Book of Abstracts

# BERLINER CHEMIE IN PRAXIS SYMPOSIUM


JCF Berlin

Gesellschaft Deutscher Chemiker

# 1. Table of Contents

## 2. Scientific Program

The BCPS offers a varied program with talks by young scientists, representatives from industry, stimulating poster sessions, catering, and many opportunities to meet and network. The schedule for the event is summarized below.

| | | |
|---|---|---|
| From 08:30 | Registration | |
| 09:00 – 09:15 | Opening Remarks | |
| 09:15 – 10:00 | Plenary Lecture | |
| | Dr. Oliver Dumele | Functional Molecules made to Order: Framework Materials and their Monomers |
| 10:00 – 10:30 | Coffee Break | sponsored by BCNP |
| 10:30 – 11:45 | 1st Session | |
| 10:30 – 10:55 | Amiera Hadi | Atmospheric-stable Phenyl Derivatives of Pentafluoroorthotellurate |
| 10:55 – 11:20 | Miriam Simon | Complexation of the cationic lipid DOTAP with oppositely charged polyelectrolytes |
| 11:20 – 11:45 | Michael Traxler | Tuning Acridine-Functionalized COFs towards Fully-Heterogenous Metallaphotocatalysts |
| 11:45 – 13:15 | Lunch Break and Poster | Session sponsored by Chemistry Europe |
| 13:15 – 14:15 | **Industry Talk** | |
| 13:15 – 13:45 | Axel Straube | Chemistry Europe – Who we are and what we do |
| 13:45 – 14:00 | Dr. Holger Bengs | Supporting decision-maker in tech companies and tech-related institutions |
| 14:00 – 14:15 | Dr. Nadia Elghobashi-Meinhardt | KNAUER GmbH |
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| 14:15 – 14:40 | Simon Djoko | Polyoxometalate boosting the light-harvesting ability of graphitic carbon nitride |
| 14:40 – 15:05 | Rahel Marschall | CO2 as a tuning parameter for the head group properties of non-ionic EO-surfactants |
| 15:05 – 15:30 | Marc Appis | BLI and dPCR – Advanced Techniques for Quantifying Biomolecules and their Interactions |
| 15:30 – 16:00 | Coffee Break | sponsored by KNAUER |
| 16:00 – 17:30 | Workshop | |
| | VAA-Workshop (job application, contracts, salary, and career) | |
| | JCF-Workshop from Team Sustainability / Start-Up | |
| 17:30 – open | Closing, Talk & Poster Prizes | |

## 3. Sponsors

**We kindly thank our sponsors!**

Communication between science and industry is of utmost importance, also with regard to career prospects. The BCPS brings young chemists together and offers a great stage for participants and companies to establish or grow contacts.

We would therefore like to thank our sponsors who make this event possible:












# Industry Lectures

## 3.1 Chemistry Europe – Who we are and what we do

Axel Straube[1]

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Founded in 1995, Chemistry Europe is an association of 16 chemical societies from 15 European countries, representing over 75,000 chemists. It publishes a family of high-quality scholarly chemistry journals, covering a very broad range of disciplines.

Its mission is to evaluate, publish, disseminate, and amplify the scientific excellence of chemistry researchers from around the globe in high-quality publications. It supports its members at every stage of their careers as they strive to solve the challenges that impact humankind. In all its work, Chemistry Europe values integrity, openness, diversity, cooperation, and freedom of thought.

In this talk, Associate Editor Axel Straube (*ChemistryOpen, Chemistry–Methods* and *ChemistrySelect*) will introduce Chemistry Europe, its family of journals and the work Chemistry Europe does to support researchers at all stages of their careers. Recent developments in Open Access publishing[1] will be highlighted with a special focus on the DEAL agreement and how Open Access works.

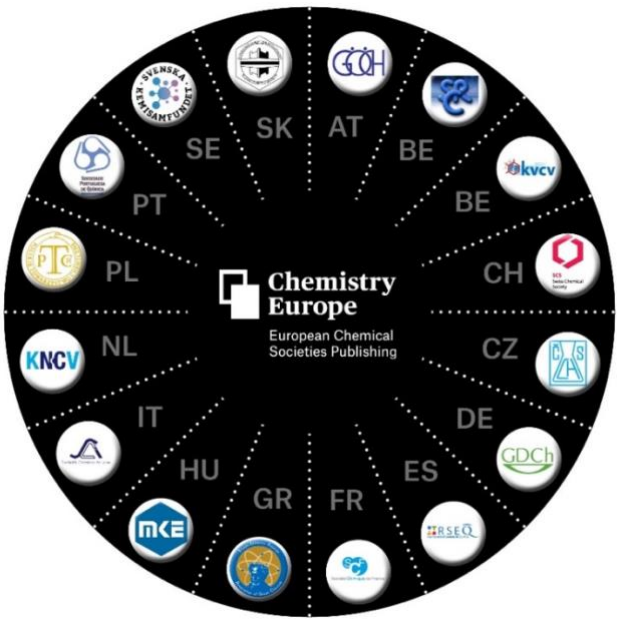


**Figure 1:** The 16 European chemical societies involved in Chemistry Europe.

**Literature:**

[1] A. Straube, F. Novara *Where is Open Access Publishing Heading?* ChemistryViews, 2022, DOI: 10.1002/chemv.202200036.

## 3.2 Supporting decision-maker in tech companies and tech-related institutions

Dr. Holger Bengs

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

BCNP, founded back in 2002, is a consultancy company specialized on the branches Biotech, Chemistry, Nanotech and Pharma.

BCNP offers market analyses, technology scouting and business planning for making strategic decisions (BCNP Strategy) and brings clients together with new potential customers (BCNP connect). Furthermore, BCNP is initiator and organizer of the European Chemistry Partnering (ECP), connecting start-ups and SME with Corporates and Investors. BCNP's customers appreciate the simultaneous understanding of technology and economy.

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

The presentation gives an insight into what types of projects are carried out at BCNP and what a working day at BCNP can look like.

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

BCNP bietet kontinuierlich bezahlte Praktikantenplätze nach Mindestlohn ab drei Monaten in Köln, Frankfurt und digital.

## 3.3 Vorstellung: KNAUER GmbH

Dr. Nadia Elghobashi-Meinhardt

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Das mittelständisches Familienunternehmen KNAUER mit Sitz in Berlin-Zehlendorf ist seit 1962 für die Wissenschaften aktiv. Mit 165 hochqualifizierten Mitarbeitenden, davon 40 % Frauen, entwickelt und produziert das Unternehmen High-Tech-Messinstrumente von höchster Präzision und Qualität mit Schwerpunkt auf Flüssigkeitschromatografie-Systemen (HPLC) und deren Komponenten. Heute liefert KNAUER hochpräzise Messinstrumente an Kunden in aller Welt.

Seit der SARS-CoV-2 Pandemie hat sich KNAUER darauf verlegt, Impingement Jets Mixing (IJM)-Skids für die Herstellung von Lipid-Nanopartikeln (LNP) zu entwerfen, zu entwickeln und weltweit zu verkaufen, insbesondere für die Herstellung von Impfstoffen auf mRNA-Basis. Diese IJM-Skids wurden von großen Pharmaunternehmen (z. B. Pfizer, BioNTech) eingesetzt, um die Produktion von mRNA-basierten Impfstoffen in großem Maßstab zu ermöglichen.

Für ihre bedeutende Rolle bei der Unterstützung der weltweiten Gemeinschaft während der Pandemie hat KNAUER weithin Anerkennung erhalten. Im Jahr 2022 wurde das Unternehmen mit dem „Innovationspreis Berlin-Brandenburg“ und dem „Großen Preis des Mittelstandes“ ausgezeichnet.

Foto: Bundeskanzlerin Angela Merkel besucht im September 2021 die Firma KNAUER.

## 4. Plenary Lecture

Constructing extended covalent frameworks based on symmetric organic small molecules is known as reticular chemistry. Such covalent organic frameworks (COFs) commonly have a 2-dimensional connectivity, resulting in stacked 2D polymers with a high degree of crystallinity and high surface areas.

Our synthetic approach leaves the flatland of two-dimensional materials. We aim at molecules that step beyond the known architectures by constructing non-planar, chiral, tubular, and electronically exotic topologies. Along this journey, we have taken detours at several stages to dig into the properties of new monomers from an optoelectronic, magnetic, and supramolecular perspective.

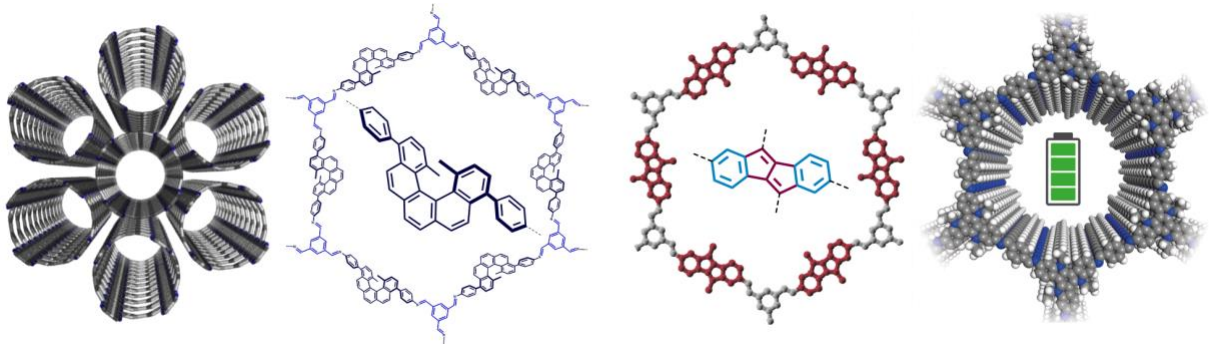

**Figure 1:** Structure of covalent organic frameworks (COFs) with new monomers for different applications.

The seminar reports on a range of molecular monomers as well as entire frameworks with surprising molecular behaviour and unexpected synthetic challenges. Unusual structures, high supramolecular affinities, and useful magnetic properties are some of the desirable characteristics of these materials.

### About the speaker

Oliver Dumele studied Chemistry at the University of Mainz and UC Berkeley (USA). After research projects at the Max Planck Institute for Polymer Research, BASF Ludwigshafen, and the National University of Singapore, he moved to Switzerland for his doctoral research. He received his PhD in chemistry from ETH Zürich under supervision of Prof. François Diederich in 2015. After a postdoc in the group of Prof. Samuel Stupp at Northwestern University (USA), he returned to Germany in 2019 as Liebig research group leader at Humboldt University Berlin.

Since 2022 he is the leader of a BMBF Junior Research Group. The focus of his work is on functional organic materials in their monomeric and framework phase to explore supramolecular binding, chirality, spin effects, magnetic switching, and energy storage.

# 5. Scientific Presentations

## 5.1 Atmospheric-stable Phenyl Derivatives of Pentafluoroorthotellurate and the First Manganese(III) Pentafluoroorthotellurate

Amiera N. Hadi[1], Daniel Wegener[1], Alberto Pérez-Bitrián[1], Sebastian Riedel[1]

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The pentafluoroorthotellurate group (teflate, $OTeF_5$) is an interesting analogue to fluoride as their electron-withdrawing properties are close to those of a fluorine atom. In addition, it is sterically demanding and resistant towards oxidation. Teflates enable strong Lewis acids and weakly coordinating anions (WCA). However, $OTeF_5$ is sensitive to hydrolysis and reduction. This circumstance limits the areas of application and necessitates inert conditions.[1] The substitution of fluorine atoms in the $OTeF_5$ group by phenyl groups results in more stable analogues. Consequently, the establishment of phenyl derivatives of the pentafluoro orthotellurate group opens the door for atmospherically stable reagents.

Similar to the fluoride, teflates are able to stabilize high oxidation states. Comparing the number of transition metal teflates with main group teflates, the latter are far better studied.[1] To date only one manganese pentafluoroorthotellurate complex has been reported, in which the metal center is in oxidation state I.[2] By utilizing $ClOTeF_5$ as a teflate transfer reagent, a novel manganese(III) pentafluoroorthotellurate could be obtained.

An atmospheric-stable phenyl-substituted derivative of the $OTeF_5$ group[3] and a synthetic pathway to obtain a novel manganese pentafluoroorthotellurate[4] are presented.

**Literature:**

[1] K. Seppelt, Angew. Chem. Int. Ed. Engl. 1982, 21,877.
[2] S. H. Strauss, K. D. Abney, K. M. Long, O. P. Anderson, *Inorg. Chem.* **1984**, *23*,1994.
[3] D. Wegener, K. F. Hoffmann, A. Pérez-Bitrián, I. Bayindir, A. N. Hadi, A. Wiesner, S. Riedel, *Chem. Commun*. **2022**, DOI: 10.1039/D2CC03936B.
[4] A. Pérez-Bitrián *et al.*, unpublished results.

## 5.2 Complexation of the cationic lipid DOTAP with oppositely charged polyelectrolytes

Miriam Simon[1] and Yeshayahu (Ishi) Talmon[1]

*[1] Department of Chemical Engineering and The Russell Berrie Nanotechnology Institute (RBNI), Technion – Israel Institute of Technology, Haifa 3200003, Israel*

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Self-assembly is a key process in forming biological materials. Especially the interaction between amphiphiles and polyelectrolytes has been widely investigated in recent years due to their potential application in industry and medicine, with a special focus on gene therapy.

Accordingly, we investigated the formation of lipoplexes by mixing liposomes with selected polyelectrolytes (PE). The cationic lipid DOTAP (1,2-dioleoyl-3-trimethylammonium-propane (chloride salt)) was mixed with different anionic polyelectrolytes, such as NaPA (sodium poly-acrylate), CMC (sodium carboxymethyl cellulose) with different degrees of substitution (DS, namely, different charge density) and DNA (deoxyribonucleic acid sodium salt). The goal of this project was to explore the influence of different system parameters, such as the charge ratio CR = [-]/[+] = [PE]/[DOTAP], the charge density of the PE or the type of PE on the morphology of the formed complexes. In additional experiments, the protein BSA (bovine serum albumin, a key blood plasma protein) was added to the lipoplexes to simulate actual transfection processes and gain information about transfection related morphology changes. The investigation of these systems was performed by cryo-transmission electron microscopy (cryo-TEM), and with small-angle X-ray (SAXS) measurements, to support our findings.

In our experiments we obtained a comprehensive picture of the formed lipoplexes, and how their structure depends on the different properties of the employed polyelectrolyte (Figure 1). Although the basic nanostructure of the complexes is usually lamellar (with some hexagonal exceptions), their detailed morphology depends strongly on parameters like the persistence length, charge density, or polymer backbone diameter. Upon addition of BSA, drastic morphology changes occur that may inhibit successful transfection. Understanding these specific interactions will allow the formation of more stable and optimized complexes as they are needed for optimized delivery.

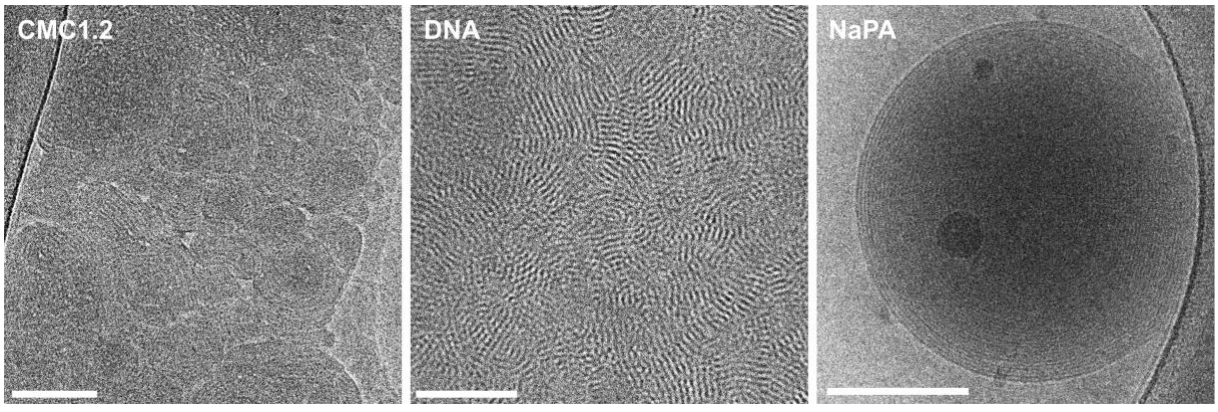


**Figure 1:** Cryo-TEM images of 1 mM DOTAP mixed with different polyelectrolytes. Left: CMC1.2, middle: DNA, and right: NaPA; all at CR=2. All samples form multilayered complexes, but the overall size of the complexes, as well as the order and the spacing of the multilayers depend on the polyelectrolyte. Scale bars are 100 nm.

## 5.3 Tuning Acridine-Functionalized Covalent Organic Frameworks (COFs) towards Fully-Heterogenous Metallaphotocatalysts

Michael Traxler[1], Sebastian Gisbertz[2], Pradip Pachfule[1], Susanne Reischauer[2], Bartholomäus Pieber[2], Arne Thomas[1]

[1] *Technische Universität Berlin, Institut für Chemie, 10623 Berlin, Deutschland*
[2] *Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Biomolekulare Systeme, 14476 Potsdam, Deutschland*

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The field of Covalent Organic Frameworks (COFs) – crystalline and porous polymers that are solely consisting of organic building blocks reticulated via covalent bonds – have gained increasing attention in the last decade.[1] COFs feature high porosity, structural tunability and the possibility to integrate functional linkers in the COF backbone and have therefore emerged as a promising materials for many applications including gas storage & separation, energy storage and catalysis. Furthermore, due to their conjugated backbone, COFs have been applied as photocatalysts for $H_2O$ and $CO_2$ conversion, however only few examples of COFs have been used to catalyze organic transformations.

Conventionally, dual-catalytic cross-coupling reactions are performed in solution by the combination of a noble metal photocatalyst with a nickel catalyst. Based on this we have in a first step synthesized a new family of porous and crystalline COFs using an acridine linker and benzene-1,3,5-tricarbaldehyde derivatives as sustainable alternative. With the broad absorption in the visible light region the COFs were applied as photocatalysts in metallaphotocatalytic C–N cross coupling. The materials showed good to excellent yields for several substrates and even catalyzed the organic transformation using green light as energy source.[2] However, the necessary nickel catalyst could not be recycled. Therefore, we aimed to develop a fully-heterogeneous metallaphotocatalytic system based on the multivariate COF approach. The material showed high activity throughout the visible light spectrum for the organic transformations and could be recycled five times without any loss in efficiency.[3]

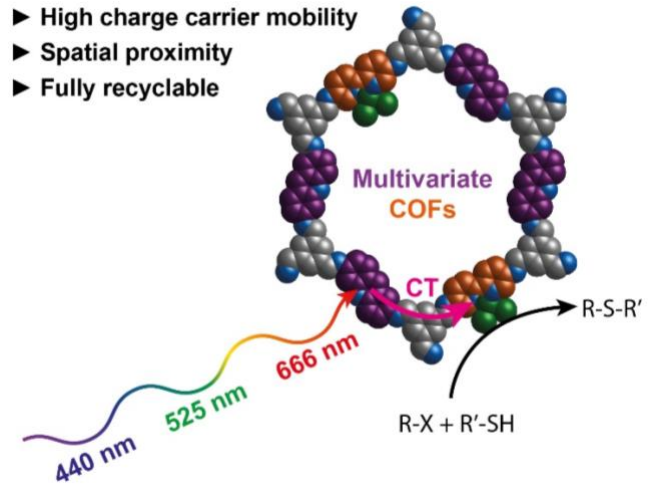


**Figure 1:** Development of a fully heterogeneous COF platform for photocatalytic cross-coupling reactions.

**Literature:**

[1] Zhao, P. Pachfule, A. Thomas, *Chem. Soc. Rev.* 50 (6871), 2021.
[2] M. Traxler, S. Gisbertz, P. Pachfule, J. Schmidt, J. Roeser, S. Reischauer, J. Rabeah, B. Pieber, A. Thomas, *Angew. Chem. Int. Ed.* 61 (e202117738), 2022.
M. Traxler, S. Reischauer, S. Vogl, J. Roeser, J. Rabeah, C. Penschke, P. Saalfrank, B. Pieber, A. Thomas, *manuscript submitted*, 2022.

## 5.4 Polyoxometalate boosting the light-harvesting ability of graphitic carbon nitride for photocatalytic water splitting: in the energy crisis context

Simon Djoko[1], Anh Dung Nguyen[1], Jin Yang[1], Hüseyin Küçükkeçeci[1], Michael Schwarze[1], Thomas Arne[1], Reinhard Schomäcker[1]

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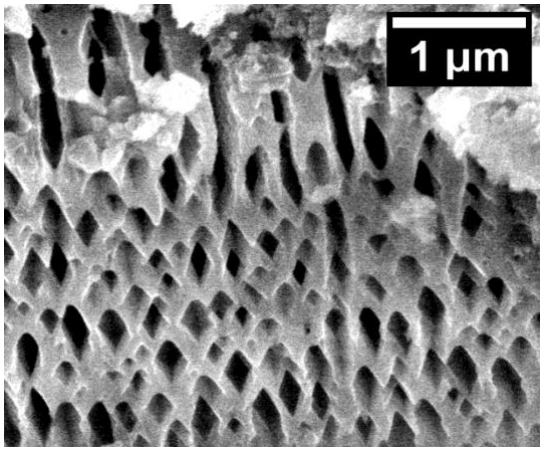
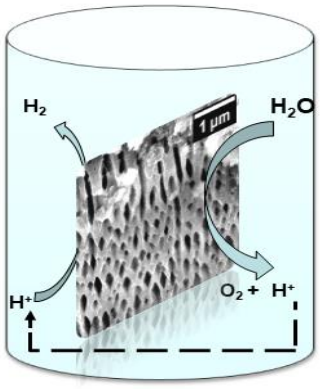
Referring to natural photosynthesis, it seems advantageous to develop artificial catalytic systems (so-called artificial leaves) that might be essential to mimic the photosynthetic reactions to produce energy carriers, just as green plants do on the surface of their leaves[1]. Thus, intending to develop g-$C_3N_4$ based photonic crystals (PCs) in the designing of an artificial leaf system, we first got a composite made up graphitic cabon nitrite and Phosphomolybdic acid (a POM compound) that is being used as precursor of our photonic crystals. We discovered that the precursor composite itself exhibited efficient enhancement of light-harvesting for photocatalytic hydrogen evolution from water splitting. Then we found interesting to first focus our investigation on the effect that a polyoxometalate might have on the light-harvesting ability of g-$C_3N_4$.

Herein, this study reports on a new improvement strategy combining 3 improvement strategies as 1 that has been applied to modify g-CN to get a new structural doped g-CN exhibiting higher activity under visible light absorption for HER from water splitting. A polyoxometalate (POM) is used in this work as coupling material to improve the photocatalytic activity of g-CN. On the other hand, when used as photocatalyst, the obtained material showed a significantly enhanced efficiency in HER from light-driven water splitting, somewhat never achieve with pristine g-CN or with other g-CN based composites[2]. The formation of porous nanosheets can most likely be ascribed to the in-situ soft-template effect of gas bubbles during thermal treatment[3]. As result of post-calcination, some molecules contain atoms are taken out of the network leaving behind ordered porous structures formed by rearrangement and hard weaving between atoms of layered nanosheets as we can observe on the figure above.




$$R_{H_2}(P-gCN/PMA_{1.5}) = \frac{3}{2} R_{H_2}(gCN)$$

**Figure :** SEM image of P-gCN/$PMA_{1.5}$

References: [1] D. G. Nocera, Acc. Chem. Res., 2012, 45, 767–776.
[2] Yun-Xiao Z., Shuang T., Wei-De Z., Yu-Xiang Y., ACS Appl. Mater. Interfaces 2019, 11, 14986−14996.
[3] Z. W. Zhao, Y. J. Sun, F. Dong, Y. X. Zhang, H. Zhao, RSC Adv., 2015, 5, 39549–39556.

## 5.5 CO2 as a tuning parameter for the head group properties of non-ionic EO-surfactants

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[1] *Technische Universität Berlin, Institute of Chemistry, 10623 Berlin, Germany*

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Investigation of carbon dioxide ($CO_2$) as sustainable resource is of fundamental interest for research and industrial applications. It can be used as a building block in chemical compounds such as polymers or surfactants.[1] Substituting ethylene oxide (EO) units in abundantly produced non-ionic EO-surfactants by $CO_2$ can increase the sustainability and save natural and fossil resources. Similarly interesting, introducing $CO_2$ gives a new tuning parameter for non-ionic surfactants, allowing to better match particular application requirements and thereby a more economical consumption and potentially even opening up pathways for novel formulations.[2]

The solubilization potential of $CO_2$ towards industrial relevant oils (decane, isopropylpalmitate, bis(2-ethylhexyl)carbonate) with different polarity has been characterized by small-angle neutron scattering (SANS) and compared with data from static and dynamic light scattering (SLS, DLS), interfacial tension measurements (IFT) and quantitative NMR (qNMR). At a given surfactant concentration, the use of $CO_2$-containing surfactants can greatly increase the solubilization capacity for oils compared to that of conventional EO-surfactants, as the incorporation of $CO_2$ into the head group renders the surfactant more effective with respect to their interfacial activity.

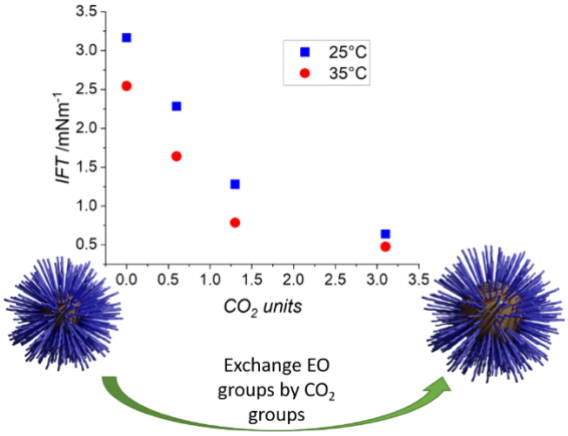


**Figure 1:** Interfacial tension of EO surfactants with varying amount of incorporated CO2 units for 25°C and 35°C. With increasing CO2 amount the interfacial tension against isopropylpalmitate is decreasing.

**Literature:**

[1] J. Langanke, J. Hofmann, K. Böhm, M. Subhani, T. Müller, W. Leitner, C. Gürtler, *Green Chem.*, 16, 1865-1870 (2014).

[2] M. Tupinamba Lima, V. Spiering, S. Kurt-Zerdeli, D. Brüggemann, M. Gradzielski, R. Schomäcker, *Colloids and Surfaces A*, 569, 156-163 (2019).

**Funding:** This project is part of “DreamResourceConti” (033R222C) and funded by the German Federal Ministry of Education and Research (BMBF) within the funding priority “r+Impuls – Innovative Technologien für Ressourceneffizienz – Impulse für industrielle Ressourceneffizienz”.

## 5.6 BLI and dPCR – Advanced Techniques for Quantifying Biomolecules and their Interactions

Part 1 (BLI): Marc Lucas Appis[1,2], Theresa Noonan[2] and Gerhard Wolber[2]
Part 2 (dPCR): Marc Lucas Appis[1,3], Michael Launspach[3] and Annette Künkele[3]

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*[2] Freie Universität Berlin, Institut für Pharmazie, 14195 Berlin, Deutschland*
*[3] Charité – Universitätsmedizin Berlin, Klinik für Pädiatrie m.S. Onkologie und Hämatologie, 13353 Berlin*

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Introduction: Quantifying the abundance of and/or interactions between biomolecules are crucial steps in every biomedical research project. Particularly, this applies for the process of drug discovery because collecting as much information about target and drug substance as possible helps improving for the desired drug properties. Here, I present recent advances in two state-of-the-art methods in quantitative biochemistry: bio-layer interferometry (BLI) and digital polymerase chain reaction (dPCR).

**Part 1:** *Shedding light into drug-target-interactions with BLI*. The screening part of a drug discovery campaign aims to identify potential binders for a given target from a large chemical library. Keeping the right balance between high throughput and precise binding measurement poses a major challenge to scientists. Certain methods like isothermal titration calorimetry (ITC) and NMR spectroscopy yield high resolution but test only with a low speed.[1] BLI can close this gap by allowing for intermediate-throughput screening and measuring three important parameters at the same time: $K_D$-, on- and off-rates.[2] We optimized BLI for an antimicrobial drug screening but faced two corresponding issues: dissociation of the protein from the sensor and unspecific binding of compounds to the reference sensor. After solving these problems, we could use the assay to experimentally test the resulting molecules of a virtual screening experimentally and even to identify a binder amongst them which is now further developed.

**Part 2:** *Absolute quantification of target DNA with dPCR*. A major improvement towards the quantitative detection of nucleic acids was the invention of real-time quantitative PCR (RT-qPCR). It relies on sequence-specific fluorescent probes which are released from linked quenching molecules by the polymerase during the amplification process. However, RT-PCR comes along with high experimental effort and is limited to relative quantification. dPCR promises an efficient strategy to overcome these challenges. It is based on the RT-qPCR principle but works via an endpoint analysis of the sample after partitioning in thousands of micro-reactions allowing for fast and absolute quantification.[3] We adapted such a dPCR protocol for the detection of transgenes in genomic DNA samples after genetical engineering with regard to assay specificity and technical parameters (imaging time and cycling number). This workflow can now be used for the assessment of genome editing efficiencies.

**Literature:**

[1] V. Kairys, et al. *Expert Opin Drug Discov* 14(8), 2019.
[2] Orthwein et al. Bio Protoc 11(17):e4152, 2021.
[3] L.L. Tan et al. *Crit Rev Biotechnol* 15 Mar 2022.

# 6. Poster Presentations

## 6.1 Cannabinoid Receptor Sub-Type Selective Fluorescent Probes

Leonard Mach[1], Malgorzata Wasinska-Kalwa[1], Anahid Omran[1], David Sykes[2,3], Yelena Mostinski[1], Thais Gazzi[1], Wolfgang Guba[4], Arne Rufer[4], Johannes Broichhagen[1], Dmitry Veprintsev[2,3], Uwe Grether[4], Marc Nazare[1]

*[1] Leibniz Research Institute for Molecular Pharmacology, 13125 Berlin (Germany);*
*[2] Division of Physiology, Pharmacology & Neuroscience, School of Life Sciences, University of Nottingham, Nottingham, NG7 2UH, UK;*
*[3] Centre of Membrane Proteins and Receptors (COMPARE), University of Birmingham and University of Nottingham, Midlands, UK;*
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**Introduction:** Fluorescent probes are emerging as powerful tools to study G-protein-coupled receptor (GPCR) pharmacology, kinetic ligand binding, visualization of dynamic GPCR processes in living systems such as internalization.[1] The cannabinoid type 1 receptor ($CB_1R$) and cannabinoid type 2 receptor ($CB_2R$) are class A GPCRs involved in various pathologies including pain, inflammation, fibrosis, neurodegenerative diseases, anxiety, obesity, and others.[2] Robust and reliable tools that allow *in vitro* and *in vivo* investigation of the CBRs in real-time under different (patho-)physiological conditions across different species are therefore urgently needed. In this work, the design, synthesis, and biological characterization of a toolbox of fluorescent $CB_1R$ and $CB_2R$ probes will be presented.

**Methods:** Capitalizing on different highly selective and potent synthetic agonists and inverse agonists, drug-derived CBR probes were elaborated by *in silico* modeling and rigorous structure-activity optimization. A general and modular synthetic approach was applied to achieve a versatile toolbox of probes for $CB_1R$ and $CB_2R$. Different fluorescent dyes allow their application in super-resolution microscopy, FACS, and other imaging techniques.

**Results:** These probes show exceptional flexibility with regard to the attached fluorophore label. Selected probes show low nanomolar binding affinity for their respective target receptor. Additionally, we have created CBR-subtype specific labeling tools to facilitate subsequent proximity-driven covalent receptor labeling. Their biological and pharmacological action is currently under investigation.

**Conclusion:** We have established a general modular synthetic approach to produce sub-type specific CBR probes. These are equipped with state-of-the-art fluorophores and labeling modalities as part of a fluorescent CBR probe toolbox. This toolbox allows the investigation of CBR dynamics in different tissues and cellular contexts.

**Literature:**
[1] C. Iliopoulos-Tsoutsouvas *et al.*, *Expert Opin. Drug Discov*. **2018**, 10, 933-947.
[2] A. Cooper *et al*., *Pharmacol. Rev.* **2017**, 69, 3.

## 6.2 The Fate of the Antibiotic Amoxicillin in the Aquatic Environment

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The environmental fate of the frequently used broad-spectrum β-lactam antibiotic amoxicillin (AMX) is of high concern regarding the potential evolution of antimicrobial resistance. Moreover, it is known that AMX is prone to hydrolysis, yielding a variety of hydrolysis products (HPs) with yet unknown effects. Studies to identify those HPs and investigate their formation mechanisms have been reported but a long-term study on their stability in real water samples was missing. In this regard, we investigated the hydrolysis of AMX at two environmentally relevant concentration levels (10 and 100 µg/L) in four distinct water types (tap water, mineral water, surface water, ultrapure water) under three different storage conditions (4 °C in the dark, 20 °C in the dark, 20 °C under irradiation by sunlight) over two months (Figure 1). Concentrations of AMX and four relevant HPs were monitored by an LC-MS/MS method revealing pronounced differences in the hydrolysis rate of AMX in tap water and mineral water on the one hand (fast) and surface water on the other (slow). In this context, the occurrence, relative intensities, and stability of certain HPs are more dependent on the water type than on the storage condition. As clarified by ICP-MS, the main difference between the water types was the content of the metals copper and zinc which are supposed to catalyze AMX hydrolysis demonstrating an effective method to degrade AMX at ambient conditions.

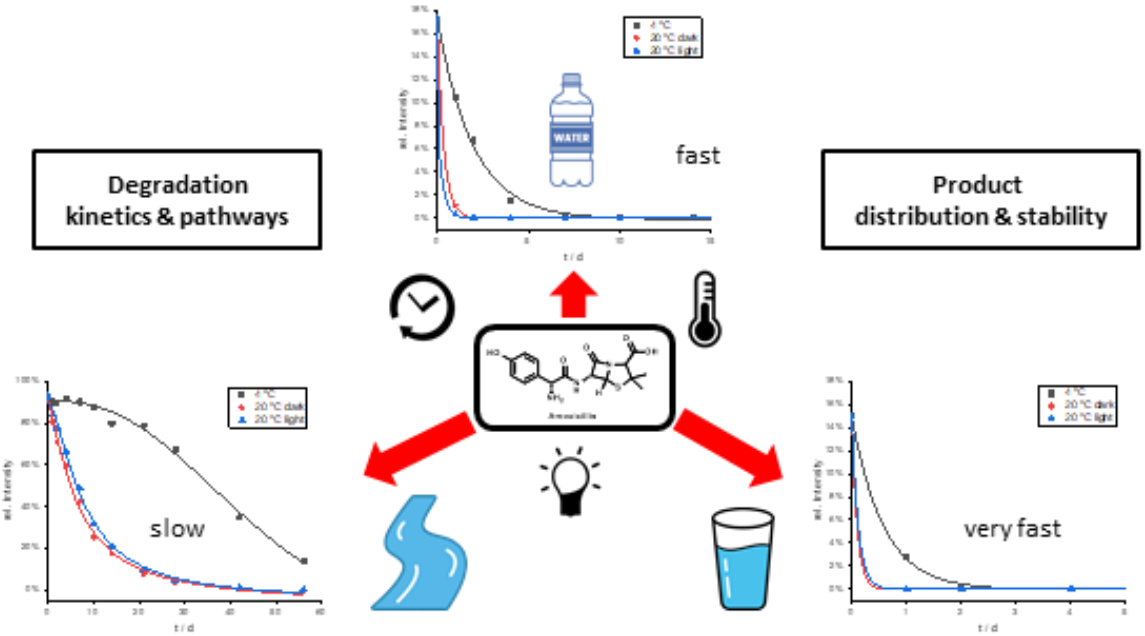


**Figure 1:** Overview of the investigated parameters for the hydrolysis of AMX and respective hydrolysis kinetics in different water types.

## 6.3 Development of highly potent and selective Fluorescent MAGL Probes with drug-like Properties

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**Introduction:** Monoacylglycerol lipase (MAGL) is a serine hydrolase that metabolizes the endocannabinoid messenger 2-arachidonic acid glycerol (2-AG) into arachidonic acid (AA) and glycerol and is therefore a key mediator at the interface of two major signal transduction pathways. 2-AG is one of the two major endogenous agonists to the cannabinoid receptors 1 (CB1) and 2 (CB2). By regulating the concentration of this neurotransmitter, MAGL thereby greatly influences the retrograde cannabinoid signaling pathways by the CB receptors that are important for learning, mood, appetite and addiction as well as regulation of immune cells. Moreover, the cleavage of 2-AG to AA is the starting point for the biosynthesis of the inflammation- and pain-mediating eicosanoids. The development of small molecular fluorescent probes that target this enzyme could help to visualize and quantify physiological processes *in cellulo* and *in vivo* across species. Enabling the visualization of the MAGL enzyme in native cells, tissues and organisms without the need of genetic engineering would give a clearer view of its functions in a spatiotemporal controlled fashion.

**Methods:** We designed a set of specific fluorescent MAGL inhibitors with drug-like properties, that allows for investigation in live cells and potentially *in vivo*. The design concept merges the structure of known potent MAGL inhibitors with fluorophore moieties to create ligands that incorporate the fluorophore into the proteins binding site. Both, favorable ADMET and photo-physical properties were simultaneously taken into account for the design process.

**Results:** The probe ligands show potencies towards MAGL in the sub-nanomolar range, high selectivity over other serine hydrolases as well as high solubility and cell permeability. The probes are active across species isoforms of the enzyme. Several co-crystal structures confirm the proposed binding mode of the novel structures. They are stable towards metabolism as well as photo bleaching and convince with bright fluorescence. The probe can be adapted to special requirements, i.e. red-shifted dyes suitable for super-resolution microscopy or covalent warheads that permanently block and label the proteins catalytic Ser122.

**Conclusion:** Here we present novel, state-of-the-art fluoroprobes for the key metabolic enzyme of the ECS with drug-like characteristics for applications such as (super resolution) live cell microscopy, TR-FRET & BRET assays, fluorescence polarization binding assays, FACS analysis etc.

## 6.4 Wasser-in-Öl Mikroemulsionen als weiche-Schablone für die Selbst-Anordnung von Nanopartikeln

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Aktuelle Trends der Entwicklung neuer hybrider Nanostrukturen verlassen sich oft auf die Selbst-Anordnung von Nanopartikeln, als ein Von-unten-nach-oben-Ansatz. Besonders die Kombination der individuellen Eigenschaften von superparamagnetischen Eisenoxid Nanopartikeln und plasmonischen Metall Nanopartikeln ist für biomedizinische, katalytische und sensorische Anwendungen interessant.

Nanopartikel Interaktionen können auf eine Flüssig-Flüssig Grenzfläche gerichtet werden, sodass sie in einer Selbst-organisierten Dispersion für die nachfolgende Selbst-Anordnung kontrolliert sind. Zu diesem Zweck wurden, unter Nutzung von Aerosol-OT (Docusat-Natrium) als Tensid, Wasser-in-Öl Mikroemulsionen formuliert. Oleyl-bedeckte Nanopartikeln wurden in der kontinuierlichen Öl-Phase eingebunden, während die Polyethylenimin-stabilisierten Nanopartikeln in den feinverteilten Wassertröpfchen begrenzt wurden. Jede Sorte Nanopartikel kann die Eigenschaften der Mikroemulsionen auf verschiedene Weise verändern, und seine Kombination führt zu synergetischen Effekten und Anordnungs-Phänomenen.[1] Zum Beispiel bildeten sich dünne Schichten von angeordneten Nanopartikeln als Filament-Netze aus, nachdem Tropfen aus der oberen Phase eines Winsor Typ II Systemes geschaffen wurden.[1,2] Detaillierte Charakterisierungen zeigten, dass diese Selbst-Anordnung auf dem kontrollierten Nanopartikel-Clustering und auf der Verlängerung der Mikroemulsion-Tröpfchen basiert.[2] Zusätzlich, wurde ein magnetisches Heterokoagulat in höherer Tensid Konzentration hergestellt, dessen Phasen-Transfer erst in Ölsäure und dann im Wasser bereitgestellt wird, wobei Öl-in-Wasser aufgeteilte Nanostrukturen erschaffen wurden, die magnetische und einschließende Eigenschaften aufweisen.[3] Dadurch wurde demonstriert, dass Mikroemulsionen geeignete weiche-Schablonen für die Selbst-Anordnung von Nanopartikeln sein können und neue Formen hybrider Nanostrukturen ermöglichen.

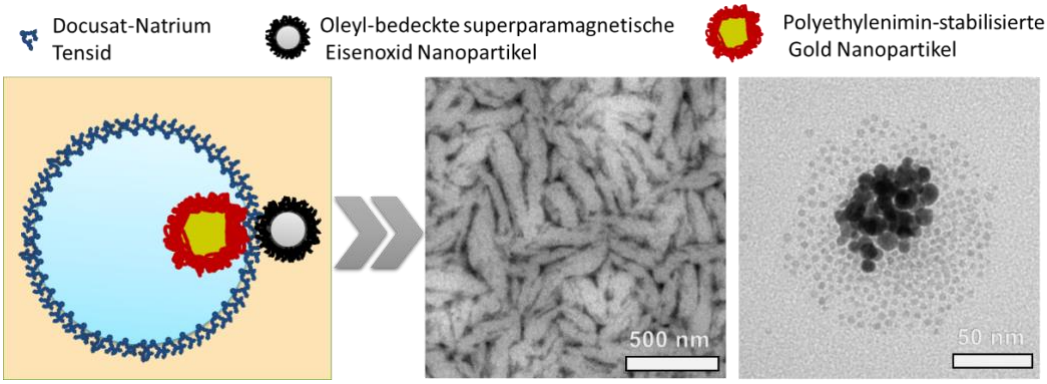


**Abbildung 1:** verschiedene Kompositionen aus ternären Mischungen von Tensid und Nanopartikeln ermöglichen verschiedene Anordnungen von Nanopartikel-Heterostrukturen.

## 6.5 Wicking of Bicontinuous Microemulsions in Porous Materials

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Wicking is the spontaneous imbibition of a liquid into a porous medium due to the neg ative capillary pressure created at the liquid-air interfaces[1]. The wicking of single fluids like water and organic solvents has been studied already for a long time[2]. We inves tigate the spontaneous imbibition of a bicontinuous microemulsion and its components into porous materials.

In this work, we study the wicking of a well-studied bicontinuous microemulsion (water/octane/C10E4) into controlled-pore glasses (CPG) with different pore diameters between 75 – 1000 Å. The naturally hydrophilic surfaces of the CPGs were hydropho bically modified to analyze the influence of the surface polarity. We observe the wick ing gravimetrically using the Lucas-Washburn equation where the advancing contact angle inside the hydrophilic and hydrophobic pores can be obtained. While the imbibi tion of water and octane strongly depends on the surface polarity of the pores, the microemulsion imbibes independently of the surface modification. These experiments are accompanied by numerical studies using COMSOL software to further characterize the wetting and imbibition in the porous network. Additionally, cryo-SEM imaging and SAXS measurements are performed to characterize the structures in bulk and inside the pores.

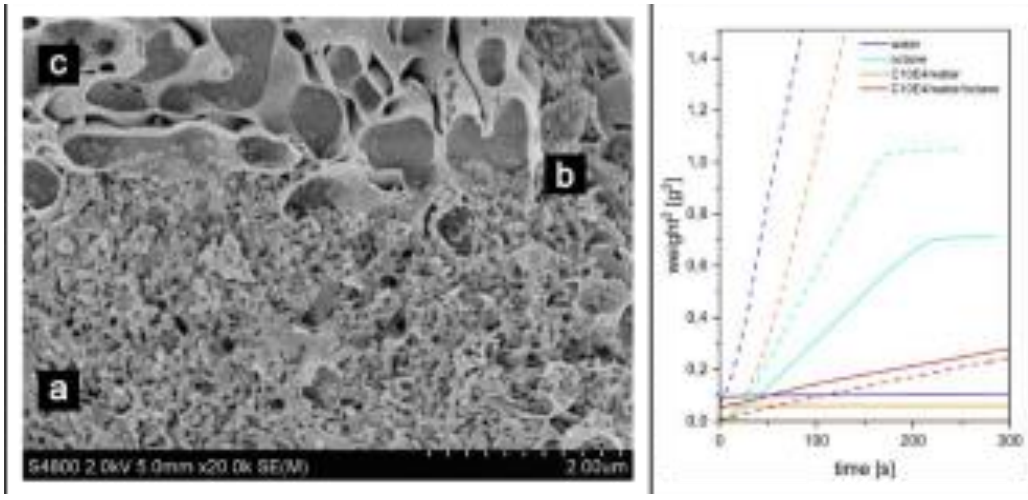


**Figure 1:** Left: Cryo-SEM micrograph of a bicontinuous microemulsion (a) imbibed (b) in a porous network with a mean pore diameter of 1000 Å (c). Right: Experimental curve of m2 vs. t of the microemulsion and its compounds on hydrophilic (dashed line) and hydrophobic (solid line) CPG with a pore diameter of 500 Å.

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## 6.6 Enhanced Solubilization of Fragrances in Solutions of Sugar Surfactants in Natural Deep Eutectic Solvents (NADES)

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Solubilization of fragrances in aqueous solutions has been already studied for a long time[1]. Interestingly, such fragrances can be also solubilized in natural deep eutectic solvents (NADES), a novel class of polar solvents that has the potential to become a non-toxic and cheap alternative to conventional organic solvents, ionic liquids, or even water. As a result of our experiments, the NADES based on choline chloride and urea, dubbed "reline", is a good candidate for solubilizing terpenoids. Both components, choline chloride, and urea are inexpensive and widely used in agriculture[2]. We were able to widen the limited scope of reline-soluble surfactants with sugar surfactants and glycolipids. They are already being industrially produced from biomass and are readily biodegradable[2]. More specifically, we examined and characterized numerous glucosides and maltosides to dissolve fragrances. With certain formulations, we achieved to dissolve terpenes such as limonene, α-pinene, eucalyptol, or menthol up to 25 wt% of the total mixture mass, see Figure 1.

All components were chosen thoroughly with the emphasis on biocompatibility, biodegradability and their low price. Some fragrances, such as menthol function also as a cosurfactant, thus affecting the internal structure and viscoelastic properties of the final mixtures, see Figure 1. Such properties could find application in cosmetics and pharmaceuticals in form of creams and topical drug delivery. These mixtures were characterized using rheological measurements and small-angle neutron scattering (SANS). The latter delivers a detailed structural picture that could directly become related to the observed rheological properties.


**Figure 1.** Left: Chemical structures of four terpenoids (limonene, a-pinene, eucalyptol and menthol) and their sources in nature (lemons, pines, eucalyptus, mint). Centre: Images of a solution of dodecyl glucoside (10 wt%) and menthol (10 wt%) in reline in unpolarized and in circularly polarized light. Right: Viscosity of the same solution at different shear rates and temperatures (25°C - 50°C). Inlet: Upside-down image of the solution demonstrating the non zero yield stress.

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## 6.7 Donor-Acceptor Co-Polymers for Photocatalytic Hydrogen Generation

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Hydrogen is considered a sustainable and clean energy source for the future and is expected to meet the energy demands by replacing fossil fuels. In this respect, the development of purely organic, i.e. metal-free photocatalysts has recently gained increasing interest.[1,2]

In this work (co-)polymers were developed that were inspired by compounds of organic electronics bearing donor-acceptor moieties which are known to facilitate charge carrier separation and stability.[3] The combination of both moieties in the polymer backbone yields a notable change in optical properties and a substantial enhancement of the catalytic performance compared to the homo-polymers.

The hydrogen evolution rate is the highest for the 2:1 Co-Polymer with on average 3.04 mmol $g^{-1}$ $h^{-1}$. The enhanced performance can be correlated to the introduction of a donor-acceptor system in the backbone of the polymer.

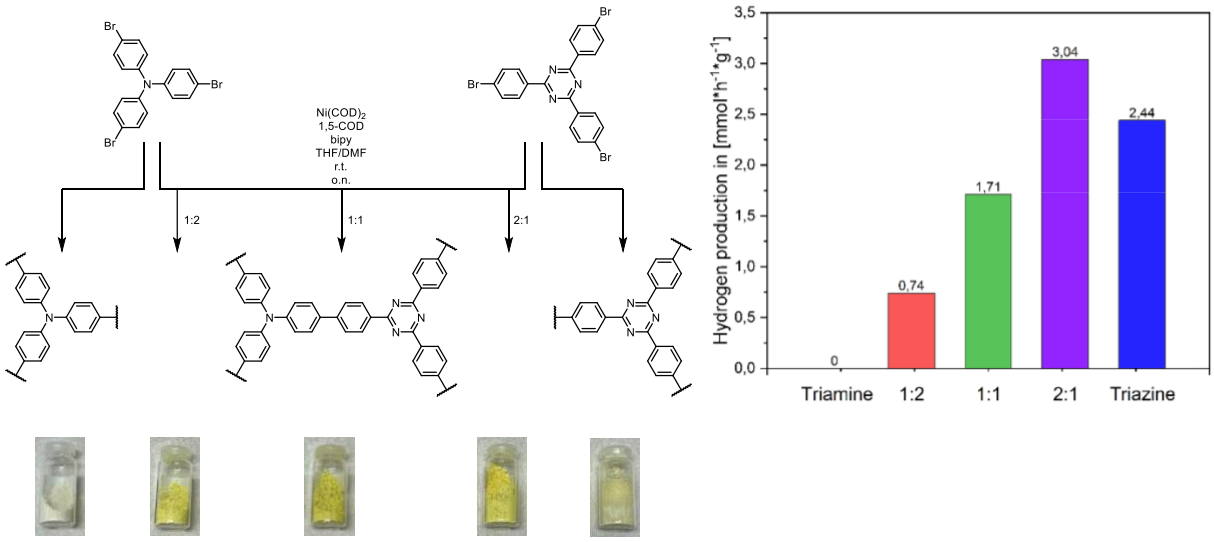


**Figure 1:** Synthesis of different (co-)polymers and their performance in the hydrogen evolution reaction (HER).

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## 6.8 Theoretical Study of the Formation, Activation and Electrochemistry of Martin's Bromane and it's Analgoues

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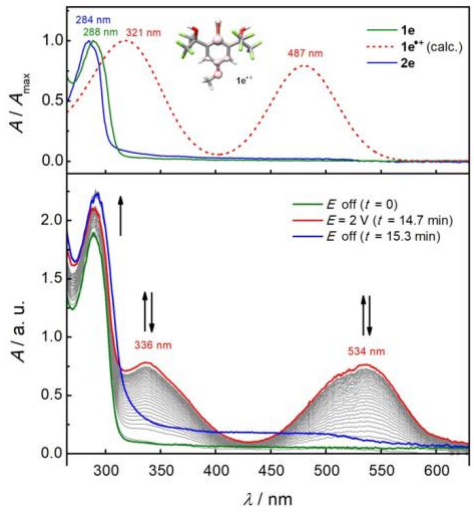


Compared to ubiquitous iodine(III)-complexes, their bromine counterparts display a higher nucleophilicity, oxidation potential, and superior reactivity. In the last year chelation-stabilized systems, prepared by electro-oxidation, have been proposed to tackle the major drawbacks of bromine(III) compounds, such as low stability and the usage of $BrF_3$ as precursor.[1] The reactivity of the chelation-stabilized systems could be tuned to yield a bench-stable product, at the cost of the need for an acid mediated activation. Herein we present a comprehensive study of the chemical and physical properties of Martin's bromane[2] and various ortho-subtituted analogues, by means of state-of-the-art electronic structure theory.[3] This work encompasses calculations of spectroscopic parameters and potential energy surfaces. Together with experimental data, our results could reveal mechanisms of the formation, activation and electrochemistry of Martin's bromane.

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