

Book of Abstracts

Berliner Chemie in Praxis Symposium

06. Oct. 2023



Greetings	3
Scientific Program	4
Location and General Information	5
Sponsors.....	6
Plenary Lecture	7
CIF Lecture	7
Oral Presentations.....	8
Workshops	18

Greetings

Welcome to the “Berliner Chemie in Praxis Symposium” (BCPS)!

Dear Friends of Chemistry,

On behalf of JCF Berlin, it is our great pleasure to extend a warm welcome to the 2nd BCPS - a fusion of the well-established "Berliner Chemie Symposium" (BCS) and "Chemie in Praxis" (ChiP). With BCPS, we aim to provide a platform for scientists to connect, discuss, and exchange ideas, bringing together diverse stakeholders from both the scientific and industrial realms.

This year, we have curated a diverse program featuring lectures, presentations and a workshop spanning various facets of chemistry. The *Book of Abstracts* in hand offers a comprehensive overview of what awaits you.

Our heartfelt gratitude goes out to all the speakers joining us today. Your contributions form the bedrock of today's scientific exchange and dialogue. We would also like to extend our thanks to our sponsors and the dedicated team at JCF Berlin, without whom BCPS would not have been possible.

We encourage you to actively participate in the discussions and workshop, pose your questions, and share your knowledge. May this symposium not only pique your curiosity but also open doors to new insights and exciting opportunities.

Wishing you an inspiring day at the symposium, we look forward to a captivating and successful BCPS! We are eager to witness the discoveries and enthusiasm that this symposium will bring and are delighted to spend this day with you.

Yours sincerely,

The JCF Berlin Team

Scientific Program

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

Time	Program Point
08:30-09:00	Registration
09:00-09:15	Opening Ceremony <i>Welcome words Larissa Doll, current chairwomen of the JCF Berlin of the German Chemical Society (GDCh)</i>
09:15-10:15	Plenary Lecture: Prof. Dr. John C. Warner Warner Babcock Institute for Green Chemistry, LLC Honorary Professor of Chemistry, Technical University Berlin
10:15-11:00	Plenary Lecture: Martin Rahmel, Chemical Invention Factory Managing Director of the Chemical Invention Factory, John Warner Center for start-ups in Green Chemistry
11:00-11:15	Break, sponsored by
11:15-12:15	Oral Presentations 1 Dr. Felix Marske: <i>“Monolithic shape-stabilized phase change materials based on silica and organic PCM for hot water storage applications”</i> Vincent Weigl: <i>“A Wittig Reaction Cycle in the Solid State”</i> Anastasia Alexandridou: <i>“Deeper access into the vitamin D metabolome using liquid chromatography tandem mass spectrometry”</i>
12:15-13:15	Lunch Break, sponsored by
13:15-14:15	Industry Lectures Carl Roth, Dr. Bettina Gebert and Daniel Gorzawski VAA, Catharina Einbacher
14:15-15:15	Oral Presentations 2 Daniel Brüggemann: <i>“Nutzung von CO₂ als modernes Synthesematerial für recyclebare Polymere und Tenside durch Ringöffnende Polymerisation”</i> Alexander Winckelmann: <i>“Multivariate data analysis for laser-induced XUV spectroscopy (LIXS)”</i> Marco Kapitzke: <i>“Novel detection approach for photometrically accurate fluorescence upconversion spectroscopy of broadly emitting dyes”</i>
15:15-15:45	Coffee Break, sponsored by
15:45-17:15	Workshops Jo Riehle: Application and leadership training CAS Workshop on Green Chemistry, Karin Färber
17:15-17:45	Closing Ceremony <i>Award ceremony for the best talk of the conference</i> <i>Closing remarks of the JCF Berlin</i>

Location and General Information

Technical University Berlin

Located in the heart of Berlin, the Technical University Berlin (TU Berlin) has offered a place for advancement in Science in Technology since 1879. TU Berlin is one of the three major universities in the city of Berlin and hosts over 33.000 students from countries across the world. Together with Freie Universität Berlin, Humboldt-Universität zu Berlin and the Charité it forms the Berlin University Alliance. Approximately 2.600 researchers work in over 100 institutes on creating new insights into natural sciences, architecture, engineering, law, art, economics and social sciences.

Chemistry at TU Berlin

The Chemistry Institute contributes to the fields of catalysis, biological and biophysical chemistry, modern molecular and synthetic chemistry, solid-state chemistry and analysis, electrochemistry and energy storage, and materials science.

In addition, the research spectrum ranges from basic research to application-oriented research. A special focus is on catalysis research. The Cluster of Excellence "Unifying Systems in Catalysis" is of particular importance here.

Location

The conference venue will be located in the Technical Chemistry building (Straße des 17. Juni 124, 10623 Berlin) in room TC006.

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.



John Warner Center
for start-ups in Green Chemistry



Plenary Lecture

Prof. Dr. John C. Warner, Warner Babcock Institute for Green Chemistry, LLC,
Honorary Professor Professor of Chemistry, Technical University Berlin

Prof. Dr. John Warner, a passionate chemist and inventor, has made groundbreaking contributions to the field of green chemistry. His commitment to sustainability and environmental protection has led to revolutionary technologies that promote a greener future. After graduating from UMASS in Boston in 1984 and earning his PhD from Princeton University in 1988, he was appointed as professor at UMASS Boston in 1996. As founder of several companies and organizations, he has spearheaded the adoption of environmentally friendly technologies. He is a professor of Green Chemistry at Monash University in Australia and an Honorary Professor at the Technical University Berlin. His commitment to education and knowledge sharing is reflected in his work with aspiring chemists. Recognizing his significant contributions, the John Warner Center for Green Chemistry start-ups was established in 2017 in Berlin in his honor for fostering innovation and providing a platform for young entrepreneurs to develop sustainable solutions that address pressing environmental challenges.



CIF Lecture

Martin Rahmel, Managing Director of Chemical Invention Factory (CIF)

Martin Rahmel, a passionate entrepreneur and environmentalist, studied Economical Engineering at TU Berlin and UC Berkeley. After gaining some industry experience during his studies and working for some years as Research Scientist at TU Berlin, he combined his passion for research and entrepreneurship he founded the DexLeChem GmbH in 2011. For 9 years, he was one of the driving forces for the company's success by implementing its business model as well as establishing a global sales system. Gaining additional managing experience later in the same company, he decided to take it a step further. Powered by his motivation of changing the chemical industry towards a circular and stable economy and willing to share his year-long experience in research and entrepreneurship, he became Managing Director of CIF in 2020. Martin now supports researchers and entrepreneurs in growing ideas towards market success based on a mutual vision of a green chemical industry and a healthy planet.



Oral Presentations

Monolithic shape-stabilized phase change materials based on silica and organic PCM for hot water storage applications

Felix Marske, Eric Matthes, Shewaye Wubetu and Patrick Richter
Technical University of Berlin, Institute of Chemistry, 10623 Berlin, Germany
E-Mail: marske@tu-berlin.de

Focus Area

Large amounts of solar energy, waste heat at peak loading processes (e.g. in electric vehicles) and off-peak electricity can easily be stored as heat via shape-stabilized phase change materials (ss-PCM). However, commercially available ss-PCMs suffer by low loading degrees of PCMs, low latent heats, leakage effects, low mechanical stabilities and thermal conductivities. Therefore, we developed a novel sol-gel synthesis¹ that generates a silica structure around nano-sized PCM droplets in water, facilitated by a structure-directing co-polymer and a surfactant. The resulting ss-PCM monoliths demonstrate the highest compressive strength (1–2 MPa) compared to the current literature (~10 kPa), at high PCM mass fractions (above 85%) and high thermal stability up to 320 °C (Fig. 1).

Research Objectives

- Shape-stabilization of paraffinic PCMs by our new sol-gel route¹ to lower market prices and enable market penetration of our monolithic ss-PCMs, formerly only synthesized with butyl stearate.
- Shape-stabilization of 100% bio-based CrodaTherm™ PCMs to fulfill 12 principles of green chemistry.
- Integration of ss-PCMs in a hot water storage prototype to increase its heat storage capacity.

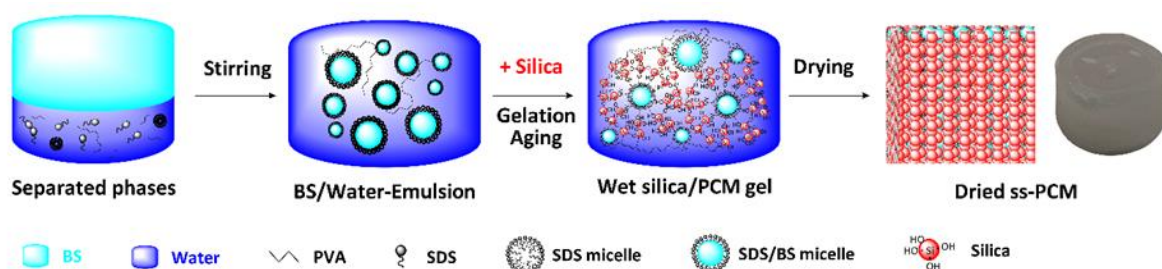


Fig. 1 Schematic presentation of the sol-gel synthesis to produce ss-PCMs.²

Key Findings

- Mixtures of hexadecane (HD) and octadecane (OD) with butyl stearate (BS) (70:30 v/v) were shape-stabilized (ss) and have highest reported compressive strengths (1.2 MPa, 5 °C) with latent heats of ~160 J/g.³
- Shape-stabilized CrodaTherm™ 21 has similar compressive strengths, spherical pore structure and latent heats (~170 J/g) as paraffinic ss-PCMs (Fig. 2).
- Storage capacity of a hot water storage tank was increased by 65% (15 wt% ss-PCM), but the ss-PCMs were not long-term stable in hot water (Fig. 2 D). Further coating or confinement is necessary.

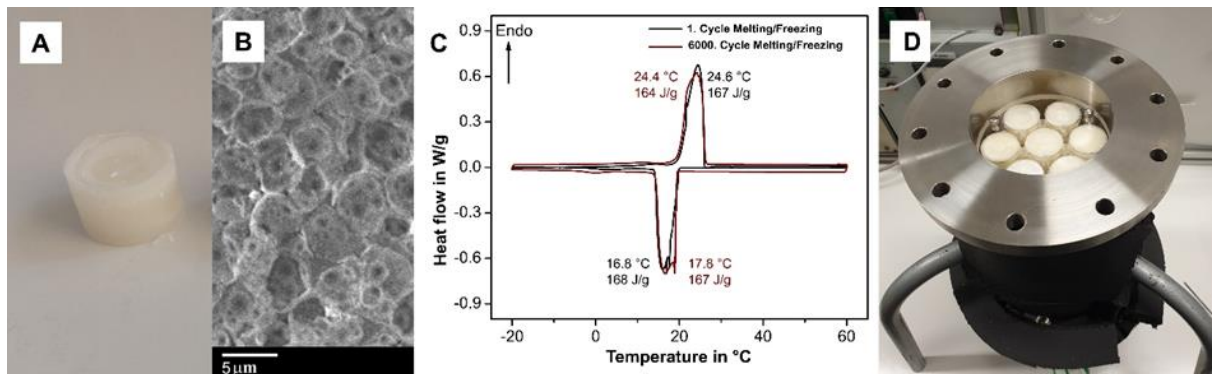


Fig. 2 A) Picture, B) SEM image and C) DSC curves of shape-stabilized CrodaTherm™ 21. D) Picture of the hot water storage prototype filled with ss-PCMs.

Literatur:

- [1] Felix Marske, Juliana Martins de Souza e Silva, Ralf B. Wehrspohn, Thomas Hahn and Dirk Enke, *RSC Adv.* 10 (2020), 3072–3083.
- [2] Felix Marske, Joe Dasler, Caroline Haupt, Kirsten Bacia, Thomas Hahn and Dirk Enke, *J. Energy Storage* 49 (2022), 104127.
- [3] Felix Marske, Caroline Haupt, Claudia Birkemeyer, Kirsten Bacia, Thomas Hahn and Dirk Enke, *J. Build. Eng.* 60 (2022), 105198.

A Triphenylphosphine-Based Microporous Polymer for a Wittig Reaction Cycle in the Solid State

Vincent Weigelt¹, Sarah Vogl¹, Johannes Schmidt¹ und Arne Thomas¹

¹ Technische Universität Berlin, Department of Chemistry/ Functional Materials, Hardenbergstraße 40, 10623 Berlin, Deutschland

E-mail: v.weigelt@tu-berlin.de

Microporous polymer networks (MPNs) are rigid and highly cross-linked polymers constructed exclusively from shape-persistent organic building blocks. This rigidity avoids space-effective packing of the polymer chains, which yields porosity and extraordinarily high surface areas.¹ Furthermore, their modular design allows to alter the building blocks which can be used to tune the chemical and physical properties of these materials. Therefore, MPNs are promising candidates for a wide range of applications including energy storage, gas storage and separation as well as heterogeneous catalysis.^{2,3} The Wittig reaction is a key step in industrial processes to synthesize large quantities of vitamin A and various other important chemicals that are used in daily life through a carbon-carbon double bond formation.^{4,5} This work reports a pathway to achieve the Wittig reaction in a microporous solid network. A highly porous triphenylphosphine-based polymer was applied as a solid Wittig reagent which underwent, in a multi-step cycle, in total six post-synthetic modifications. This allowed to regenerate the starting material and reuse it for the same reaction cycle again. Of particular industrial relevance is that the newly developed material also enables a simple way of separating the product by filtration. Therefore, additional costly and difficult separation and purification steps are no longer needed.⁶

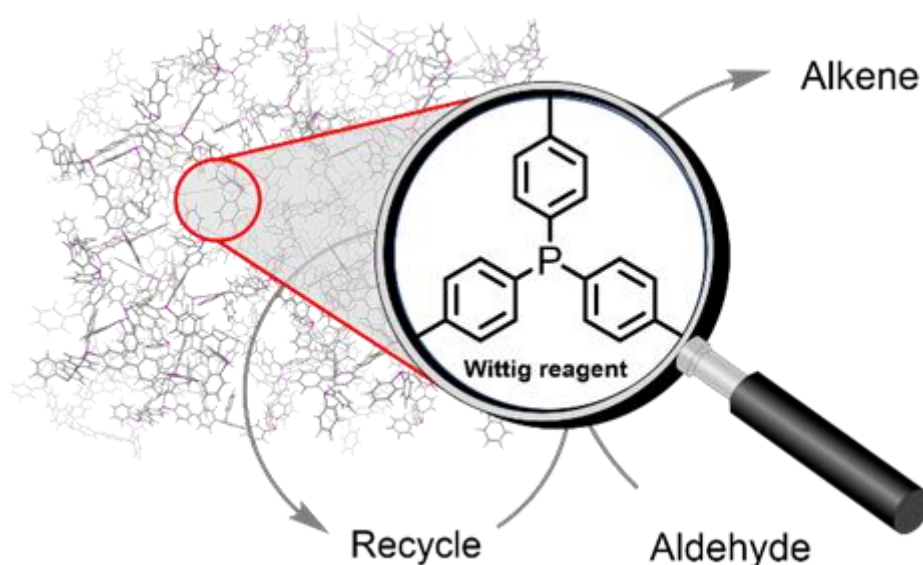


Figure 1: Structure of the solid, microporous Wittig reagent.

Literatur:

- [1] N. Chaoui, M. Trunk, R. Dawson, J. Schmidt & A. Thomas, *Chem Soc Rev* **2017**, *46*, 3302–3321.
- [2] H.-P. Liang, Q. Chen & B.-H. Han, *ACS Catal.* **2018**, *8*, 5313–5322.
- [3] Q. Chen, M. Luo, P. Hammershoj, D. Zhou, Y. Han, B. W. Laursen, C.-G. Yan & B.-H. Han *J. Am. Chem. Soc.* **2012**, *134*, 14, 6084–6087.
- [4] W. Reif & H. Grassner, *Chemie-Ing.-Techn.* **1973**, *45*, 646–652a.
- [5] BASF SE. Presse-Information BASF erweitert World-Scale-Formulierungsanlage für Vitamin A in Ludwigshafen (**2022**). At www.basf.com.
- [6] V. Weigelt, S. Vogl, J. Schmidt & A. Thomas, *Angew. Chem. Int. Ed.* **2023**, e202307818.

Deeper access into the vitamin D metabolome using liquid chromatography tandem mass spectrometry.

Anastasia Alexandridou¹, Dietrich A. Volmer¹

¹ Bioanalytical Chemistry, Department of Chemistry, Faculty of Mathematics and Natural Sciences, Humboldt University of Berlin, Brook-Taylor-Strasse 2, 12489 Berlin, Germany

E-mail: alexanda@hu-berlin.de

Vitamin D compounds belong to a group of secosteroids which are found in human biological samples in very low concentrations spanning from picomolar to nanomolar levels [1]. For this reason, the applied analytical methods should be very sensitive and selective. Liquid chromatography/tandem mass spectrometry (LC-MS/MS) is considered to be the ideal analytical method for vitamin D assessment and is characterised as the “gold standard” technique [2,3].

Vitamin D measurement can be very challenging due to the lack of readily ionizable groups of vitamin D metabolites, the presence of interfering endogenous compounds and the low abundances in human serum [4]. Chemical derivatisation can enhance the detection sensitivity by increasing the ionization efficiency, shifting the mass to higher *m/z* values with less isobaric noise and providing specific fragmentation patterns for MS/MS. Moreover, derivatisation can also have a positive effect on the selectivity of LC separation.

In our study, we compared the detection sensitivity and LC separation of vitamin D₃, 3β-25(OH)D₃, 3α-25(OH)D₃, 1,25(OH)₂D₃ and 24,25(OH)₂D₃ using four dienophile reagents (4-phenyl-1,2,4-triazoline-3,5-dione (PTAD), 4-[2-(6,7-dimethoxy-4-methyl-3-oxo-3,4-dihydroquinoxaliny)ethyl]-1,2,4-triazoline-3,5-dione (DMEQ-TAD), Amplifex, 2-nitrosopyridine (PyrNO)) as well as two reagents targeting hydroxyl groups (isonicotinoyl chloride (INC) and 2-fluoro-1-methylpyridinium-p-toluenesulfonate (FMP-TS)). In addition, a combination of dienophiles and hydroxyl group reagent was examined. We also present separation of isomers and epimers utilizing C-18 and PFP HPLC columns as well as different compositions of the mobile phase. Moreover, the short-term and long-term stability of the derivatives in serum extracts were tested. The measurements were conducted using Sciex QTRAP 6500+.

Derivatisations using Cookson-type reagents are well established but often lead to problems during chromatographic separation. More than a single peak for each vitamin D analyte is present at the chromatogram as a result of diastereomer (R and S) formation during reaction. This can be problematic when different diastereomer's peaks coelute. Moreover, the existence of more than one peaks has a negative impact on the sensitivity of the method.

Derivatization reagents targeting hydroxyl group can be an alternative offering advantages and disadvantages. Depending on the stereochemical hindrance of each hydroxyl group and the amount of derivatization reagent used, one or more hydroxyl groups can be derivatised resulting in 1-3 different precursor ions depending on the structure of each analyte.

With respect to detection sensitivity, the optimum derivatization reagent for the profiling of multiple metabolites was Amplifex. Nevertheless, FMP-TS, INC, PTAD, or PTAD combined with an acetylation reaction showed very good performance for selected metabolites. These reagent combinations provided signal enhancements on the order of 3- to 295-fold depending on the compound. Chromatographic separation of the dehydroxylated vitamin D₃ species was readily achieved using any of the derivatization reactions, while for 25(OH)D₃ epimers, only PyrNO, FMP, INC, and PTAD combined with acetylation enabled complete separation. To our knowledge, no systematic comparison of multiple derivatising agents for MS analysis of vitamin D metabolites has ever been presented. This information is important and can serve as a useful tool to help analytical and clinical scientists decide which derivatization reagent to choose for their application.

Literatur:

- [1] Volmer DA, Mendes LR, Stokes CS., *Mass Spectrometry Reviews*, 34 (2015) 2.
- [2] Sempos CT, Betz JM, Camara JE, Carter GD, Cavalier E, Clarke MW, Dowling KG, Durazo-Arvizu RA, Hoofnagle AN, Liu A, Phinney KW., *Journal of AOAC International*, 100 (2017) 1230.
- [3] van den Ouweland JM., *Trends in Analytical Chemistry*. 1 (2016) 117.
- [4] Alexandridou A, Schorr P, Volmer DA., *Analytical and Bioanalytical Chemistry*, 415 (2023) 4689.

Multivariate data analysis for laser-induced XUV spectroscopy (LIXS)

Alexander Winckelmann^{1,2,3}, Adrian Wichser², Carlos Abad¹ and Davide Bleiner^{2,4}

¹Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Str. 11, 12489 Berlin, Germany

²Swiss Federal Laboratories for Materials Science and Technology (Empa), Ueberlandstr. 129, 8600 Dübendorf, Switzerland

³Department of Chemistry, Humboldt Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

⁴Department of Chemistry, University of Zurich, Winterthurststr. 190, CH 8057 Zurich, Switzerland

E-mail: alexander.winckelmann@bam.de

The application of multivariate data analysis is essential in extracting the full potential of laser-induced XUV spectroscopy (LIXS) for high-precision elemental mapping. LIXS offers significant advantages over traditional laser-induced breakdown spectroscopy in UV-vis (LIBS), including higher precision and a wider dynamic range,^[1,2] while making it possible to determine light elements like lithium and fluorine. However, it is challenged by the presence of unresolved transition arrays (UTAs) for heavier elements. These UTAs add considerable complexity to the spectral data, often concealing crucial information. In this study, we employ well-established multivariate data analysis techniques and intensive data preprocessing to unravel this contained information.

The refined analysis reveals a high level of detail, enabling the precise identification of inhomogeneities within material samples. Our approach has particular relevance for studying aging processes in lithium-ion batteries (LIBs), specifically in relation to varying cathode materials and fluorine-containing polymer binder content. By combining elemental distribution with structural information, this improved method can offer a more comprehensive understanding of sample inhomogeneities and aging processes in LIBs, contributing to the development of more reliable and sustainable battery technologies.

Literatur:

[1] Bleiner, D.; Qu, D.; Kraft, K.; Shlyakhtun, O. Laser-induced XUV spectroscopy (LIXS): From fundamentals to application for high-precision LIBS. *Spectrochim. Acta, Part B* **2023**, 204, 106668. DOI: <https://doi.org/10.1016/j.sab.2023.106668>.

[2] Qu, D.; Ohannessian, N.; Wyder, C.; Trottmann, M.; Wichser, A.; Lippert, T.; Bleiner, D. High-precision mapping of fluorine and lithium in energy materials by means of laser-induced XUV spectroscopy (LIXS). *Spectrochim. Acta, Part B* **2021**, 181, 106214. DOI: <https://doi.org/10.1016/j.sab.2021.106214>.

Nutzung von CO₂ als modernes Synthesematerial für recyclebare Polymere und Tenside durch Ringöffnende Polymerisation

Daniel Brüggemann^{1,2}, Reinhard Schomäcker¹

¹ Technische Universität Berlin, Institut für Chemie – Technische Chemie, Straße des 17. Juni 124, 10623 Berlin, Deutschland

² Covestro Deutschland AG, Kaiser-Wilhelm-Alle 60, 51373 Leverkusen, Deutschland

E-Mail: d.brueggemann@campus.tu-berlin.de

Die chemische Industrie fertigt den überwiegenden Teil der Produkte seit jeher auf der Basis von Rohöl. Darunter fallen mit einem großen Prozentsatz Polymere und Tenside. Allein im Jahr 2016 wurden in Deutschland für Anwendungen in Haushalten und industriellen Prozessen insgesamt ca. 1,29 Mio. Tonnen Tenside hergestellt. Davon machen 1,10 Mio. Tonnen kationische, anionische und nichtionische Tenside aus [1]. Nichtionische Tenside stellen dabei den größten Anteil von 41%, die primär aus langkettigen Fettalkoholen und Ethylenoxid (EO) hergestellt werden. Mit einem Umsatzwert von 894 Mio. Euro zählen nichtionische Tenside zu den wichtigsten chemischen Erzeugnissen [1,2].

Unter diesen Gesichtspunkten führt die Möglichkeit Kohlenstoffdioxid (CO₂) als Synthesematerial für die Herstellung einzusetzen, zu einem großen Mehrwert für die Umwelt, nicht zuletzt wegen der vereinfachten Möglichkeit des Recyclings. Für Rohöl basierte Produkte erfolgt das Recycling meist über energieintensives Steamcracking, in ihre die Plattformchemikalien. Durch den Einbau von CO₂ werden Sollbruchstellen geschaffen, die die Aufarbeitung erleichtern und eine einfache Rückgewinnung der Monomere ermöglicht. Die Herstellung geeigneter Monomere für diese Polymere und Tenside sind durch moderne Synthesemethoden zugänglich (siehe Abbildung 1).

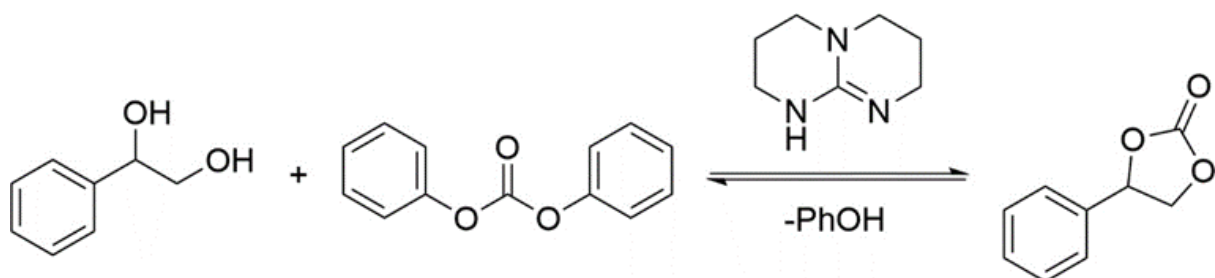


Abbildung 1: Organokatalyse eines CO₂-haltigen Monomers.[3]

Diese Monomere eignen sich nicht nur zur Herstellung von CO₂-haltigen Polymeren, mittels einer kontrollierbaren ringöffnenden Polymerisation, sondern sind auch zur Herstellung von Tensiden geeignet (siehe Abbildung 2).

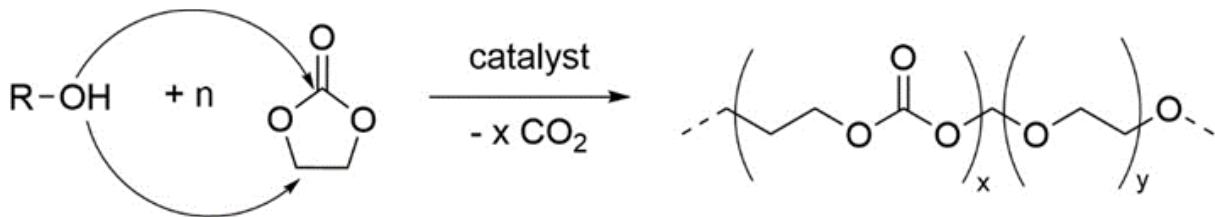


Abbildung 2: Herstellung von CO₂-haltigen Tensiden mittels ringöffnender Polymerisation.[4]

Diese Tenside herzustellen und dabei gleichzeitig die Produkteigenschaften zu steuern, ist durch die Nutzung eines CO₂-Bausteins wie z.B. cyclischen Ethylencarbonaten (cEC) möglich. Das Verständnis der Steuerungsmöglichkeiten bei der ringöffnenden Polymerisation [6], führt für die Nutzung von z.B. cyclischen Ethylencarbonaten, zu einstellbaren funktionalen nichtionischen Tensiden, die sowohl durch ihre Umweltfreundlichkeit, als auch durch gute biologische Abbaubarkeit überzeugen können. Dabei haben diese Produkte mindestens gleiche, teils bessere Eigenschaften als ihre klassischen rohölbasierten Äquivalente. So haben sich diese Tenside bereits zum Aufreinigen von Mikroplastik Verunreinigungen im Wasser bewährt [5].

Dieser Vortrag hat das Ziel, die Ergebnisse einer dreijährigen Dissertation zusammenzufassen und dem Hörer näher zu bringen.

Literatur:

[1] Statistisches Bundesamt, Statistisches Bundesamt Produzierendes Gewerbe, 2016. [https://www.destatis.de/DE/Publikationen/Thematisch/IndustrieVerarbeitendesGewerbe/Strukturdaten/Kostenstruktur2040430107004.pdf? blob=publicationFile](https://www.destatis.de/DE/Publikationen/Thematisch/IndustrieVerarbeitendesGewerbe/Strukturdaten/Kostenstruktur2040430107004.pdf?blob=publicationFile).

[2] M.. Patel, A. Theiß, E. Worrell, Surfactant production and use in Germany: resource requirements and CO₂ emissions, Resour. Conserv. Recycl. 25 (1999) 61–78. [https://doi.org/10.1016/S0921-3449\(98\)00063-9](https://doi.org/10.1016/S0921-3449(98)00063-9).

[3] E.R. Baral, J.H. Lee, J.G. Kim, Diphenyl Carbonate: A Highly Reactive and Green Carbonyl Source for the Synthesis of Cyclic Carbonates, J. Org. Chem. 83 (2018) 11768–11776. <https://doi.org/10.1021/acs.joc.8b01695>.

[4] N. Von Seggern, T. Schindler, S. Naumann, Dual Catalytic Ring-Opening Polymerization of Ethylene Carbonate for the Preparation of Degradable PEG, Biomacromolecules. 21 (2020) 2661–2669. <https://doi.org/10.1021/acs.biomac.0c00360>.

[5] D. Brüggemann, T. Shojamejer, M. Tupinamba Lima, D. Zukova, R. Marschall, R. Schomäcker, The Performance of Carbonate-Modified Nonionic Surfactants in Microplastic Flotation, Water. 15 (2023) 1000. <https://doi.org/10.3390/w15051000>.

[6] D. Brüggemann, M. Machat, R. Schomäcker, M. Mojgan The importance of elementary steps induced by catalyst monomer interactions in ring opening polymerization of cyclic ethylene carbonate for determining polyether carbonate polyols characteristics: a DFT metadynamics study validated by kinetic measurements, (2023), [Manuscript in preparation].

Novel detection approach for photometrically accurate fluorescence upconversion spectroscopy of broadly emitting dyes

Marco Kapitzke¹, Samuel Palato¹, Julia Stähler¹

¹Humboldt-Universität Berlin, Department of Chemistry, Brook-Taylor-Strasse 2, 12489 Berlin, Germany

Broadband fluorescence upconversion spectroscopy (FLUPS) stands as a powerful method to monitor ultrafast emission processes like intramolecular and vibrational cooling or solvation dynamics. It is capable of recording background-free fluorescence spectra in the visible range with an impressive time resolution of approximately 100 fs.^[1,2] However, because FLUPS is based on phasematching (PM), a compromise between spectral coverage and signal strength is ubiquitous. Particularly, for broadly emitting fluorophores, extensive spectral coverage requires thin upconversion crystals and, thus, significant compromises in signal strength. Figure 1a illustrates that sufficient coverage cannot be achieved for some systems, leading to a distortion of the lineshape and potentially to erroneous conclusions.

We introduce a novel measurement strategy that relies on recording the upconversion signal at different PM angles, as shown in Figure 1b. Using the push-pull dye 4-Dimethylamino-4'-nitrostilbene (4-DANS) in tetrahydrofuran, we demonstrate that both spectral coverage and signal-to-noise improve simultaneously through a 3-angle detection scheme with subsequent superposition of all angular contributions. Unlike other multi-angle approaches that rely on spectral reconstruction, our spectra undergo a photometric correction procedure, ensuring the display of accurate lineshapes. Furthermore, we validate the reproducibility of the 3-angle method through a blind comparison between two independent laboratories.

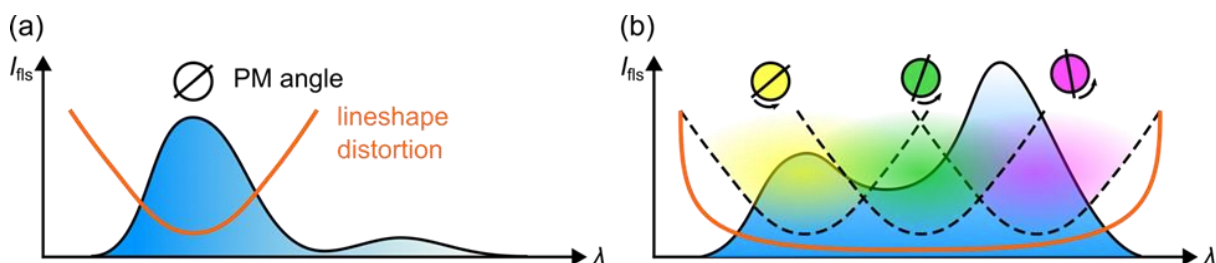


Figure 1: Comparison of a) conventional FLUPS, in which the spectral coverage for a fixed PM angle may not be sufficient and b) our new approach, that synthesizes broadband transient spectra with accurate lineshapes using spectra at different PM angles combined with a photometric correction procedure.

References:

[1] Zhao, L.; Lustres, J. L. P.; Farztdinov, V.; Ernsting, N. P. Femtosecond fluorescence spectroscopy by upconversion with tilted gate pulses. *PCCP* **2005**, *82*, 1716-1725

[2] Zhang, X.-X.; Würth, C.; Zhao, L.; Resch-Genger, U.; Ernsting, N. P.; Sajadi, M. Femtosecond broadband fluorescence upconversion spectroscopy: Improved setup and photometric correction. *Rev. Sci. Instrum.* **2011**, *82*, 063108

Workshops

Application and Leadership training with Jo Riehle

CAS workshop on green chemistry, Karin Färber

Everyone is talking about sustainability and the word “green“. But what does that mean for chemistry? It is not only about the toxicity of the used solvents or the utilization of better catalyst. It is thinking about each step even about the “reusability“ of your reaction flasks. But how can I transfer my good working synthesis to “greener“ alternative? The way to go is the CAS Indexing and SciFinder-n. This workshop will help you to find greener approaches and will leverage your synthesis to a new environmental friendlier level.

You will learn how:

- How to apply the relevant concepts to your green chemistry search
- How to unveil more efficient reaction with less impact on our environment
- Save money by improving reaction condition with less burden to your equipment