzene-1,3,5-tricarboxamide (BTA) monomers, typically forming 1D supramolecular polymers, can transition into liquid droplets through competitive interactions with surfactants, offering innovative opportunities for creating phase-separated droplets of small molecules.

Elisha Krieg (Technical University Dresden) Tuesday, February 27, 9.45 AM

Programmable polymer materials empowered by DNA nanotechnology

Biological tissues are self-organized, responsive, and genetically programmed to execute a vast array of functions. Intriguingly, the field of DNA nanotechnology has recently opened new possibilities for creating synthetic materials with attributes and a level of control reminiscent of those found in biological matter. In this talk, I will discuss our progress in developing such programmable materials and elucidate their interactions with living cells and tissues. Due to their customizable mechanical properties and predictable responsiveness, these fully synthetic matrices help guide and interrogate cellular development and morphogenesis.

Ivan Huc (Ludwig Maximilian University of Munich) Tuesday, February 27, 10.00 AM

Engineering molecular shape with synthetic oligomers

Aromatic oligomers constitute a distinct and promising class of synthetic foldamers. Their structures are, to a large extent, predictable, show unprecedented conformational stability in essentially all solvents, and represent convenient building blocks to elaborate protein-sized architectures. Cavities can be designed within aromatic foldamers that enable them to act as artificial receptors, and their surface can be decorated for the selective recognition of protein surfaces.

Fabien Cougnon (University of Jyväskylä) Tuesday, February 27, 11.30 AM

Foldaknots

Synthesising fully organic, multiply entangled macromolecules without resorting to metal templation represents a formidable challenge. In this presentation, I will discuss the efforts of our group to develop reliable metal-free methodologies to access multiply entangled macromolecules. We have notably demonstrated that the hydrophobic effect could be exploited to direct the folding of exceptionally compact entangled macromolecules. This methodology is easy to implement, generally high yielding and allows for the synthesis of macromolecules with different topologies.

Brigitta Duzs (University of Mainz) Tuesday, February 27, 12.00 AM

Mechano-Adaptive Hydrogels with Metamaterial Strain Gates and Reaction-Diffusion Signaling

Highly autonomous life-like behavior in functional materials can be achieved by embedding nonlinear chemical or physical dynamical elements, i.e., chemical reaction networks and metamaterial unit cells. Herein we introduce a platform concept to realize the sensor-processor-actuator paradigm in soft robots and mechanical materials. We integrate mesoscale metamaterial unit cells as binary strain-gate sensory units, the reaction-diffusion dynamics of the pH-autocatalytic urea-urease chemical reaction network as the information processing element, and adaptive downstream macromolecular processes for actuator response. Our approach allows for advanced local-to-global information transmission and mimosa-like system-level adaptivity induced by local forces in closed, free-standing multi-material hydrogels.

Guido Clever (Technical University Dortmund) Tuesday, February 27, 12.15 AM

From Heteroleptic Coordination Cages to Complex Molecular Systems

Advanced self-assembly strategies enable the targeted synthesis of supramolecular systems and materials with increasing structural and functional complexity. We develop non-statistical assembly strategies such as “shape complementary assembly” (SCA) and “coordination sphere engineering” (CSE) to obtain heteroleptic metallosupramolecular structures. In this way, several functions can be combined and ‘complex systems’ behaviour can emerge. For example, we study cage interconversions, guest-binding/release cascades and propagation of chiral information.

Poster numbers and presenters

Host-Guest-Chemistry

1	**Robert Hein**	*Ion-Dependent Conformational Switching of Bisthioxanthylidenes*
2	**Léa Lefrancois**	*Acridinium receptors: π-π stacking and anion-π interactions*
3	**Swapnil Ghule**	*Synthesis and Supramolecular Binding Properties of Cytosine-Functionalized Macrocyclic Receptor.*
4	**Veronika Stoianova**	*Synthesis and VCD-Spectroscopy of Chiral Azacryptands*
5	**Mark Spektor**	*Macrocyclic hosts based on triphenylamine*
6	**Sebastiano Casalino**	
7	**David Ocklenburg**	*Flexibility drives oxalate recognition within neutral L_2Zn_2 containers.*
8	**Rafał Grzelczak**	*Calix[n]phyrin condensation: A Tool for the Construction of Mechanically Interlocked Porphyrinoids*
9	**Nilima Manoj Kumar**	*SUPRABANK – The Repository for Supramolecular Interactions*
10	**M. A. Niyas**	*Bilayer nanographene with a benzene defect shows evidence for halide permeation*
11	**David Van Craen**	*Charge-neutral metallocontainers for anion recognition*
12	**Clara Schritt**	*A constricted helically chiral open-chain tetrapyrrole*
13	**Lena Beiersdörfer**	*Selective Recognition of Sucrose in Water by a Synthetic Receptor*
15	**Jessica Rühe**	*A Terrylene Bisimide based Universal Host for Aromatic Guests to Derive Contact Surface-Dependent Dispersion Energies*
16	**Maximilian Notheis**	*Allosterically controlled metallo-supramolecular spin crossover complexes*
17	**Boris Morozov**	*Macrocyclic Conformational Switch Coupled with Pyridinium-Induced PET for Fluorescence Detection of Adenosine Triphosphate*
18	**Janos Wasternack**	*Spectroscopic Investigation of a Redox-Active Squaraine Rotaxane*

Self-Assembly

19	**Jack Davies**	*Imaging Self-Assembled Metal-Organic Networks at the Solid-Liquid Interface with (Sub)Molecular Resolution.*
20	**Tiffany Guitton-Spassky**	*Beyond Assembly: Fluorinated Amphiphiles Tailored for Diverse Functionalities*
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