Nordic Polymer Days 2019

Book of Abstracts

5-7 June 2019

Trondheim, Norway

EDITORS

Rita de Sousa Dias

Sulalit Bandyopadhyay

PARTNERS AND SPONSORS

NTNU

SINTEF

The Research Council of Norway

TRONDHEIM KOMMUNE

polymers

ThermoFisher SCIENTIFIC

BioMACROMOLECULES

NKS

EXHIBITORS

TA Instruments

matriks KJEMISK TEKNOLOGI

METTLER TOLEDO

NETZSCH

NERLIENS MESZANSKY

Welcome to Trondheim

Dear colleagues,

The members of the Nordic Polymer Days 2019 Organizing Committee extend a warm welcome to all participants of the Nordic Polymer Days meeting.

Nordic Polymer Days is the premier Nordic annual conference where researchers and professionals gather to confer around new polymer science developments and applications. Now in its 56th year, the Nordic Polymer Days continues to foster a collaborative environment and facilitate networking opportunities at the intersection of polymer science and technological development. We aim at continuing the success of previous editions by providing a stimulating environment for discussions and brain-storming.

In addition to the oral program, the poster section will take place adjacent to the lecture rooms. The posters will be up throughout the meeting and a dedicated session will take place on Thursday afternoon. In the same space you will find the commercial exhibitors. Visit them to see the latest in analytical techniques related to polymer science.

The participation of young researches has been a priority and, as recognition of the work put into their presentation, MDPI Journal “Polymers” and ACS Journal “Biomacromolecules” are kindly sponsoring awards to a total of 3 oral and 4 poster presentations. In addition, we encourage all participants to submit their regular manuscript on the topic of their presentation at NPD2019 to the Special Issue “Nordic Polymer Days" of the MDPI Journal “Polymers”.

Behind the success of this year’s “Nordic Polymer Days” lies the extensive efforts, commitment, and dedication of myriad individuals and organizations. We first acknowledge our established polymer science community in the Nordic countries, who have collectively sustained this conference series, in terms of both scientific rigor and event hosting, for over half a century. We have thereby enjoyed the fruits of a robust scientific platform and outstanding professional network upon which to build this year’s gathering. Second, we acknowledge the essential contributions of the knowledgeable and dedicated program committee members in devising a successful strategy for this year’s conference.

Financial premises of this year’s conference were secured by our direct sponsors, including the Research Council of Norway, NTNU, SINTEF, Thermo Fisher Scientific, and the Norwegian Chemical Society. Essential scientific and technical competence contributions were provided by several exhibitors, including T-A Instruments, METTLER TOLEDO, NETZSCH Group, Nerliens Meszansky and Matriks AS.

Finally, this conference would not be possible without the participants contributions and involvement. We are pleased and grateful that 130 participants registered for this year’s Nordic Polymer Days conference, which is emblematic of the essential role that polymers play in the Nordic industries.

Sincerely, NPD Organizing Committee

Kristofer Paso, NTNU

ORGANIZATION

Program Committee

Bjørn Torger Stokke, NTNU (Chairman)
Kristofer Gunnar Paso, NTNU
Bjørn E Christensen, NTNU
Marit Sletmoen, NTNU & NKS Makro
Kurt I Draget, NTNU
Rita S Dias, NTNU
Andreas Echtermeyer, NTNU
Kenneth Knudsen, IFE
Reidar Lund, UiO& NKS Makro
Heidi Johnsen, SINTEF
Erik Andreassen, SINTEF
Pontus Lundberg, Thermo Fisher
Wilhelm Glomm, SINTEF
Sulalit Bandyopadhyay, NTNU

Organizing Committee

Kristofer Gunnar Paso, NTNU (Chairman)
Kurt I Draget, NTNU
Rita S Dias, NTNU
Bjørn Torger Stokke, NTNU
Sulalit Bandyopadhyay, NTNU
Heidi Johnsen, SINTEF

Conference Secretariat

NTNU Videre, Mila Knoff

GENERAL INFORMATION

Conference Site

The conference site is the Electrical Engineering Building located on the main campus of the Norwegian University of Science and Technology, NTNU, at Gløshaugen. The street address is O.S. Bragstads plass 2. The plenary lectures will be presented in lecture halls EL5. The parallel session with oral presentations will be held in lecture halls EL5 and EL6. The poster sessions will take place in the foyer outside the lecture hall. A post office, a small food store and a bookstore are conveniently located on campus in Central Buildings I and II. Opening hours are 08:00-15:00. Please note that smoking is not allowed in any of the campus buildings.

Registration

Registration will take place on Wednesday June 5, 10:00-12:00 at the Conference Secretariat, Electrical Engineering Building, NTNU, Gløshaugen.

Secretariat During the Conference

The Secretariat during the conference is located in the Electrical Engineering Building, room 21 in the foyer outside auditorium EL5. The Secretariat will be happy to assist you with any practical information during your stay in Trondheim. The following telephone numbers can be used to leave messages for the participants during the conference: + 47 9137 4177 and +47 4507 1041.

Opening Hours of the Secretariat

Wednesday, June 5	1000-1230
Thursday, June 6	1000-1230

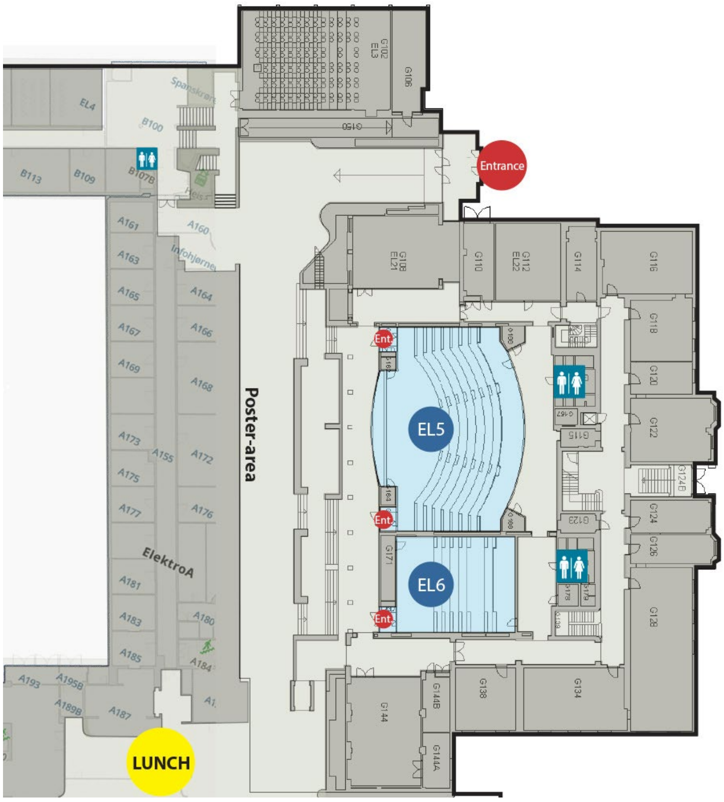
Badges

Please, wear your Nordic Polymer Days 2019 badge which you received upon registration during all conference sessions and associated activities.

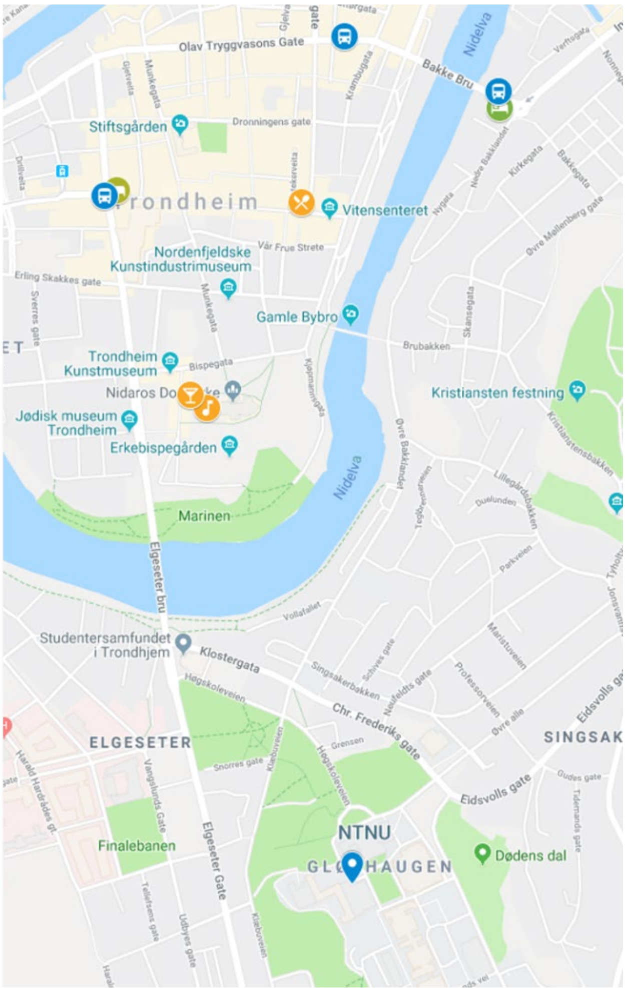
Wifi Networks

Eduroam and ntnuguest.

MAPS



- NPD 2019 Venue
- Organ concert in the Nidaros Cathedral
- Reception at Café To Tårn
- Conference dinner at Banksalen
- Scandic Nidelven
- Scandic Bakklandet
- Quality Hotel Augustin
- Line 5 - Bus stop: Kongens gate K2
- Line 22 - Bus stop "Bakkegata"
- Line 22 - Bus stop "Nova Kino"



SCIENTIFIC SESSIONS

Oral Presentations

All lectures will be presented in lecture hall EL5 or EL6, located in the Electrical Engineering Building situated on the main campus of the Norwegian University of Science and Technology, NTNU, at Gløshaugen. The lecture halls are equipped with overhead projector. All speakers are encouraged to wear the microphone provided to ensure that everyone can hear the presentation. Preview facilities is provided in the room of the Secretariat (room 21).

The total presentation time for invited lectures are 30 minutes **including** 5 minutes for discussion, and 20 minutes **including** 5 minutes for discussion for oral contributions. Speakers are encouraged to strictly respect this time allocations to both allow time for discussion, and to keep the program on schedule.

Poster Presentations

The poster session will take place in the foyer outside the lecture halls EL5 and EL6 on Thursday June 6, 16:10- 18:00. Authours of posters are requested to mount their posters before 12:20 on Wednesday June 5 on their assigned poster board. Suitable mounting aids will be provided. All posters will be displayed during the conference from Wednesday afternoon to Friday.

IMPORTANT: All posters must be removed from the poster boards by 13:00 on Friday June 7. The organizers can not take any responsibility for posters not removed by this time.

Publication of Papers

All participants are encouraged to submit their regular manuscript on the topic of their presentation at NPD2019 to the Special Issue “Nordic Polymer Days" of the MDPI Journal “Polymers” with a submission deadline of **25 October 2019**). More information can be found at: https://www.mdpi.com/journal/polymers/special_issues/Nordic_Polymer_Days

SOCIAL PROGRAM

Wednesday, June 5

Organ Concert at Nidaros Cathedral 19:00 – 19:30

Concert with the Steinmeyer organ including an official welcome from a representative of Trondheim Municipality

Evening Reception at Café To Tårn 19:30 – 21:00

Café To Tårn is located adjacent to Nidaros Cathedral

Thursday, June 6

Conference Dinner at Banksalen Restaurant (Kongens gate 4) 19:00 – 22:00

Program Nordic Polymer Days 2019, June 5-7 2019, Trondheim, Norway

Wednesday, 5 June 2019

10:00	Registration			
11:00 – 12:00	Lunch			
12:00 – 12:20	Opening/welcome (room EL5) Chairperson: Bjørn Torger Stokke			
12:20 – 12:50	PL1	Kell Mortensen, Anine L. Borger, Jacob J.K. Kirkensgaard, Kristoffer Almdal, Qian Huang, Ole Hassager and Masahiko Annaka **SANS Studies of Star-Polymers and Star-Polymer Gels Exposed to Stretch**		
12:50 – 13:20	PL2	Kristiina Oksman **Bio-based nanomaterials, their isolation, properties and composites**		
13:25 –	**Parallel session. Topic 1: Polymer characterization** (room EL5) Session co-chairs: Kell Mortensen, Dag Werner Breiby		**Parallel session. Topic 2: Polymer Composites** (room EL6) Session co-chairs: Kristiina Oksman, Andreas Echtermeyer	
13:25 – 13:45	O1.1	Matthias Amann, Jakob Stensgaard Diget, Jeppe Lyngsø, Jan Skov Pedersen, Theyencheri Narayanan and Reidar Lund **The Kinetic Pathway for Polyelectrolyte Coacervate Formation revealed by Time-resolved Synchrotron SAXS**	O2.1	Tahani Kaldéus, Lars Berglund, Eva Malmström and Giada Lo Re **Molecular engineering of CNF/PCL interface for high toughness bio-nanocomposites**
13:45 – 14:05	O1.2	S. Bayati, L. Galantini, K. D. Knudsen and K. Schillén **A combined SAXS and SANS study of interactions between bile salt and a triblock copolymer**	O2.2	Karolina Gaska and Roland Kádár **Thermal and electrical properties of graphene polypropylene composites**
14:05 – 14:25	O1.3	Sindre Olufsen, Arild Holm Clausen and Odd Sture Hopperstad **In-Situ X-ray tomography for investigation of void growth in mineral-filled PVC using a conventional X-ray source: A plausibility study**	O2.3	Ravindra Reddy Chowreddy and Katrin Nord-Varhaug **Recycled Poly (Ethylene Terephthalate) Nanocomposites: Rheology, Thermal and Mechanical Properties**
14:25 – 14.55	Coffee & break			
14:55 – 15:15	O1.4	Vegar Ottesen, Per Tomas Larsson and Kristin Syverud **Swelling of Individual Cellulose Nano-Fibrils: Does Crystallinity affect Swellability?**	O2.4	Karolina Gaska and Roland Kádár **Nonlinear rheological signatures and percolation in nano-filled polymers**
15:15 – 15:35	O1.5	Josefine Eilsø Nielsen, Victoria Ariel Bjørnestad, Abdullah Lone, Håvard Jenssen, Tania Kjellerup Lind, Marité Cardenas and Reidar Lund. **Probing the Structure of Antimicrobial Peptides and their Interaction with Lipid Membranes using Small-angle X-ray and Neutron Reflectivity Methods**	O2.5	Lilian Forsgren, Karin Sahlin-Sjövold, Abhijit Venkatesh, Johannes Thunberg, Roland Kadar, Antal Boldizar, Gunnar Westman and Mikael Rigdahl **Composites with surface-grafted cellulose nanocrystals (CNC)**
15:35 – 15:55	O1.6	Ekkehard Füglein **Characterization and Classification of Polymers and Polymer Mixtures by Means of DSC and an Advanced Software Database**	O2.6	Tony Tiainen, Marina Lobanova, Erno Karjalainen and Sami Hietala **Nanodiamond reinforced polyelectrolyte films**
15:55 – 16:15	O1.7	Stephanie Haider, Lukas Kammerer, Michael Aigner, Sabine Hild and Gabriel Kronberger **Using Elastic Net Regularization for the Identification and Quantification of Raman Spectra in Mechanical Polymer Recycling.**	O2.7	Shiyu Geng, Daniela Wloch, Natalia Herrera and Kristiina Oksman **High-strength, high toughness polylactic acid-based nanocomposites reinforced with well-dispersed cellulose nanocrystals**
16:15 – 16:35	O1.8	Christian Andersen, Niels Jørgen Madsen and Anders E. Daugaard **Method of Making Polymer Surface Modifications Through the use of Screening Platforms**	O2.8	Yingwei Ouyang, Massimiliano Mauri, Ida Östergren, Thomas Gkourmpis, Per-Ola Hagstrand, Oscar Prieto and Christian Müller **In-situ Formation of a Polyethylene-Polypropylene Copolymer through Reactive Compounding**
16:35 – 16:55	O1.9	C. W. Karl, A. Lang, M. Klüppel and U. Giese **Characterization of modified elastomer surfaces by wetting**	O3.1	Kerstin Steyrl, Blanca Maria Lekube, Thomas Hofstätter and Christoph Burgstaller **Melt filtration of polymers**.
17:00 – 17:30	PL3	Susie Jahren (room EL5) Chairperson: Kristofer Paso **The war on plastics**		
19:00	Organ concert followed by reception			

Thursday, 6 June 2019

08:30 – 09:00	PL4	Monika Österberg (room EL5) Chairperson: Reidar Lund **Surface-tailored functional and ecological materials from wood polymers**		
09:00 – 09:30	PL5	Dag W. Breiby **Quantitative 4D X-ray Microscopy and Its Future in Polymer Science**		
09:40 onwards	**Parallel session. Topic 4: Biopolymers** (room EL5) Session co-chairs: Monika Österberg, Pontus Lundberg		**Parallel session. Topic 5: Other Topics in Polymer Science** (room EL6) Session co-chairs: Reidar Lund, Heiki Tenhu	
09:40 – 10:00	O4.1	Erfan Oliaei, Pär Lindén, Qiong Wu, Fredrik Berthold, Lars Berglund and Tom Lindström **Fibrillation of unbleached Kraft softwood pulp to lignin-containing microfibrillated cellulose**	O5.1	Els Verdonck and Philip Davies **The Thermal Analysis Toolkit for Characterising Polylactic Acid**
10:00 – 10:20	O4.2	Eleonora Parelius Jonasova and Bjørn Torger Stokke **Responsive hydrogels as recognition and transducing elements in biosensing: Spatiotemporal response of DNA-co-acrylamide hydrogels**	O5.2	Erik Andreassen, Ivanna Baturynska, Marius Johansen and Marius Andersen **Mechanical properties of polyamide 12 parts made by powder bed fusion (additive manufacturing)**
10:20 – 10:50	Coffee & break			
10:50 – 11:10	O4.3	Jiayuan Wei, Shiyu Geng, Olli Pitkänen, Topias Järvinen, Krisztian Kordas and Kristiina Oksman **Making good use of lignin – from a low-value biopolymer to energy storage devices**	O5.3	Jonna Hynynen, Emmy Järsvall, Renee Kroon, Yadong Zhang, Stephen Barlow, Seth R. Marder, Martijn Kemerink, Anja Lund and Christian Müller **Enhanced Thermoelectric Performance of the Conjugated Polymer Poly(3-hexylthiophene) through Tensile Drawing**
11:10 – 11:30	O4.4	Mihaela Tanase Opedal, Eduardo Espinosa Víctor, Johnny Kvakland Melbø, Alejandro Rodríguez Pascual and Gary Chinga-Carrasco **Lignin – a biopolymer from forestry biomass for biocomposites and 3D printing**	O5.4	Karsten Leucker, Janosch Amtmann and Dirk W. Schubert **Revealing correlations of bonding area and pilling behaviour of polypropylene non-wovens using a novel objective test method**
11:30 – 11:50	O4.5	Linn Berglund and Kristiina Oksman **Direct preparation of alginate/nanofiber hybrid-ink from seaweed**	O5.5	Markus Schubnell and Jürgen Schawe **Investigating crystallization and thermal stability of polymers by fast scanning calorimetry**
11:50 – 12:10	O4.6	Mika H. Sipponen, Tao Zou, Alexander Henn and Monika Österberg **Lignin-lipid capsules as renewable hybrid materials for sustainable material applications**	O5.6	Shaoquan Wang, Kaspar Lasn, Christer Westum Elverum and Andreas T. Echtermeyer **A novel approach for in-situ measurement of residual strain in FDM using Optical Backscatter Reflectometry**
12:10 – 12:30	O4.7	Julien Navarro and Ulrica Edlund **Functionalized CNF for materials and biomarker sensing**	O7.1	Andrey E. Krauklis, Anton G. Akulichev, Abedin I. Gagani and Andreas T. Echtermeyer **Creep of Epoxy in Water: Time-Temperature-Concentration Superposition**
12:30 – 13:30	Lunch			
13:30 – 14:00	PL6	Stefan Hervø-Hansen, Richard Chudoba and Mikael Lund (room EL5) Chairperson: Rita S Dias **Ion Specific Effects on Polymer Interactions**		
14:10 –	**Parallel session. Topics 4 & 6: Biopolymers and Functional Polymers** (room EL5) Session co-chairs: Sulalit Bandyopadhyay, Finn Knut Hansen		**Parallel session. Topic 7: Polymer Theory and Modelling** (room EL6) Session co-chairs: Rita S Dias, Mikael Lund	
14:10 – 14:30	O4.8	Muhammad Farooq, Tao Zou, Guillaume Riviere, A. Seppälä, Mika H. Sipponen and Monika Österberg **Thermal and water barrier properties of CNF based aerogels and nanocomposites**	O7.2	Anna-Maria Persson, Erik Andreassen, Kristian Martinsen and Einar L. Hinrichsen **Thermoplastic elastomers – Long-term mechanical properties for sealing applications**
14:30 – 14:50	O5.7	Xinfeng Wei, Ulf W.Gedde and Mikael S. Hedenqvist **Degradation of polyamide-based multilayer fuel line exposed to bio and petroleum diesel under "in-vehicle" conditions**	O7.3	Arne Ilseng, Victorien Prot, Bjørn H. Skallerud and Bjørn T. Stokke **Effect of initial thickness for the onset of buckling in hydrogel plates.**

14:50 – 15:10	O6.1	Marius Sandru, Per Stenstad, Eugenia Sandru, Jing Deng and Liyuan Deng **Novel polymer architectures for CO_2 selective membranes**	O7.4	Dirk W. Schubert **Revealing novel power laws and quantization in electrospinning considering jet splitting – towards predicting fiber diameter and its distribution**
15:10 – 15:30	O6.2	Xiaomin Qian, Fabian Itel, Noga Gal and Brigitte Städler **Stimuli-responsive polymers as functional materials to discriminate complex mixtures**	O7.5	Raju Lunkad, Anastasiia Murmiliuk, Milan Boublík, Pavel Dubský, Pascal Hebbeker, Miroslav Štěpánek and Peter Košovan **Quantitative understanding of ionization of weak polyelectrolytes and weak polyampholytes: simulations vs. experiment**
15:30 – 15:50	O6.3	Eugenia Sandru, Wilhelm Glomm, Le Thuy Truong, Peter Molesworth and Heidi Johnsen **Microencapsulation by complex coacervation of oil soluble vitamins**	O7.6	Hyejeong Cheon, Morten Stornes, Costanza Tedesco and Rita S. Dias **Monte Carlo simulation of halloysite nanotube and polyelectrolyte**
15:50 – 16:10	O6.4	Vikram Baddam and Heikki Tenhu **Counterion turns poly(ionic liquid)-PEG copolymer thermoresponsive**	O7.7	Pablo M. Blanco, Josep Lluís Garcés, Francesc Mas and Sergio Madurga **Exploring mechanically-induced charge regulation in weak polyelectrolytes by computer modelling**
16:10 – 18:00	**Poster session** (including coffee)			
19:00	Conference dinner			

Friday, 7 June 2019

09:00 –	**Parallel session. Topic 8: Biomedical Applications** (room EL5) Session co-chairs: Wilhelm Glomm, Søren Hvilsted		**Parallel session. Topic 6: Functional Polymers** (room EL6) Session co-chairs: Erik Andreassen, Heidi Johnsen	
09:00 – 09:20	O5.8	Muhammad Ahsan Bashir, Martin Gjerde Jakobsen and Vivian B. Farstad **The Effect of Extender Particle Size on the Glass Transition Temperatures of Cured Epoxies**	O6.5	Anastasiia Murmiliuk, Sergey K. Filippov, Zdeněk Tošner, Michael Gradzielski, Stergios Pispas, Athanasios Skandalis and Miroslav Štěpánek **Three-layered onion micelles with soft poly(lauryl acrylate) core: co-assembly and morphological transition**.
09:20 – 09:40	O8.1	Viktor Granskog, Mathieu Arseneault, Daniel Hutchinson and Michael Malkoch **Utilizing Thiol-ene and Thiol-yne Chemistry to Create New Materials for Dental and Skeletal Repair**	O6.6	Kjartan Tobias Boman, Cecilia Winander and Marit Dahling **Polyoxalates for marine antifouling coatings**
09:40 – 10:00	O8.2	Edit Brodszkij, Carina A. Ade, Bo Thingholm and Brigitte Stadler **pH responsive polyanions to aid cytosolic placement of nanoreactors**	O6.7	Yizhi Zhuo, Jianying He and Zhiliang Zhang **Self-healing polymers for durable icephobicity**
10:00 – 10:20	O8.3	Geir Fonnum and Pontus Lundberg **Improving health with monodisperse beads**	O6.8	Libor Zverina, Manuel Pinelo, John M. Woodley and Anders E. Daugaard **From ultrafiltration to nanofiltration by controlled pore collapse of modified polyethersulfone membranes**
10:20 – 10:40	O8.4	Wilhelm R. Glomm, Eugenia M. Sandru, Peter P. Molesworth, Hanne Haslene-Hox, Andrea D. Hoel and Masahiro Yasuda **Polymer particles as scaffolds for 3D cell culture systems**	O6.9	Anna Gruszkiewicz and Szczepan Zapotoczny **Low-bandgap donor-acceptor polymer brushes**
10:40 – 11:10	Coffee			
11:10 – 11:40	PL7	Session chairperson: Kristofer Paso (room EL5) Michael Malkoch **Click composites as future standard-of-care materials for bone fractures and dental restorations**		
11:40 – 12:10	PL8	Piotr Stanislaw Mazurek, Liyun Yu and Anne Ladegaard Skov **Glycerol-silicone elastomers – application perspectives**		
12:10	Closing ceremony			
12:40	Lunch			

PLENARY LECTURES

ORAL PRESENTATIONS

Topic 1: Polymer Characterization

Topic 2: Polymer Composites

Topic 3: Environment Aspects of Polymers

Topic 4: Biopolymers

Topic 5: Other Topics in Polymer Science

Topic 6: Functional Polymers

Topic 7: Polymer Theory and Modelling

Session 8: Polymers for Biomedical Applications

POSTER PRESENTATIONS

Topic 1: Polymer Characterization

Topic 2: Polymer Composites

Topic 3: Environment aspects of polymers

Topic 4: Biopolymers

Topic 5: Other Topics in Polymer Science

Topic 6: Functional Polymers

Topic 7: Polymer Theory and Modelling

Session 8: Polymers for Biomedical Applications

ABSTRACTS

PL1

SANS Studies of Star-Polymers and Star-Polymer Gels Exposed to Stretch.

*Kell Mortensen**[1], *Anine L. Borger*[1], *Jacob J.K. Kirkensgaard*[1],
Kristoffer Almdal[2], *Qian Huang*[2] *and Ole Hassager*[2]. *Masahiko Annaka*[3]

[1]*University of Copenhagen.*, [2]*Technical University of Denmark*, [3] *Kyushu University, Japan*

* kell@nbi.ku.dk

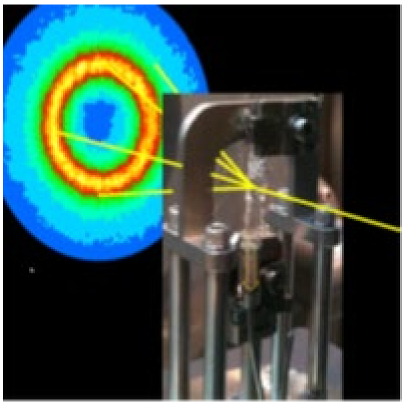


Figure 1: SANS scattering experiment on a 30% aqueous crosslinked TAT-TNT network sample mounted for in-situ stretching experiments.

One of the major challenges in polymer physics is the fundamentals of the unique visco-elastic properties characterizing soft materials, and their relation to the molecular structure. Small-Angle Neutron Scattering is, using the unique H-D substitution, the one and only method to address the molecular conformation and have accordingly been the basis for a number of studies. Still, however, the understanding is only limited. We have recently extended such results, studying the effect of very high flow rates [1,2]. We have studied the effect of polydispersity [3], the effect of branched complex polymer architecture [4], and the structural properties when cross-linked into well-defined network structures [5]. The linear chains show typically 2D-SANS pattern with Lozenge shaped contour [1,3], and clear evidence of chain-expansion and subsequent retraction upon relaxation [2]. The three-armed polystyrene star-polymer with short deuterated segments at the end of each arm shows novel, unexpected correlations perpendicular to the flow axis. We show that the form factor of the three-armed star molecules in the relaxed state agrees very well with that of the random phase approximation of Gaussian chains. Upon exposure to large extensional flow conditions, the star polymers change conformation resulting in a highly stretched structure of a fully extended three-armed tube. The cross-linked star-polymers show novel response to strain. While the mechanical properties appear as expected with linear stress-train relationship, the SANS pattern shows an apparent unchanged structure. The latter is attributed to a local layered organization of the star-molecules [5].

Acknowledgements

This work was funded from the Independent Research Fund Denmark, the Danish Research Infrastructure via DANSCATT. PSI (CH) and ANSTO (Au) are acknowledged for SANS beam time.

References

[1] O. Hassager et al. *Rheologica Acta* 51, 385, 2012
[2] A. Borger, et al. *Manuscript* 2019
[3] J. Kirkensgaard et al. *Phys. Rev. E* 94, 020502(R), 2016
[4] K. Mortensen et al., *Phys. Rev. Lett.* 120, 207801 2018
[5] K. Mortensen, M. Annaka *ACS Macro Lett.* 7, 1438, 2018

PL2

Bio-based nanomaterials, their isolation, properties and composites.

Kristiina Oksman

Luleå University of Technology, Luleå, Sweden

Kristiina.Oksman@ltu.se

Bionanomaterials such as cellulose and chitin nanofibers and nanocrystals, have gained large interest during the last 10-15 years both in research society and in industry. These fascinating bionanomaterials, isolated from plants, algae, sea crustaceans are interesting for packaging, medical, transportation and construction applications. Cellulose and chitin nanofibers and nanocrystals are very small, the width can be as small as 3 nm and the length can vary from hundreds of nanometers to micrometer level. They own many interesting properties, such as high mechanical strength and stiffness, they are of lightweight, biodegradable, transparent and they can also self-organize to strong layered networks. These properties are making them interesting as reinforcing agents and when combining them with polymers we can obtain composites which new properties. The lecture is giving an insight to these bionanomaterials and their isolation processes as well as some ideas about how these materials can be used to make composites and what type of properties can be achieved. Composites manufacturing processes such as liquid-assisted extrusion, in-situ polymerization and impregnation of nanofiber networks are discussed.

PL3

The War on Plastics.

Susie Jahren

SINTEF Industry, Forskningsveien 1, 0314 Oslo, Norway

Susie.Jahren@sintef.no

In 2018 Eric Solheim and the UN decreed a war on plastic. But it was actually a war that put us on this path in the first place. It wasn't until World War II that plastic products began to be mass-produced as they are today. The war accelerated the need for new technologies, and plastics came to revolutionise the way we live – providing us with durable, mass-produced and inexpensive commodities. They promised men of the 1950s a vision of the future, and their housewives an easier life. And plastics more than fulfilled their promise.

Today, 70 years on from the post-war plastic revolution, we produce more than 300 million tonnes of plastic goods each year. Our planet is quite literally drowning in it. What we need indeed is a war on plastics. However, the answer is not to ban plastic, but to use it and all other materials more intelligently and more responsibly. We need to take a look at the events that have bought us here and the events that are now starting to make the tide turn on plastic. Beach cleaning and paper straws are great but the real solution in the hands of plastics researchers and technologists. By creating the materials, products and systems that take care of our resources instead of dumping them , we can solve our plastic problem. Let's roll up our sleeves and see what we need to do.

PL4

Surface-tailored functional and ecological materials from wood polymers.

Monika Österberg

Aalto University, Department of Bioproducts and Biosystems, School of Chemical Engineering

monika.osterberg@aalto.fi

There is an acute lack of clean water, especially in countries that lack resources for efficient water purification. We furthermore, need to decrease the amount of waste we produce. This can be done for example by replacing synthetic materials in packaging, textiles and furniture by degradable/recyclable materials from renewable resources. However, we are not willing to make compromises in comfort, functionality or price. Hence, the sustainable solutions needs to be competitive in performance and price.

In this presentation, some examples of our recent work preparing sustainable and functional materials from wood polymers and other natural sources will be presented. The common denominator in these examples are that simple, green and scalable methods were applied to tailor the surface properties and control interfacial interactions. Cationic colloidal lignin particles (CLPs) were demonstrated to be efficient in removing viruses from water. Using chitosan as the cationic component, amphiphilic particles that were able to stabilize olive oil-water emulsions were prepared. Ionic cross-linking with sodium triphosphate formed microcapsules that could be dried and rewetted without disruption [1]. These capsules were demonstrated to have potential for delivery of hydrophobic drugs. Hybrid materials also demonstrate interesting properties and we have combined CLPs and cellulose nanofibrils to produce various hybrid materials like nanobiocomposite films demonstrating antioxidative and UV-protective properties beneficial for packaging applications [2], hybrid hydrogels suitable for 3D bioprinting and phase changing materials with potential for energy storage. Lastly, examples of non-toxic, material efficient, surface modification approaches that introduce protection against water or bacteria, while retaining the comfortable feel and breathability of cellulosic materials will be shown [3,4].

References:

1. Zou, T., Sipponen, MH, Österberg, M. Natural shape-retaining microcapsules with shells made of chitosan-coated colloidal lignin particles *Frontiers in Chemistry* Under review

2. Farooq, M, Zou, T., Riviere, G. Sipponen, MH, Österberg, M. Strong, ductile and waterproof cellulose nanofibril composite films with colloidal lignin particles *Biomacromolecules* **20** (2019), 693.

3. Hassan, G. Forsman, N., et al Dehydroabietylamine-based Cellulose Nanofibril Films: A new Class of Sustainable Biomaterials for Highly Efficient, Broad-Spectrum Antimicrobial Effects" *ACS Sustainable Chemistry & Engineering* **7** (2019) 5002.

4. Forsman, N., Lozhechnikova, A., Khakalo, A., Johansson, L.-S., Vartiainen, J. and Österberg, M. Layer-by-layer assembled hydrophobic coatings for cellulose nanofibril films and textiles, made of polylysine and natural wax particles" *Carbohydrate Polymers* **173** (2017) 392.

PL5

Quantitative 4D X-ray Microscopy and Its Future in Polymer Science.

Dag W. Breiby

Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway
Institute for Microsystem Technology, University of South-Eastern Norway (USN), Horten, Norway

dag.breiby@ntnu.no

X-ray scattering and diffraction are firmly established tools for unraveling the structural secrets of polymers and other soft materials. The penetrating nature of X-rays facilitates using complex sample environments combined with thick samples. For example, small-angle scattering (SAXS) allows the pore structure and phase transitions in surfactant-templated mesoporous films to be followed *in situ* as function of relative humidity [1].

Despite the wealth of information that can be obtained by traditional scattering methods, techniques able to retrieve real-space *images* (2D, 3D) or *movies* (4D) of nanostructured soft materials are in increasing demand. A critical review, demonstrating the upcoming possibilities for studies of soft materials, will be given. A shared feature of many new microscopy schemes is that computers are used actively in the image-forming process itself, so-called *computational imaging*. Rather than relying solely on beam attenuation for image contrast, one can employ phase and scattering as contrast mechanisms, allowing fine variations in composition and morphology to be observed. Raster scanning of a pencil-shaped beam is a conceptually simple, yet powerful, way to map out structures in polymeric samples, even using home laboratory equipment [2]. By utilizing specialized synchrotron X-ray sources, high-resolution (down to 10 nm) and quantitative phase-contrast nanoscopy can be carried out. Ultrafast tracking of structural dynamics triggered for example by laser pulses is now feasible [3]. Our recent efforts towards 4D microscopy of soft materials will be presented, highlighting in situ studies of natural organic fibers exposed to humidity [4], cement exposed to CO_2-rich brine [5], flash annealing of polymeric films [6], and 3D orientation mapping in samples ranging from fossil bones [7], via semiconducting microwires [8], to injection molded polypropylene [9].

1. Chavez E.A., Granlund H., Sztucki B., O. Konovalov, Breiby D.W., Gibaud A. *ACS Appl. Mater. & Interf.* **2014**, *6*, 2686-2691
2. Granlund H., Andreassen E., Skjønsfjell E.T., Høydalsvik K., Diaz A., Breiby D.W. *J. Polym. Sci. B.* **2014**, *52*, 1157-1167
3. Lemke H.T., Breiby D.W., Ejdrup T., Hammershøj P., Cammarata M., Khakhulin D., Rusteika N., Adachi S.I., Koshihara S., Kuhlman T.S., Mariager S.O., Nielsen T.N., Wulff M., Sølling T.I., Harrit N., Feidenhans'l R., Nielsen M.M. *ACS Omega*, **2018**, *3*, 9929–9933
4. Esmaeili M., Fløystad J.B., Diaz A., Høydalsvik K., Guizar-Sicairos M., Andreasen J.W., Breiby D.W. *Macromolecules*, **2013**, *46*, 434
5. Chavez E.A., Torsæter M., Gawel K., Bjørge R., Gibaud A., Yang Y., Bruns S., Zheng Y., Sørensen H.O., Breiby D.W. *Environmental Science & Technology*, **2017**, *51*, 9344-9351
6. Patil N., Skjønsfjell E.T.B., Van den Brande N., Chavez E.A., Classens R., Guizar-Sicairos M., Van Mele B, Breiby D.W. *PLoS ONE*, **2016**, *11*, e0158345
7. Mürer F.K., Sanchez S., Álvarez-Murga M, Di Michiel M., Pfeiffer F., Bech M., Breiby D.W. *Scientific Reports*, **2018**, *8*, 10052
8. Coucheron D.A., Fokine M., Patil N., Breiby D.W., Buset O.T., Healy N., Peacock A.C., Hawkins T., Jones M., Ballato J., Gibson U.J. *Nature Comm.* **2016**, 13265
9. Skjønsfjell E.T., Kringeland T., Granlund H., Høydalsvik K., Diaz A., Breiby D.W. J Appl Cryst, **2016**, *49*, 902-908

PL6

Ion Specific Effects on Polymer Interactions.

*Stefan Hervø-Hansen, Richard Chudoba, Mikael Lund**

Lund University, Division of Theoretical Chemistry, Sweden

* mikael.lund@teokem.lu.se

Through intermolecular and intramolecular interactions, the stability of (bio)polymers in aqueous solution is influenced by the presence of salt. Not only does the salt *concentration* or ionic strength play an important role, but so does the salt *type*. The latter observation can be traced back to early works of Franz Hofmeister and the underlying molecular mechanisms was later studied via a combination of atomistic computer simulations and high resolution experimental techniques.

In this presentation we propose a new model for describing ion specific effects in aqueous solution of polymers and other macromolecules. The model combines macroscopic and microscopic observables from experiment or all-atom MD simulations into a coarse grained model where large length and time scales can be studied. Our model include transfer free energy terms for describing salting out, i.e. when salt is excluded from the solute surface and can cause a polymer collapse and/or induce aggregation. To capture salting in, i.e. when ions bind to the solute surface we use a two-state binding parametrised via NMR experimental data. We demonstrate how the model, based on the Metropolis Monte Carlo algorithm, can be applied to aqueous solutions of PEG, caffeine, and proteins.

PL7

Click composites as future standard-of-care materials for bone fractures and dental restorations.

Michael Malkoch

KTH Royal Institute of Technology, Dept Fibre and Polymer Technology, Div of Coating Technology

Hospital visits are a continuous reminder to Humans on how fragile the body is. At any given time our body tissue can be compromised due to various unfortunate events. Careless children, athletes, physical professions and elderly are high risk groups with frequent hospital visits. In this case, bone fractures belong to most typical accidents and surgeons are often faced with more challenging surgeries that require metal implants fixators. Harsh mechanical drilling into healthy bone with screws and metal plate, for adequate fixation of the fracture, is a painful and long journey for any patient. Consequently, surgeons are one lookout for alternative fixation methods that eliminate the use of old-fashion metal-based implants.

This presentation will focus on current research activities that capitalizes on a novel materials concepts and surgical methodologies for fixation of bone fractures and dental restorations. In this context, highly robust click reactions are utilized for selective buildup of “Fiber Reinforced Adhesive Patches” (FRAP)[1] - as a modular, facile and mild fixation methodology for an array of bone fractures that today are considered inaccessible due to sensitive locations, near joints or when drilling is not an option. The FRAPs are accomplished by introducing a phosphonic primer layer as a critical component, that is programmed to strongly adhere to wet bone surfaces and “on-fracture-site” bind two a two-component resin system with imbedded hydroxyapatite and PET fibre mesh. From surgical viability point-of-view, the FRAP is produced under physiologically benign conditions using dental High-Energy Visible light applicator as a benign curing source. As an implant, the FRAP is biocompatible, none-degradable composite fixator that deliver unprecedented adhesion to bone, with a shear bond strength of 9.4 MPa, and that can withstand a minimum of 1000 cycles in fatigue tests. The adhesion strength of the FRAP surpasses commercially available dental restoration materials and can compete with metal fixation implants for an array of common fractures *e.g.* finger, radius, ankle and maxillofacial. Collectively, these high-performance “clickable” adhesive fixators can match the unlimited demand from the healthcare sector including dentistry[2] with the ultimately goal of increasing the quality of life for patients, reducing rehabilitation time and the overall healthcare costs.

References:

[1] V. Granskog, S. García-Gallego, J. von Kieseritzky, J. Rosendahl, P. Stenlund, Y. Zhang, S. Petronis, B. Lyvén, M. Arner, J. Håkansson and M. Malkoch. “High-Performance Thiol–Ene Composites Unveil a New Era of Adhesives Suited for Bone Repair”. Adv. Func. Mtrls., **2018**, 26, https://doi.org/10.1002/adfm.201870180.

[2] M. Arseneault, V. Granskog, S. Khosravi, I. M. Heckler, P. Mesa-Antunez, D. Hult, Y. Zhang and M. Malkoch. “The Dawn of Thiol-Yne Triazine Triones Thermosets as a New Material Platform Suited for Hard Tissue Repair”. Adv. Mtrls., **2018**, 30, https://doi.org/10.1002/adma.201804966.

PL8

Glycerol-silicone elastomers – application perspectives.

*Piotr Stanislaw Mazurek, Liyun Yu, Anne Ladegaard Skov**

Danish Polymer Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

* al@kt.dtu.dk

Glycerol and silicone polymers are two virtually immiscible liquids [1]. However when sufficiently high shear forces are applied to a mixture of both then the glycerol phase breaks down to micro-size droplets evenly distributed within the silicone pre-polymer phase thus a glycerol-in-silicone emulsion is produced [2]. Upon cross-linking of the silicone pre-polymer free-standing silicone elastomers with incorporated glycerol droplets are obtained. Interestingly, mechanical properties of these composites are not compromised as the glycerol loading increases [3]. Glycerol-silicone elastomers has become a platform for creating multiple functional smart materials, e.g. drug delivery wound care membranes, silicone foams, water absorbing silicones or magnetochromic films. Here some of the most interesting examples of glycerol-silicone elastomers applications will be presented and briefly explained elucidating the great potential of this "impossible" composition that, however, is extremely easy to work with.

References:

1. Mazurek, P.; Brook, M. A.; Skov, A. L. Glycerol-silicone elastomers as active matrices with controllable release profiles. *Langmuir*, **2018**, *34*, 11559–11566
2. Mazurek, P.; Ekbrant, B. E. F.; Madsen, F. B.; Yu, L.; Skov, A. L. Glycerol-silicone foams – Tunable 3-phase elastomeric porous materials. *European Polymer Journal,* **2019**, *113*, 107–114
3. Mazurek, P.; Yu, L.; Gerhard, R.; Wirges, W.; Skov, A. L. Glycerol as high-permittivity liquid filler in dielectric silicone elastomers. *Journal of Applied Polymer Science,* **2016**, *133*, 1–8

O1.1

The Kinetic Pathway for Polyelectrolyte Coacervate Formation revealed by Time-resolved Synchrotron SAXS.

Matthias Amann[1]*, Jakob Stensgaard Diget*[1] *, Jeppe Lyngsø* [2] *Jan Skov Pedersen*[2]*, Theyencheri Narayanan*[3] *and Reidar Lund*[1,*]

1Department of Chemistry, University of Oslo, Norway.
2Department of Chemistry and iNANO, Aarhus University, Langelandsgade 140, 8000 Aarhus, Denmark
3ESRF - The European Synchrotron, 71 Avenue des Martyrs, 38043 Grenoble, France

Reidar.lund@kjemi.uio.no

The kinetic pathways for coacervation and micelle formation are still not fully understood [1]. Driven by electrostatic interactions and entropically driven counter-ion release, complexation of oppositely charged macromolecules lead to the formation of micellar nanostructures. Here we study the coacervation process, from initial formation and growth of stable micelles, on a nanometric length scale using time-resolved small-angle X-ray scattering (TR-SAXS). The micellar coercevates are formed through the complexation of anionic polyelectrolyte poly(sodium 4-styrene sulfonate) (PSSS) and cationic block–copolymer poly(ethylene oxide)-block-poly((vinylbenzyl)trimethyl-ammonium chloride) (PEO-b-PVBTA). Mixing the polyelectrolytes in a stoichiometric 1:1 charge ratio resulted in the formation of stable spherical core-shell micellar-like coacervates consisting of a central core of complexed PSSS and PVBTA with a PEO corona. The results reveal that the formation polyelectrolyte coacervates follows a two-step process; i) first, metastable large-scale aggregates are formed upon a barrier-free complexation immediately after mixing; ii) Subsequently the clusters undergo charge equilibration upon chain rearrangement and exchange processes yielding micellar-like aggregates with net neutral charge that are pinched off to yield the final stable micelle-like coacervates. Interestingly, the overall kinetic process was essentially concentration independent, indicating that the rearrangement process is mainly accomplished via noncooperative chain rearrangement and chain exchange processes. This mechanism is in contrast to the kinetic pathways for block copolymer micelle formation which follows a nucleation & growth mechanism without cluster formation [3].

Literature references:

[1] Lund, R., Willner, L., & Richter, D. (2013). Kinetics of Block Copolymer Micelles Studied by Small-Angle Scattering Methods. Vol. 259, pp. 51–158

[2] Voets, I. K., de Keizer, A., & Cohen Stuart, M. A. (2009). Complex coacervate core micelles. Advances in Colloid and Interface Science, 147-148, 300–318.

[3] Lund, R., Willner, L., Monkenbusch, M., Panine, P., Narayanan, T., Colmenero, J., & Richter, D. (2009). Structural Observation and Kinetic Pathway in the Formation of Polymeric Micelles. Physical Review Letters, 102(18), 188301–4.

O1.2

A combined SAXS and SANS study of interactions between bile salt and a triblock copolymer.

S. Bayati[1]*, L. Galantini*[2]*, K. D. Knudsen* [3]**, K. Schillén* [1]

[1]*Department of Chemistry, Lund University, SE-221 00 Lund, Sweden,*
[2]*Department of Chemistry, University of Rome, 00185 Rome, Italy,*
[3]*Institute for Energy Technology, 2027 Kjeller, Norway*

Small angle X-ray and neutron scattering techniques can be very useful for extracting information about structural parameters as well as interparticle interactions in solutions of polymers and polymer complexes. We have investigated mixed complexes formed between micelles of the nonionic amphiphilic PEO-PPO-PEO copolymer and the anionic bile salt (NaGDC) in aqueous solution. The aim of the work was to gain understanding of how thermoresponsive PEO-PPO-PEO block copolymers interact with bile salts, in order to make predictions concerning their potential as a new class of bile salt sequestrants in the treatment of bile-salt related diseases. It was found that the NaGDC molecules are preferentially associated to the PEO corona of the P123 micelle and - due to their amphiphilic nature - are located close to the core/corona interface. Because of this association the micelles become charged, causing their interparticle repulsions in solution to increase. Modelling of the SAXS and SANS experimental data made it possible to extract information on changes in both the core and total radius, as well as on the (de)hydration of the "P123 micelle-NaGDC" complexes, demonstrating the usefulness of small angle scattering techniques for this and similar types of polymer systems.

References:

4. Bayati, S.; Galantini, L.; Knudsen, K. D.; Schillén, K. Effects of Bile Salt Sodium Glycodeoxycholate on the Self-Assembly of PEO-PPO-PEO Triblock Copolymer P123 in Aqueous Solution. *Langmuir* 31, 13519-13527, **2015**
5. Bayati, S.; Galantini, L.; Knudsen, K. D.; Schillén, K. Complexes of PEO-PPO-PEO Triblock Copolymer P123 and the Bile Salt Sodium Glycodeoxycholate in Aqueous Solution: A Small Angle X-Ray and Neutron Scattering Investigation. *Colloids and Surfaces A* 504, 426-436, **2016**

O1.3

In-Situ X-ray tomography for investigation of void growth in mineral-filled PVC using a conventional X-ray source: A plausibility study.

Sindre Olufsen[1], Arild Holm Clausen[1], Odd Sture Hopperstad[1]*

[1]Structural Impact Laboratory (SIMLab), Department of Structural Engineering, NTNU, Norwegian University of Science and Technology,NO-7491 Trondheim, Norway

*sindre.n.olufsen@ntnu.no

Void nucleation and growth have been identified for a range of polymers subjected to deformation. The presence of voids is linked to a pressure sensitive material behaviour, non-isochoric deformation and failure. *In-situ* measurements yielding spatial void volume fraction distributions during a deformation process have been achieved [1,2], but rely on the use of synchrotron radiation facilities. We propose a method for measuring spatial void volume fraction distributions during tensile testing, employing a conventional lab-grade X-ray CT setup. The method exploits the axisymmetric nature of the tensile specimens, allowing for *in-situ* measurements with lab-scale equipment. The capabilities of the method are demonstrated by investigating a $CaCO_3$ filled PVC, previously found to sustain substantial dilation caused by void nucleation and growth before failure [3].

References:

1. P. A. Poulet, G. Hochstetter, A. King, H. Proudhon, S. Joannès, L. Laiarinandrasana, *Observations by in-situ X-ray synchrotron computed tomography of the microstructural evolution of semi-crystalline Polyamide 11 during deformation*, Polymer Testing 56 (**2016**) 245–260.
2. N. Brusselle-Dupend, E. Rosenberg, J. Adrien, *Characterization of cavitation development while tensile testing PVF2 using 3D X-ray microtomography*, Materials Science and Engineering A 530 (1) (2011)36–50
3. S. Olufsen, A. H. Clausen, O. S. Hopperstad, *Influence of strain rate and triaxiality on stress-strain behaviour and dilation of mineral-filled PVC*, Polymer Testing 75 (**2019**) 350-357

O1.4

Swelling of Individual Cellulose Nano-Fibrils: Does Crystallinity affect Swellability?

Vegar Ottesen[1], Per Tomas Larsson[2], Kristin Syverud[1,3]

[1]Norwegian University of Science and Technology, Dept. of Chemical Engineering
[2]RISE Bioeconomy
[3]RISE PFI

* vegar.ottesen@ntnu.no

Cellulose nanofibrils were prepared from cotton linter with two degrees of crystallinity (DoC) by high pressure homogenization. The fibrils had high (65 ± 2 %) or low (44 ± 2 %) DoC. By atomic force microscopy (AFM) high resolution micrographs can be recorded of these fibrils in air or submerged in liquid. By imaging the same fibrils in air and de-ionized water high precision measurements of swelling of individual nanofibrils were recorded and swelling was assessed (See Figure). We found no statistically significant ($p=0.3143$) difference between swelling of high and low DoC fibrils. Loess regression of swelling versus dry diameter revealed no clear correlation between the size of the nanofibril and the swelling of same.

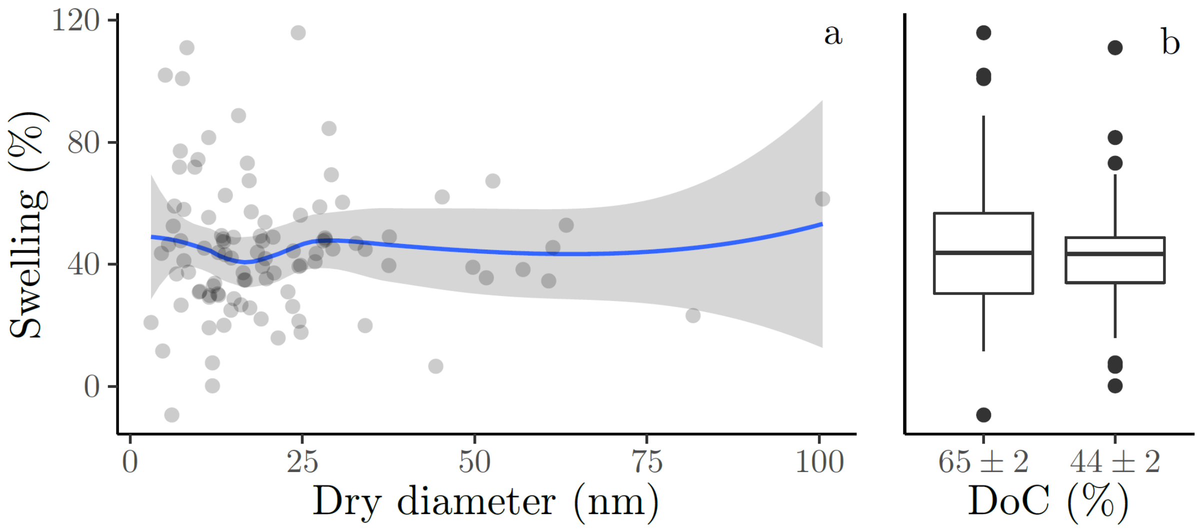


Figure 1 Loess regression of dry diameter versus swelling of fibrils (a) and Tukey box-plot (b). Both plots have the same y-axis. Each data point in a shown for clarity. Ribbon in a shows 95 % confidence interval, as reported by loess (in R). DoC in b refers to Degree of Crystallinity, as measured by ^{13}C NMR

O1.5

Probing the Structure of Antimicrobial Peptides and their Interaction with Lipid Membranes using Small-angle X-ray and Neutron Reflectivity Methods.

Josefine Eilsø Nielsen[1*], *Victoria Ariel Bjørnestad*[1], *Abdullah Lone*[2], *Håvard Jenssen*[2], *Tania Kjellerup Lind,*[3] *Marité Cardenas*[3] *and Reidar Lund*[1]

[1]*Department of Chemistry, University of Oslo, Norway.*
[2]*Department of Science and Environment, Roskilde University, Denmark.*
[3]*Department of Biomedical Sciences and Bio Films, Malmö University, Malmö, Sweden.*

* j.e.nielsen@kjemi.uio.no

Antibiotic resistance is one of the biggest threats to global health, according to WHO. AMPs seem to be able to evade much of the bacterial resistance mechanisms and are therefore promising candidates for future antibiotics. Instead of blocking specific biochemical pathways as most available antibiotic agents today, most AMPs act physically on the cytoplasmic membrane itself. [1-2] The precise microscopic mechanism for the disturbance of the membrane has not fully been proven but several theories has been suggested including membrane deformation and pore formation. Here we have used state of the art neutron and x-ray scattering techniques to investigate the microscopic mechanism of action of AMPs with model bacterial membranes. SAXS measurements on a model peptide, Indolicidin together with lipid vesicles have shown that Indolicidin interacts with the membrane. Based on analysis of the results we can see that the peptide does not seem to affect the structure of the bilayer significantly but situates in the interface between the lipid head group and the tail in the outer leaflet in the bilayer.[3] This causes and slight alteration in the lipid chain packing as seen by calorimetry but does not lead to any significant membrane thinning or similar. This is further confirmed by Neutron Reflectivity and Atomic Force Microscopy on planar supported bilayers.[4] Combining these techniques has given us a new important insight into how the peptide interact with the bilayer. Rather than supporting any specific structural model, we speculate that the mechanism is compatible with the disordered model proposed by Wimley.[5]

Literature references:

[1] Hancock, R. E.; Rozek, A., *FEMS microbiology letters* **2002,** *206* (2), 143-149.
[2] Jenssen, H.; Hamill, P.; Hancock, R. E., *Clinical microbiology reviews* **2006,** *19* (3), 491-511.
[3] Nielsen, J. E.; Bjørnestad, V. A.; Lund, R., *Soft Matter,* **2018**, 14, 8750-8763.
[4] Nielsen, J. E.; Bjørnestad, V. A.; Lone, A.; Lind, T. K.; Gerelli, Y.; Hansen, P. R.; Jenssen, H.; Cardenas, M; Lund, R., *(BBA) – Biomembranes*, **2019** (accepted for publication)
[5] Wimley, W. C., *ACS chemical biology,* **2010,** *5* (10), 905-917.

O1.6

Characterization and Classification of Polymers and Polymer Mixtures by Means of DSC and an Advanced Software Database.

Ekkehard Füglein

NETZSCH-Gerätebau GmbH, Wittelsbacherstraße 42, 95100 Selb, Germany

ekkehard.fueglein@netzsch.com

Differential Scanning Calorimetry (DSC) is a very commonly used analytical technique to quickly characterize polymers, blends and mixtures. Inspection of incoming goods, production and quality control as well as research and material development are typical application areas for DSC. To cope with the challenge of automated routine analysis procedures on one hand and highest flexibility in usability and evaluation on the other, an advanced software was introduced recently [1, 2].

Comparing analysis results with reference data is an established procedure in research and materials characterization. Spectroscopic techniques such as infrared spectroscopy (FT-IR) or mass spectrometry (MS) allow those comparisons via the software for decades. Numerous spectra libraries are available to compare measurement results with reference data. With the new evaluation tool of the NETZSCH *Proteus*® software, this capability is now also available for thermoanalytical data. Along with reference data, this thermoanalytical library allows for visual comparison of measured data with reference data. Recent works could demonstrate the use of this library functionality for different polymers, polymer mixtures and even for recycled polymers [3, 4]. The measurement results obtained with DSC, of course, strongly depend on the compatibility of the mixture. In case the single components do not form mixed phases, mixtures will present DSC signals of each single component according to its quantity. This work presents examples for the characterization of polymer samples and mixtures by means of DSC results and subsequent comparison of these results with library data.

References:

1. Schindler, A.; Strasser, C.; Schmoelzer, S.; Bodek, M. Senuita, R., Wang, X. Database-supported thermal analysis involving automatic evaluation, identification and classification of measurement curves. *J Therm Anal Calorim*, **2016**, *123*, 2405 (doi.org/10.1007/s10973-015-5026-x)
2. Schindler, A.; Doeth, M.; Gezgin, S.; Menzel, J. Schmoelzer, S. Identification of polymers by means of DSC, TG, STA and computer-assisted database search. *J Therm Anal Calorim*, **2017**, *129*, 833 (DOI: 10.1007/s10973-017-6208-5)
3. Fueglein, E.; Kaisersberger, E. About the development of databases in thermal analysis. *J Therm Anal Calorim*, **2015,** *120***,** 23 (DOI: 10.1007/s10973-014-4381-3)
4. Fueglein, E. About the use of IDENTIFY – a thermoanalytical database – for characterization and classification of recycled polyamides. *J Therm Anal Calorim*, **2015**, *121*, 1353 (DOI: 10.1007/s10973-015-4583-3)

O1.7

Using Elastic Net Regularization for the Identification and Quantification of Raman Spectra in Mechanical Polymer Recycling.

Stephanie, Haider[1,3]; Lukas, Kammerer[2], Michael, Aigner[1]; Sabine, Hild[3], Gabriel, Kronberger[2]

[1]*EREMA Engineering Recycling Maschinen und Anlagen Ges.m.b.H*
[2]*FH Oberösterreich – HEAL – Heuristic and Evolutionary Algorithms Laboratory*
[3]*Johannes Kepler University – Institute for Polymer Science*

In polymer processing (sorting, extrusion, injection molding) Raman spectroscopy is becoming more and more popular for material identification, quantification and quality detection. In fulfilling EU-requirements concering increasing recycling rates, the technology is gaining importantance in mechanical recycling. Although the waste streams are already sorted well in advance a 100% pure material stream cannot be guaranteed. Therefore it is necessary to obtain information about the composition of the material stream. For this purpose a Raman Spectrometer was added to the preconditioning unit (PCU) of an EREMA extrusion line.

In state of the art detection algorithms a multivariate approach is often used for the identification and quantification of Raman spectra. This method amends for a calibration for every possible mixture. As this is not possible for recycling materials a generalized model must be used. The algorithm developed can be divided in three steps. At first the inline recorded spectra must be pre-processed using baseline fit, a normalization and an interpolation for achieving spectrometer independent conditions. In a second step the possible materials are selected from a library depending on peak positions. Peak shifts can occur due to temperature differences in the process and must be considered for material selection [1]. The last step is the quantification of the acquired spectra. The pre-selected library spectrum of each material group is used as covariate and the relative amount as unknown parameter. A regularized linear regression model is used to estimate the unknown weights [2].

In dependence of the result of the material characterization, adjustments on the process (temperatures, screw speeds, additivation) can be performed. At the end of the day the recycler knows the composition of the recycled material and benefits from that information in further processing steps.

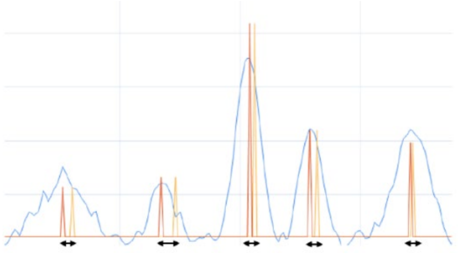


Figure 2: example of selection criteria for material identification.

References:

1. Haider, S., Aigner, M., Hild, S. Detection of changes in Raman spectra of thermoplastic polymers caused by temperature. *ICORS*. Jeju, Korea, August 26-31, **2018**.
2. Hastie, T., Tibshirani, R., Friedman; J. The Elements of Statistical Learning: Data Mining, Inference, and Prediction. *Springer*, California, **2009**, 661-668.

O1.8

Method of Making Polymer Surface Modifications Through the use of Screening Platforms.

Christian Andersen[1], *Niels Jørgen Madsen*[2], *Anders E. Daugaard*[1].

[1] *Danish Polymer Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, 2800 Kongens Lyngby, Denmark*
[2]*Coloplast A/S, Holtedam 1-3, 3050 Humlebæk.*

Chrand@kt.dtu.dk

Surface modifications have been used extensively to expand the applicability of various polymer materials. This includes everything from chemical resistance in tubing and pipelines to biocompatibility in cell scaffolds. The development of novel surface materials is, however, a tedious process requiring testing of almost endless numbers of different formulations in order to obtain optimized properties to fit a desired application. A way to accelerate development is by the use of screening platforms. Many existing solutions utilize automated systems, conducting polymerization on glass slides under inert atmosphere. These methods are both fast and efficient but the procedure is not directly translatable to industrial methods were inert conditions are difficult to achieve and the small volume used makes the process run exclusively in bulk[1,2]. The method and platform presented here is able to run UV-initiated free radical polymerization directly on a flexible polyurethane substrate under normal atmosphere while also allowing for testing of the influence of solvents and monomer concentrations.

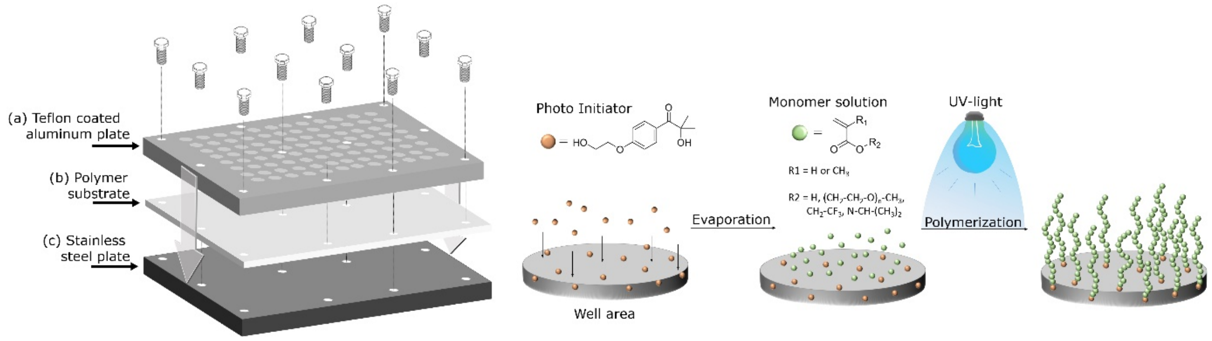


Figure 1: Schematic representation of screening platform (left) and grafting procedure (right).

References:

1. Hook AL, Williams PM, Alexander MR, Scurr DJ. Multivariate ToF-SIMS image analysis of polymer microarrays and protein adsorption. *Biointerphases*. **2015**; 10 (1),19005.

2. Celiz AD, Smith JGW, Patel AK, et al. Chemically diverse polymer microarrays and high throughput surface characterisation: A method for discovery of materials for stem cell culture. *Biomater Sci*. **2014**; 2(11), 1604-1611.

O1.9

Characterization of modified elastomer surfaces by wetting.

C. W. Karl[1*], A. Lang[2], M. Klüppel[2], U. Giese[2]

[1*]SINTEF Industry, Forskningsveien 1, 0373 Oslo
[2]Deutsches Institut für Kautschuktechnologie e. V. (DIK), Eupener Str. 33, 30519 Hannover

[*]Christian.Karl@sintef.no

Surface and interface phenomena play a very important role in many technical processes, including bonding and coating processes, surface printing, friction and wear behavior. A well-known natural surface phenomenon is the lotus effect, which can be attributed to the surface microstructure and hydrophobic properties of epicuticular waxes [1]. The design and surface structures are an important factor in the development of dirt-repellent surfaces. Applications of (super)hydrophobic surfaces are self-cleaning roofing tiles, textile surfaces, coatings [2], hoses, seals and profiles [3], as well as icephobic coatings [4]. Previous studies have shown that contact angle hysteresis values, which represent a measure of the roughness and chemical heterogeneity of a surface, correlate well with roughness factors for different smooth and rough coated elastomers [5-7]. Roughness parameters such as R_a (arithmetical mean roughness) are mainly used for the quantitative characterization of the roughness of smooth surfaces (1-10 µm) [8-9]. To address this issue, contact angle hysteresis values of surface modified elastomers were compared with roughness parameters obtained from white light interferometry measurements. Future work provides the investigation of rough elastomer and polymer surfaces (R_a >10 µm) in order to compare surface descriptors (cut-off lengths and fractal dimensions) [10] with hysteresis values from contact angle measurements (modified Wilhelmy balance technique). Furthermore the characterization of samples with varied roughness and chemical heterogeneity is of particular interest to get a better understanding of wetting processes of elastomer surfaces.

References:

1. M. Yamamoto, N. Nishikawa, H. Mayama, Y. Nonomura, S. Yokojima, S. Nakamura, K. Uchida. *Langmuir*, **2015**, *26*, 7355
2. J. Drelich, A. Marmur. *Surface Innovations*, **2013**, *2*, 211
3. A. Wildberger, H. Geisler, R. H. Schuster. *KGK rubberpoint*, **2007**, *60*, 24
4. K. Golovin, S. P. R. Kobaku, D. Hyun Lee, E. T. DiLoreto, J. M. Mabry, A. Tuteja. *Science Advances,* **2016**, *2*, 3
5. C. W. Karl, M. Klüppel. *Chem. Listy*, **2011**, *105*, 233-CL-12
6. C. W. Karl, A. Lang, A. Stoll, A. Weiße, M. Stoll, M. Klüppel. *KGK rubberpoint*, **2012**, *65/4*, 44
7. C. W. Karl, W. Rahimi, A. Lang, U. Giese, M. Klüppel, H. Geisler. *KGK rubberpoint*, **2018**, *09*, 19
8. S. Palzer, C. Hiebl, K. Sommer, H. Lechner. *Chemie Ing. Technik*, **2001**, *73*, 1032
9. L. Busse, K. Peter, C. W. Karl, H. Geisler, M. Klüppel. *Wear,* **2011**, *271*, 1066
10. Y. Nonomura, E. Seino, S. Abe, H. Mayama. *J. Oleo Sci*., **2013**, *8*, 587

O2.1

Molecular engineering of CNF/PCL interface for high toughness bio-nanocomposites.

*Tahani Kaldéus[1], Lars Berglund[2], Eva Malmström[2], and Giada Lo Re[1,3]**

KTH Royal Institute of Technology, [1]Fibre and Polymer Technology, [2]WWSC,
[3]Chalmers University of Technology, Department of Industrial and Materials Science

* giadal@chalmers.se

The potential of a "bottom-up" design of a molecularly engineered water-borne reactive compatibilizer for the tuning of the polycaprolactone (PCL)/cellulose nanofibril (CNF) interface has been highlighted in this work, with the aim to tailor the mechanical properties of the corresponding nanocomposite. This design allowed for self-assembly in aqueous medium into nanoparticles of the synthesized amphiphilic random copolymer with hydrophilic quaternized ammonium and hydrophobic reactive groups (methacrylate moieties). The reactive compatibilizer adsorbed onto CNF in water dispersion forming a uniform core-shell nanohybrid due to electrostatic interactions as confirmed by AFM. The mixture of polymer matrix and the core-shell nanohybrid in water dispersion allowed for a wet feeding approach with an efficient evaporation of the water during the melt compounding, [1, 2] as schematically shown in Figure 1. A remarkable improvement of the mechanical properties is demonstrated. The Young's modulus and toughness of the polycaprolactone containing 10 wt.% CNF increased 80%, and an impressive 1000%, respectively, when a low amount of reactive compatibilizer (< 5 wt%) was used. Our results contribute to a deeper understanding of the interfacial design for future nanocellulose-based composite materials.

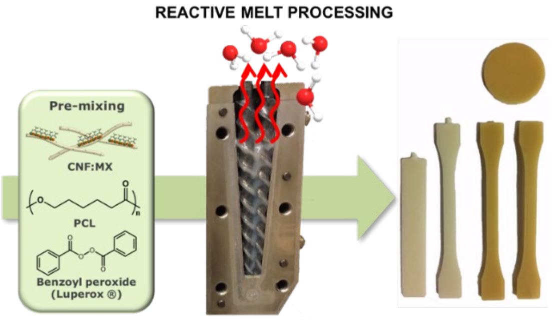


Figure 1. Schematic overview of the reactive wet feeding melt processing of the bio-nanocomposites. The PCL radicals are formed by hydrogen abstraction by the peroxide (Luperox®).

References:

[1] G. Lo Re, et al. Poly(ϵ-caprolactone) Biocomposites Based on Acetylated Cellulose Fibers and Wet Compounding for Improved Mechanical Performance, ACS Sustain. Chem. Eng. 6 (2018) 6753–6760.
[2] G. Lo Re, et al. Improved Cellulose Nanofibril Dispersion in Melt-Processed Polycaprolactone Nanocomposites by a Latex-Mediated Interphase and Wet Feeding as LDPE Alternative, ACS Appl. Nano Mater. 1 (2018) 2669–2677.

O2.2

Thermal and electrical properties of graphene polypropylene composites.

Karolina Gaska[1*], *Roland Kádár*[1].

[1]*Chalmers University of Technology, Department of Industrial and Materials Science,*
SE-412 96 Göteborg, Sweden

* gaskak@chalmers.se

Graphene having superb electrical conductivity, high thermal conductivity as well as high aspect ratio has attracted significant scientific and commercial attention as a potential conductive filler in polymer nanocomposites [1]. Adding graphene into polymer matrix leads to enhanced performance and therefore wide range of potential industrial applications. As an example, electromagnetic shielding, anti-static components, gas barrier, thermally conductive layers [2].

In this research we have used melt-mixing which is one of the most economically advantageous method of dispersing a filler in a thermoplastic matrix and is frequently used in a large-scale industrial environment. A proper dispersion and uniform distribution have a huge impact on the macroscopic properties of polymer nanocomposites. In this work, the influence of graphene on electrical and thermal properties of polypropylene based nanocomposites were investigated. The used graphene leads to achieving very low percolation threshold especially in comparison with commercially available graphene nanoplatelets where significantly higher filler content is needed [3]. Thermal conductivity increases significantly with the increasing filler content. The influence of graphene on polypropylene nucleation has been also investigated.

References:

1. Kim, H.; Abdala A.; Macosko, C, Graphene Polymer Nanocomposites. *Macromolecules*, **2010**, *43* (16), 6515– 6530
2. Das, T.; Prusty, S.; Graphene-Based Polymer Composites and Their Applications. *Polymer Plastics Technology and Engineering*, **2013**, 52(4), 319-331
3. Gaska, K.; Xu, X.; Gubanski, S.; Kádár, R.; Electrical, mechanical, and thermal properties of LDPE graphene nanoplatelets composites produced by means of melt extrusion process. *Polymers*, **2017**, 9(1), 1-12,

O2.3

Recycled Poly (Ethylene Terephthalate) Nanocomposites: Rheology, Thermal and Mechanical Properties.

Ravindra Reddy Chowreddy[1]* *and Katrin Nord-Varhaug*[1]

[1]*Norner Research AS, Asdalstrand 291, 3962 Stathelle, Norway*
* ravindra.chowreddy@norner.no

Polymer nanocomposites (PNCs) containing nano-fillers have attracted great interest from both academia and industry due to their unique characteristics. Incorporation of small quantities of nano-fillers into polymeric matrices is known to improve the mechanical, electrical, barrier and thermal properties [1–3]. In the present study, the effect of adding nano-fillers such as multi-wall carbon nanotubes and clay to recycled poly (ethylene terephthalate) (PET) has been investigated. Although incorporation of nano-fillers, especially, CNTs has been extensively investigated for a wide variety of polymers, there are not many studies with recycled PET. The nanocomposites were prepared through melt compounding via masterbatch dilution method and the masterbatch and the nanocomposites were processed in a twin-screw extruder. It is challenging to obtain a homogeneous distribution of nano-fillers in nanocomposites, therefore it has been important to characterize the morphology of the PET-nanocomposites. The rheology as well as thermal and mechanical properties were investigated on the PET-nanocomposites.

Incorporation of nano-fillers into recycled PET increases the viscosity significantly. Significant increase in viscosity was achieved at reasonably lower concentrations of CNTs compared to the clay. The incorporated nano-fillers in the recycled PET increase the degree of crystallinity and crystallization temperature through heterogeneous nucleation. The tensile properties of recycled PET increased with incorporation of nano-fillers. The property enhancement in PET-nanocomposites was observed at low concentrations of CNTs. Whereas in case of PET-nanocomposites containing clay, higher amounts of clay were needed to achieve similar property enhancement as with CNT. Morphological investigation indicated homogeneous dispersion of the nano-fillers.

References:

1. Okada, A.; Usuki, A.; Twenty years of polymer–clay nanocomposites. *Macromolecular Materials Engineering,* **2006,** 291(12), 1449–1476
2. Paul, D.; Robeson, L.M.; Polymer nanotechnology: nanocomposites. *Polymer,* **2008**, 49(15), 3187–3204
3. Kim, H.; Abdala, A.A.; Macosko, C.W.; Graphene/polymer nanocomposites. *Macromolecules,* **2010**, 43(16), 6515–6530

O2.4

Nonlinear rheological signatures and percolation in nano-filled polymers.

*Karolina Gaska, Roland Kádár**

Chalmers University of Technology, Department of Industrial and Materials Science,
Division of Engineering Materials, SE-412 96 Gothenburg, Sweden

* roland.kadar@chalmers.se

Filled polymer systems remain essential for improving and/or inducing new functional properties otherwise unavailable in plastics. Of particular importance are conductive anisotropic high aspect ratio fillers. Particularly, from rheological point of view, the flow-field - filler interactions in the presence of small and large deformation / deformation rates is crucial for understanding the tailoring of filler concentration, dispersion and morphology to achieve enhanced nanocomposite properties. Here, we focus on nonlinear rheological material properties in relation to the percolation behaviour in nanocomposites. The types of nanofillers investigated in this framework include carbon nanotubes, graphene / graphite-nanoplatelets, hybrid compositions, boron nitride, special hierarchical structures etc. in a variety of polymers. Some of the compositions stand out in terms of dispersion and consequently percolation, whereas in other cases the fillers are difficult to disperse into the polymers. The comparison is not systematic, rather common nonlinear features of nanocomposites above percolation are highlighted. The nonlinear rheological analysis was performed in oscillatory shear experiments in the framework of Fourier-transform Rheology and Tschebyshev polynomial stress decomposition. Complementary, comprehensive complementary tests were performed including electrical, thermal, mechanical and microstructural analysis. Overall, the rheological percolation thresholds are determined with superior sensitivity using nonlinear material parameters, based on the relative increase on the magnitude of nonlinearities recorded. However, by carefully emphasising the effect of strain-rate in strain sweep experiments distinct nonlinear signatures could be recorded at and above percolation. The distinct signatures are captured both in the scaling behavior of the third relative higher harmonic from Fourier spectra as well as by the third relative viscous Tschebyshev coefficients.

References:

1. Lim, H.T.; Ahn, K.H.; Hong, J.S.; Hyun, K. Nonlinear viscoelasticity of polymer nanocomposites under large824 amplitude oscillatory shear flow. Journal of Rheology*,* **2013**, 57, 767–789
2. Kádár, R., Abbasi, M., Figuli, R., Rigdahl, M., Wilhelm M. Linear and nonlinear rheology combined with dielectric spectroscopy of hybrid polymer nanocomposites for semiconductive applications. Nanomaterials*,* **2017**, *7*, 2
3. Gaska, K.; Kádár, R.; Rybak, A.; Siwek, A.; Gubanski, S.; Gas barrier, thermal, mechanical and rheological properties of highly aligned graphene-LDPE nanocomposites. Polymers*,* **2017**, 9 (7), 294

O2.5

Composites with surface-grafted cellulose nanocrystals (CNC).

Lilian Forsgren[1], *Karin Sahlin-Sjövold*[2,3], *Abhijit Venkatesh*[1], *Johannes Thunberg*[1], *Roland Kadar*[1,3], *Antal Boldizar*[1,3]*, *Gunnar Westman*[2,3], *Mikael Rigdahl*[1,3]

[1] *Department of Industrial and Materials Science, Chalmers University of Technology, 412 96 Gothenburg, Sweden,*
[2] *Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 412 96 Gothenburg, Sweden*
[3] *Wallenberg Wood Science Center, Chalmers University of Technology, 412 96 Gothenburg, Sweden,*

*antal.boldizar@chalmers.se

To construct strong, lightweight materials with reduced fossil content, Cellulose and in particular cellulose nanocrystals (CNC) are potentially interesting as reinforcements in polymer composites. Cellulose is available in large volumes, renewable, biodegradable, lightweight, have good specific mechanical properties and low abrasion towards processing equipment, which indicate cellulose or CNC to be an interesting alternative to fossil based reinforcing materials.

But using CNC as a reinforcing element in a polymer matrix might imply challenges as: limited adhesion between the hydrophilic fibres and the in most cases hydrophobic polymer matrix, moisture uptake, poor dispersion of the fibres in the matrix and low thermal stability of the cellulose causing degradation at normal processing temperatures used for thermoplastic forming. To potentially reducing these challenges, a surface treatment of the cellulosic elements were performed in this study.

Hydroxyazetidinium salts were used to surface-modify cellulose nanocrystals (CNC) by grafting the salts onto the sulphate ester groups on the CNC surfaces. Three different surface modifications of CNC have been used at three different concentration levels; 0.1%, 1% and 10 weight-% CNC in an EAA (copolymer of ethylene and acrylic acid) matrix. An aqueous dispersion of CNC was mixed with an EAA dispersion and dried into flakes before compression moulded to produce a composite. A strong positive effect on the stiffness of the composite could be seen, with an increase in modulus from around 300 MPa to up to more than 900 MPa for samples with 10% untreated CNC. The results of the mechanical testing are discussed in terms of interactions between the grafted units and the matrix material and between the grafted groups themselves. The thermal stability was improved by 100 °C for the composites reinforced with surface-treated CNC compared to the composite with unmodified CNC.

O2.6

Nanodiamond reinforced polyelectrolyte films.

Tony Tiainen, Marina Lobanova, Erno Karjalainen, Sami Hietala

Department of Chemistry, University of Helsinki, PB 55, FIN-00014 HU

* Sami.Hietala@helsinki.fi

Nanodiamonds[1] (ND) are 4-5 nm sized diamond particles possessing many beneficial properties such as high thermal conductivity, hardness, modifiable surface chemistry and biocompatibility. These make them attractive materials for a variety applications for example in biomaterials[2] and nanocomposites[3].

In this work ND-polymer nanocomposite polyelectrolyte films were prepared by photopolymerization of acrylic monomers. Their mechanical and thermal properties were adjusted by varying the ratios of monomers ((butyl acrylate (BA) and dimethylaminoethyl methacrylate (DMAEMA)), ND content and by use of a compatibilizing block copolymer to disperse the NDs. Incorporation of NDs enhances the mechanical properties of the films especially when copolymer was included, Figure 1.

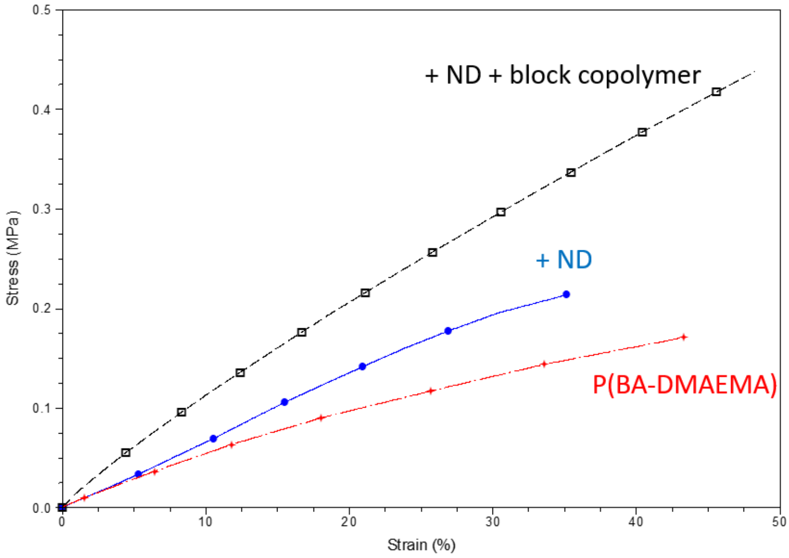


Figure 1. Stress-strain curves of P(BA-DMAEMA) films.

References:

1. Mochalin, V N.; Shenderova, O.; Ho, D.; Gogotsi, Y. The Properties and Applications of Nanodiamonds. Nature Nanotechnology, **2012**, *7*, 11–23.
2. Neburkova, J.; Vavra, J.; Cigler, P. Coating nanodiamonds with biocompatible shells for applications in biology and medicine. Current Opinion in Solid State and Materials Science **(2017)** *21*, 43–53.
3. Zhang, Y.; Rhee, K. Y.; Hui, D.; Park, S.-J. A critical review of nanodiamond based nanocomposites: Synthesis, properties and applications. Composites Part B: Engineering **(2018)**, *143*, 19–27.

O2.7

High-strength, high toughness polylactic acid-based nanocomposites reinforced with well-dispersed cellulose nanocrystals.

Shiyu Geng[1]*,Daniela Wloch*[1]*, Natalia Herrera*[1]*, Kristiina Oksman*[1,2]*

[1] *Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Luleå SE-971 87, Sweden*
[2] *Fibre and Particle Engineering, University of Oulu, Oulu FI-90014, Finland*

* E-mail address: kristiina.oksman@ltu.se

Bio-based nanocomposites have recently recieved lots of attention due to the environmental issues caused by fossil-based materials. Burgeoning research activites have been reported and are on going in the field of biodegradable polymers reinforced by nanocellulose, a material owning abundant resources, high integrity and biodegradability.[1] However, the reinforcing efficiency of nanocellulose in some biopolymer matrices, such as poly(latic acid) (PLA), is limited by compatibility and dispersion issues, resulting in unsatisfied mechanical performance of the nanocomposites.[2] Moreover, PLA has its own drawbacks, especially high brittleness, posing obstacles for applications. Hence, in this present work, the dispersion of cellulose nanocrystals (CNCs) in PLA matrix is improved by *in-situ* polymerization, and interestingly, solid-state drawing is found to significantly enhance the unidirectional mechanical properties of the PLA/CNC nanocomposites not only in strength but also in elongation at break, resulting in much higher toughness compared to the undrawn samples. The highly aligned structure in the drawn nanocomposites are confirmed by polarized optical microscopy and scanning electron microscopy. The mechanical properties of the aligned nanocomposites are investigated by tensile testing. Moreover, the aligned nanocomposite containing 0.2 wt% *in-situ* dispersed CNCs outperforms the one reinforced by the same amount of native CNCs in ultimate strength and elongation at break by 18.6% and 13.4%, respectively, which is attributed to the better dispersion of the CNCs achieved by the *in-situ* emulsion polymerization process.

References:

1. Jonoobi, M.; Mathew, A. P.; Oksman, K. Natural Resources and Residues for Production of Bionanomaterials. In *Handbook of Green Materials: 1 Bionanomaterials: separation processes, characterization and properties*; World Scientific: 2014; pp 19-33.
2. Lee, K.-Y.; Aitomäki, Y.; Berglund, L. A.; Oksman, K.; Bismarck, A. On the use of nanocellulose as reinforcement in polymer matrix composites. *Compos. Sci. Technol.* **2014,** *105*, 15-27.

O2.8

In-situ Formation of a Polyethylene-Polypropylene Copolymer through Reactive Compounding.

Yingwei Ouyang[1]*, Massimiliano Mauri*[1]*, Ida Östergren*[1]*, Thomas Gkourmpis*[2]*, Per-Ola Hagstrand*[2]*,*
Oscar Prieto[2] *and Christian Müller*[1]

[1]*Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 41296 Göteborg, Sweden*
[2]*Innovation & Technology, Borealis AB, 44486 Stenungsund, Sweden*

* christian.müller@chalmers.se

Polyethylene (PE) is the most widely used plastic. For more demanding applications such as hot water pipes and power cables, crosslinking is often required to improve the material's thermomechanical properties. Polyethylene crosslinking usually involves peroxides, resulting in the formation of unwanted by-products which compromises the cleanliness of the material. It is therefore of interest to develop other means of improving the thermomechanical properties of polyethylene. One way is to introduce a polymer with a higher melting point like polypropylene (PP). However, PE and PP are immiscible which is detrimental to the mechanical properties of PE/PP blends. We address this by blending small amounts of a compatibiliser into an LDPE matrix that form a PE-PP copolymer in-situ via reactive compounding. The resulting material exhibits thermomechanical properties superior to neat LDPE as a result of compatibilisation and the presence of PP crystals. Furthermore, the material is thermoplastic and recyclable, which is a further advantage over crosslinked polyethylene.

O3.1

Melt filtration of polymers.

Kerstin Steyrl[*1], Blanca Maria Lekube[1], Thomas Hofstätter[2], Christoph Burgstaller[1].*

[1]Transfercenter für Kunststofftechnik, Franz-Fritsch-Straße 11, 4600 Wels, Austria,
[2]EREMA Engineering Recycling Maschinen und Anlagen GmbH, Unterfeldstraße 3, 4052 Ansfelden, Austria

* kerstin.steyrl@tckt.at

Recycling plastics became more important over the last few years, due to plastic waste and CO_2 emission discussions. One of the major problems in plastics recycling are contaminations of the material, due to colour or unwanted materials, like labels or wooden splinters from pallets. Due to economic reasons and legislations at European level there is the necessity to recycle more materials, and also to produce recycylates with high quality to find applications for them. One the major problem is still the handling of the plastic waste. Pre-procssing steps like washing, milling, grinding and sorting steps improve the materials quality, but there are still at least some contaminants left. To further improve the materials quality, compounding or re-melting are common steps to remove contaminants, reduce the size to flakes and process plastics into granulate which is easier to converte than flakes (1) (2).

The aim of this work was to investigate the capabilities of using melt filtration to separate contaminants from plastics, in this case polypropylene (PP). As model substances, glass beads, wood particles, PET powder and zeolite were used. These materials were added as a dry-blend as much as 1% to the PP and then filtered by processing the mix with a Haake Rheocord 19 mm single-screw extruder at 210 °C and 20 rpm, equipped with a melt filtration setup where a filter with 100 µm nominal size was inserted. The mass temperature and the pressure before and after the sieve were recorded. After some extrusion time, the experiments were stopped and the machine cooled down to pull the screw, to see the remaining particles in the sieve and also in the screw.

We found, that it is possible to filter the different materials, but the efficiency depends on the size and elasticity of the contamination. While the filtration worked well to remove wood particles, the PET powder was less retained by the filter. Also, for efficient filtration the amount of contaminants as well as a possibility to renew the filter surface will be imperative for real life application.

---

1. **Kim Ragaert, Laurens Delva.** Mechanical and chemical recycling of solid plastic waste. *Waste Managament.* 2017.

2. European Commission - Press Release Database. *http://europa.eu/rapid/press-release_IP-18-3846_de.htm.* [Online] 22. Mai 2018. http://europa.eu/rapid/press-release_IP-18-3846_de.htm.

O4.1

Fibrillation of unbleached Kraft softwood pulp to lignin-containing microfibrillated cellulose.

Erfan Oliaei[1,2*], Pär Lindén[2], Qiong Wu[2], Fredrik Berthold[1], Lars Berglund[2], Tom Lindström[3]

[1]*RISE, Division of Bioeconomy, Stockholm, Sweden.*
[2]*Wallenberg Wood Science Center, Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden.*
[3]*KTH Royal Institute of Technology, Stockholm, Sweden.*

* Erfan.oliaei@rise.se

Microfibrillated cellulose (MFC) due to its unique features has attracted a lot of attention in recent years. Preparation of MFC is generally difficult, but it may be facilitated by preventing full delignification as the remaining lignin contains charge (Sarkanen and Ludwig 1971). However, in the native cell wall, lignin is intermixed with cellulose fibrils and cements them together (Sjöström 1993), thereby making fibrillation difficult. Therefore, we investigated the yield of fibrils as a function of pulp lignin content. Geometry of the resultant fibrils was studied, as well. A series of Kraft pulp fibres with falling Kappa numbers (an indication of the remaining lignin) was prepared from spruce wood. All the fibres were then mechanically beaten and homogenized. During homogenization, the fibres were mechanically disintegrated into lignin-containing microfibrillated cellulose (L-MFC) with different lignin content. Thereafter, the nano-sized fibrils' fraction of the L-MFC:s were carefully separated using a centrifugation method. The observed yields suggest that fibres with a moderate Kappa number (in a range of 30-70) give a higher fibrillation yield compared to the fibres with either very low or very high Kappa number. This observation correlates well with the trend of water retention value versus Kappa number of the fibres. The pulp fibres with a Kappa number of 65 (11 % lignin) combined high lignin content with ease of fibrillation. This "optimum" is due to a suitable combination of charge and lignin content. The L-MFC from these pulp fibres constituted a fraction of 40-60 % of nano-sized fibrils with widths in the range of 2.5-70 nm. L-MFC fibrils were heterogenous in width and showed some branching, especially at the ends. Thin L-MFC films were prepared and showed high optical transparency. Despite the fairly wide distribution in L-MFC size, the tensile strength and modulus were as high as 240 MPa, and 12.5 GPa, respectively. The present L-MFC:s are of technical and scientific interest, since there is no complexity in the production procedure.

References:

Sarkanen K. V., Ludwig C. H. Lignins: occurrence, formation, structure and reactions. John Wiley & Sons, New York, United States, **1971**.
Sjöström E. Wood polysaccharides. In: Wood chemistry. Academic Press, San Diego, United States, **1993**.

O4.2

Responsive hydrogels as recognition and transducing elements in biosensing: Spatiotemporal response of DNA-co-acrylamide hydrogels.

Eleonora Parelius Jonasova[1*], *Bjørn Torger Stokke*[1]

[1]*Norwegian University of Science and Technology (NTNU), Norway*

* eleonora.jonasova@ntnu.no

Responsive hydrogels alter their state due to changes in their environment. Additionally, this class of polymeric materials can also be biocompatible. Thus, they are good candidates for biomedical applications such as sensing, targeted delivery and scaffolding. In the present work, we focus on application of responsive hydrogels as recognition and transducing elements that, when combined with an appropriate read-out platform, can make up a biosensor. Particularly, incorporation of deoxyribonucleic acid (DNA) in responsive hydrogels offers many advantages due to the predictable nature of the DNA base pairing and consequently its predictable and controllable higher order structure and interaction with other (both DNA and non-DNA) molecules. The hydrogels that are the topic of this presentation consist of a covalently crosslinked polyacrylamide network with added partially hybridized DNA strands covalently linked to the network with one end, thus making up physical crosslinks. These additional crosslinks can be opened by an invading target strand in a process of competitive displacement. The resulting swelling of the hydrogel is monitored using an interferometric setup allowing determination of the optical length of the ~50 μm radius hemi-spherical hydrogels attached to optical fibers with a resolution of 2 nm. The swelling is the last step of a cascade of processes that take place within the gel following the addition of the target molecule. Starting from the migration of the target, through its binding and crosslink opening, ending with the swelling of the gel, the hydrogel serves to amplify the effect of processes on the molecular level, bringing them to the (microscopic) level of the hydrogel and allowing efficient readout and monitoring. The interplay of the underlying cascading processes influences the rate of hydrogel's swelling and is the focus of our work. Using a combination of interferometry and confocal laser scanning microscopy (CLSM), we explored the effect of toehold length on hydrogel swelling, target migration and binding, showing how longer toehold increases the binding rate as expected but slows down the target migration within the gel and thus provides only a moderate increase in the gel's overall swelling rate.

O4.3

Making good use of lignin – from a low-value biopolymer to energy storage devices.

Jiayuan Wei[1]*, Shiyu Geng*[1]*, Olli Pitkänen*[2]*, Topias Järvinen*[2]*, Krisztian Kordas*[2] *and Kristiina Oksman*[1,3,*]

[1]*Department of Engineering Sciences and Mathematics, Luleå University of Technology, Luleå, Sweden*
[2] *Microelectronics Research Group, University of Oulu, Oulu, Finland*
[3]*Fibre and Particle Engineering Research Group, University of Oulu, Finland*

* Kristiina.oksman@ltu.se

Lignin is the second most abundant natural biopolymer on Earth [1]. Despite its abundancy and easy accessibility, lignin has long been treated as a low-value byproduct during the pulping process, and value-added products derived from lignin have seldom been seen. Recently, researches about lignin-derived biocarbon are developing rapidly because of the dominant aromatic units endowing high carbon content in lignin, which propose promising applications such as carbon fiber reinforcement in composites and carbon electrodes in energy storage devices [2]. In this study, we are targeting on developing lignin-based carbon electrodes, *i.e.* lignin has been electrospun together with poly (vinyl alcohol) (PVA) into nanofiber networks which are then carbonized at different temperatures (800, 1000, 1200 and 1400 °C) to obtain lignin-based carbon nanofiber networks (LCNs). Effects of the carbonization temperature on the fiber structure, specific surface area, carbon structure, electrochemical performance, *etc.* are analyzed. Moreover, an all-solid-state flexible supercapacitor coded as FS1000 using the obtained LCN as electrodes and solid-state PVA/H_3PO_4 as electrolyte is assembled. The FS1000 shows brilliant mechanical properties and outstanding electrochemical performance which enable its potential use in wearable electronics. A device capacitance of up to 60.4 F g^{-1} is achieved, which outperforms most of the reported all-solid-state flexible supercapacitors. Meanwhile, FS1000 has an energy density of 2.7 Wh kg^{-1} while the power density reaches 500 W kg^{-1}, which meets the characteristics of typical carbon-based electrostatic double layer capacitors [3].

References:

1. Ian, D. and Kadla.J. F., *Handbook of Green Materials: Processing Technologies, Properties and Applications (in 4 volumes)*, in *Handbook of Green Materials*, Oksman K, Mathew A. P, Bismarck A, Rojas O, and Sain M,, Editors. 2014, World Scientific: Singapore.
2. Norgren, M. and H. Edlund, *Lignin: Recent advances and emerging applications.* Current Opinion in Colloid Interface Science, 2014. **19**(5): p. 409-416.
3. Lu, M., *Supercapacitors: materials, systems, and applications*. 2013: John Wiley & Sons.

O4.4

Lignin – a biopolymer from forestry biomass for biocomposites and 3D printing.

Mihaela Tanase Opedal[1], *Eduardo Espinosa Víctor*[2], *Johnny Kvakland Melbø*[1], *Alejandro Rodríguez Pascual*[2], *Gary Chinga-Carrasco*[1]*.

[1] *RISE PFI, Høgskoleringen 6b, 7491 Trondheim, Norway.*
[2] *Chemical Engineering Department, Faculty of Science, Universidad de Córdoba, Building Marie-Curie, Campus de Rabanales, 14014, Spain.*

*gary.chinga.carrasco@rise-pfi.no

Polymers from forestry biomass are promising for the sustainable development of new biobased materials [1]. As such, lignin and fibre-based biocomposites are plausible alternatives to petrochemical-based products. Biocomposites based on various biopolymers and reinforcing wood fibres have major potential for 3D printing operations, as we have recently demonstrated [2]. In this study, we have obtained lignin from Spruce biomass through a pulping process. The lignin was used for manufacturing biocomposite filaments containing 20 and 40% lignin, and using polylactic acid (PLA) as matrix material. Dogbones for mechanical testing were 3D printed by fused deposition modelling. The lignin and the corresponding biocomposites were characterized in detail, including TGA, DSC, FTIR and SEM. The results demonstrate the potential of lignin as a component in biocomposites materials, which are adequate for 3D printing operations.

Figure 1: Left) PLA/lignin pellets. Middle) Extrusion of PLA/lignin filament. Right) 3D printed dogbones of PLA and PLA/lignin biocomposites.

References:

1. Brodin, M.; Vallejos, M.; Tanase-Opedal, M.; Area, M.C.; Chinga-Carrasco, G. Lignocellulosics as sustainable resources for production of bioplastics – a review. *Journal of Cleaner Production,* **2017**, *162*, 646-664

2. Filgueira, D.M.; Holmen, S.; Melbø, J.K.; Moldes, D.; Echtermeyer, A.T.; Chinga-Carrasco, G. Enzymatic-assisted modification of TMP fibres for improving the interfacial adhesion with PLA for 3D printing. *ACS Sustainable Chem. Eng.*, **2017**, *5* (10), 9338–9346.

4.5

From the seaweed forest to multifunctional, bio-inspired foams.

Linn Berglund[1*], Lucas Gerardin[1], Boris Valldecabres[1], Kristiina Oksman[1,2,3]

[1]Division of Materials Science, Luleå University of Technology, 97187, Luleå, Sweden,
[2]Fibre and Particle Engineering, University of Oulu, Oulu, Finland
[3]Mechanical and Industrial Engineering, University of Toronto, ON, Canada

* linn.berglund@ltu.se

Laminaria digitata is a large brown seaweed, or algae that grows in underwater forests along the coasts. The lamella-structured seaweed grows in the upper sublittoral zone in rocky, wave-exposed localities and it is well adapted to this because of its flexibility. The cell wall structure is different to that of other plants, though cellulose is present; the major polysaccharide is alginate, forming a rigid yet flexible structure able to withstand the forces from the sea.[1]

Current commercial uses of brown seaweed is as a raw material source for alginate extraction.[1] Alginate is a biopolymer used in a variety of applications due to its favorable properties, such as biocompatibility, non-toxicity, and gel formation ability. Moreover, alginate-based biocomposites have been prepared to achieve multifunctional properties for uses such as, adsorbents for ionic dyes[2], antibacterial films[1], and wound healing materials[3], in form of hydrogel, film and foam structures.

The aim of the present study is to explore seaweed's inherently robust and flexible layered structure by maintaining its natural architecture for preparation of bio-inspired foams. The porosity of the foam could be adjusted by swelling of the purified natural hydrogel prior to freeze-drying, thus obtaining a porosity between 93-98%. The foams could furthermore be successfully crosslinked, thus kept their structural integrity in water, while swelling to a degree of about 160%. By exploiting, the natural architecture of the raw materials the processing can be carried out without extensive fractionation and still combine multifunctional properties.

Acknowledgement: Funding from EU Interreg Nord – European Regional Development Fund; and Bio4Energy– a strategic research environment appointed by the Swedish government.

References:

1. Mišurcová, L., (2012). Chemical Composition of Seaweeds. In Handbook of Marine Macroalgae: Biotechnology and Applied Phycology, 1st ed.; Se-Kwon, K., Ed.; JohnWiley & Sons, Ltd.: New Delhi, India, 181-182.
2. Sui, K., et al. (2012). Carbohydrate Polymers, 90, 399–406.
3. Naseri, N., et al. (2016). Biomacromolecules, 17, 3714-3723.

O4.6

Lignin-lipid capsules as renewable hybrid materials for sustainable material applications.

Mika H. Sipponen[1*], Tao Zou,[1] Alexander Henn[1], Monika Österberg[1*]

[1] *Department of Bioproducts and Biosystems, Aalto University, School of Chemical Engineering,*

* mika.sipponen@aalto.fi; monika.osterberg@aalto.fi

Lignin is an abundant and low-cost renewable resource for the production of colloidal lignin particles (CLPs) that exhibit antioxidant and UV-shielding properties. CLPs can be surface-modified by simple adsorption approaches,[1–3] and there are many promising applications such as controlled drug delivery[4] and functional nanocellulose composites.[5] Here we describe production and characterization of micro- and nanoscaled capsules by using lignin-based particles as building blocks. Shape-retaining Pickering emulsion microcapsules were prepared by assembling chitosan-coated CLPs on olive oil droplets followed by electrostatic cross-linking. In addition, hybrid nanocapsules were prepared by nanoprecipitation of lignin in the presence of fatty acids. The CLPs and capsules were characterized by an array of techniques such as DSC, AFM, TEM, and Laser Doppler Micro-Electrophoresis. Our results show that the stable and uniform micro- and nanocapsules are excellent candidates for controlled storage and release of active ingredients and latent heat. Prospective applications include controlled drug delivery and phase-change materials in thermal energy storage. Overall, our results show that the combination of the two natural materials – lignin and lipids – opens up new avenues for the development of future sustainable materials.

References:

(1) Lievonen, M.; Valle-Delgado, J. J.; Mattinen, M.-L.; Hult, E.-L.; Lintinen, K.; Kostiainen, M. a.; Paananen, A.; Szilvay, G. R.; Setälä, H.; Österberg, M. Simple Process for Lignin Nanoparticle Preparation. *Green Chem.* **2016**, *18*, 1416–1422.

(2) Sipponen, M. H.; Smyth, M.; Leskinen, T.; Johansson, L.-S.; Österberg, M. All-Lignin Approach to Prepare Cationic Colloidal Lignin Particles: Stabilization of Durable Pickering Emulsions. *Green Chem.* **2017**, *19*, 5831–5840.

(3) Leskinen, T.; Witos, J.; Valle Delgado, J. J.; Lintinen, K. S.; Kostiainen, M. A.; Wiedmer, S. K.; Österberg, M.; Mattinen, M.-L. Adsorption of Proteins on Colloidal Lignin Particles for Advanced Biomaterials. *Biomacromolecules* **2017**, *18*, 2767–2776.

(4) Sipponen, M. H.; Lange, H.; Ago, M.; Crestini, C. Understanding Lignin Aggregation Processes. A Case Study: Budesonide Entrapment and Stimuli Controlled Release from Lignin Nanoparticles. *ACS Sustain. Chem. Eng.* **2018**, *6* (7), 9342−9351.

(5) Farooq, M.; Zou, T.; Riviere, G.; Sipponen, M. H.; Österberg, M. Strong , Ductile and Waterproof Cellulose Nanofibril Composite Films with Colloidal Lignin Particles. *Biomacromolecules* **2019**, *20* (2), 693–704.

O4.7

Functionalized CNF for materials and biomarker sensing.

*Julien Navarro, Ulrica Edlund**

Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

* edlund@kth.se

Cellulose nanofibrils (CNF) offer many interesting properties meriting their use in advanced and high-end applications. The scope of applications can be further extended by engineering the chemistry of the CNF surface. Graft polymerization routes to produce hydrophobic CNF with improved compatibility, processability, and good dispersion in plastic composite matrices will be presented along with the use of modified CNF as a filler in plastic matrices where a major challenge is the dispersion of CNF into the matrix, possibly overcome by modifying the CNF with a hydrophobic surface [1-3].

To assure an unprejudiced introduction of new materials, human health and environmental risks need to be assessed in parallel with material development. The few toxicological studies with wood-derived CNF have so far not shown any indications of toxicity. However, different raw materials, processes and chemical modifications may alter physicochemical properties, highlighting the need for case-by-case studies. To assess eco-toxicological aspects, a combination of standard tests and feeding experiments to was used to study the effects of CNF exposure on the feeding and life-history traits in the cladoceran *Daphnia magna*. CNF with a luminescent probe was synthesized by surface-initiated controlled radical polymerization to allow for bio-marker sensing in *D. magna* [1,4].

References:

1. Navarro, J.; Wennmalm, S.; Godfrey, J.; Breitholtz, M.; Edlund, U. A Luminescent Nanocellulose Platform: from Controlled Graft Block Copolymerization to Bio-marker Sensing. *Biomacromolecules* **2016**, *17*, 1101–1109.
2. Navarro, J.; Edlund, U. A surface-initiated controlled radical polymerization approach to enhance nanocomposite integration of cellulose nanofibrils. *Biomacromolecules* **2017**, *18*, 1947–1955.
3. Edlund, U.; Lagerberg, T.; Ålander, E. Admicellar Polymerization Coating of CNF enhances Integration in Degradable Nanocomposites. *Biomacromolecules* **2019**, *20*, 684–692.
4. Ogonowski, M.; Edlund, U.; Gorokhova, E.; Linde, M.; Ek, K.; Liewenborg, B.; Könnecke, O.; Navarro, J.R.G.; Breitholtz, M. Multi-level toxicity-assessment of engineered cellulose nanofibrils in Daphnia magna. *Nanotoxicology*, **2018**, *12* (6), 509-521.

O4.8

Thermal and water barrier properties of CNF based aerogels and nanocomposites.

Muhammad Farooq[1], Tao Zou[1], Guillaume Riviere[1], A. Seppälä[2] , Mika H. Sipponen[1] , and Monika Österberg[1]

[1] *Aalto University, School of Chemical Engineering, Department of Bioproducts and Biosystems, Espoo, Finland*
[2] *Aalto University, School of Engineering, Department of Mechanical Engineering, Thermodynamics and Combustion Technology Espoo, Finland*

* monika.osterberg@aalto.fi

Demand for ecological and environmentally friendly substitutes to fossil fuel-based materials have inspired the exploration of materials from renewable lignocellulosic biomass [1]. In this regard, cellulose in the form of nanofibrillated cellulose (CNF) and lignin as colloidal lignin particles (CLPs) are plausible candidates as standardized building blocks. CNF offers impressive properties such as low thermal conductivity, low thermal expansion, high strength and elastic modulus and biocompatibility. Here we describe the use of CNF for the production of thermal insulation material and free-standing films. The inherent drawbacks of CNF were overcome by incorporation sodium bicarbonate (SBC) as flame retarding agent and CLPs for water barrier enhancer.

CNF aerogels containing SBC exhibited a distinctly lower burning rate. The average combustion velocity of pure CNF aerogel was 5.84 cm s^{-1}, whereas at 10 wt % loading of SBC (C-SB10), the burning velocity was reduced to 0.33 cm s^{-1} along with a self-extinguishing behavior after 5 s of initial burning [2] . On the other hand , inclusion of CLPs into CNF significantly improved the water barrier properties of CNF films. An optimum 10 wt % content of colloidal lignin particles (CLPs) rendered the films waterproof with nearly double the toughness compared to a CNF film without lignin. Incorporation of CLPs also provided antioxidant activity and UV-shielding with better visible light transmittance [1].

References:

[1] M. Farooq, T. Zou, G. Riviere, M. H. Sipponen, and M. Österberg, “Strong, Ductile, and Waterproof Cellulose Nanofibril Composite Films with Colloidal Lignin Particles,” *Biomacromolecules*, vol. 20, no. 2, pp. 693–704, Feb. **2019**.

[2] M. Farooq, M. H. Sipponen, A. Seppälä, and M. Österberg, “Eco-friendly flame retardant cellulose nanofibril aerogels by incorporating sodium bicarbonate,” *ACS Appl. Mater. Interfaces*, p. acsami.8b04376, **2018**.

O5.1

The Thermal Analysis Toolkit for Characterising Polylactic Acid.

Els Verdonck, Philip Davies*

TA Instruments, a division of Waters

* everdonck@tainstruments.com

The combination of various thermal analysis techniques is providing complementary information in understanding how a material is behaving when heated. Polylactic acid (PLA) is investigated as a case study.

The first step in the characterisation process is the use of TGA (Thermo Gravimetric Analysis) to detect in which temperature region the material starts decomposing, and check if and how much volatiles it contains. Subsequently with DSC (Differential Scanning Calorimetry) the Tg can be measured, as well as cold crystallisation and melting. In case that it’s not obvious to calculate the crystallinity of the as-received material from the DSC thermogram, MDSC (Modulated DSC) provides the solution. The DSC can be equipped with a microscope to add more visualisation to the data (see Figure). DMA (Dynamic Mechanical Analysis) allows measuring changes in the viscoelastic parameters. With TMA (Thermo Mechanical Analysis) dimension changes are measured. If relaxation effects overlap on the CTE, MTMA (Modulated TMA) allows separating them from the CTE.

Combining multiple techniques allows to obtain a clearer picture of what is happening in a material when heating it. It’ll minimise the risk of misinterpreting the data and help to explain the events occurring during processing of the material.

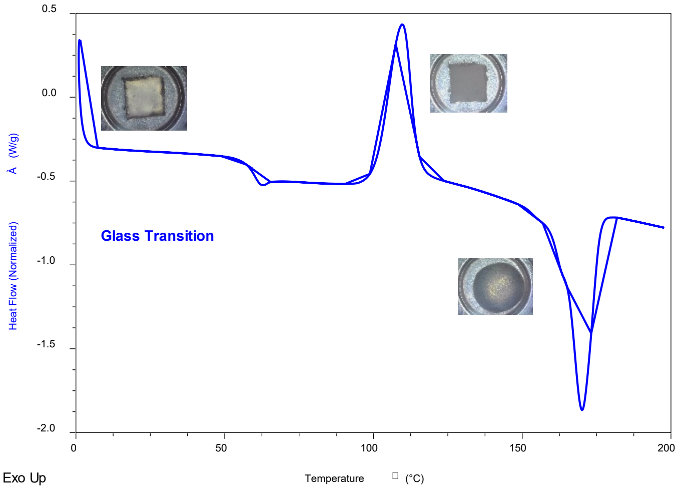


Figure. DSC thermogram and microscope images of PLA

O5.2

Mechanical properties of polyamide 12 parts made by powder bed fusion (additive manufacturing).

Erik Andreassen[1,2,*], *Ivanna Baturynska*[3], *Marius Johansen*[1], *Marius Andersen*[4]

[1]*SINTEF Industry, Department of Materials and Nanotechnology, Oslo, Norway*
[2]*University of South-Eastern Norway, Department of Microsystems, Vestfold Campus, Norway*
[3]*NTNU, Department of Manufacturing and Civil Engineering, Gjøvik, Norway*
[4]*SINTEF Industry, Department of Materials and Nanotechnology, Trondheim, Norway*

* erik.andreassen@sintef.no

Industrial use of additive manufacturing (often referred to as 3D printing) for end-use parts in polymer materials is increasing. There are many recent developments regarding materials, machines and software for numerical simulations. However, there are still challenges, e.g., when it comes to predictable and repeatable mechanical properties.

One important category of additive manufacturing processes for polymer materials is powder bed fusion (PBF). PBF uses thermoplastic polymer materials and the manufactured parts have quite good mechanical properties. The cost per manufactured part is among the lowest for additive manufacturing processes, but the machine cost is high. In PBF, powder particles (with diameter < 0.1 mm) are fused together, layerwise, into a 3D part. The energy for this fusion is typically delivered by a CO_2 laser beam (this sub-category of PBF is often referred to as laser sintering, but there are also other PBF technologies for polymer materials).

This presentation will summarize results from studies of the mechanical behaviour of parts made by PBF, using polyamide 12 materials and two different PBF processes. These topics will be covered:

- *Mechanical properties of parts made by PBF vs. parts made by injection moulding with the same powder*. The main difference is the lower strain at break of the former parts.
- *Variation in part properties due to the parts' position and orientation in the build chamber, and repeatability from build to build.* The main finding is that the repeatability is good, but parts from some build positions have inferior properties. The effect of orientation is large and well-known from other studies.
- *A comparison between the mechanical properties achieved by the conventional laser PBF process and the more recent Jet Fusion PBF process (technology from HP).* The latter process gives somewhat better mechanical properties, but larger variation from part to part.
- *Effects of stress triaxiality on the mechanical response − studied by testing notched round bar specimens with different notch radii.* Stress triaxiality affects the mechanical response of these specimens, and the results can be used to predict the performance of real parts, which often have stress triaxiality.

These studies were supported by the Research Council of Norway (grant no. 248243/MKRAM).

O5.3

Enhanced Thermoelectric Performance of the Conjugated Polymer Poly(3-hexylthiophene) through Tensile Drawing.

Jonna Hynynen[1], Emmy Järsvall[1], Renee Kroon[1], Yadong Zhang[2], Stephen Barlow[2],*
Seth R. Marder[2], Martijn Kemerink[3], Anja Lund[1], Christian Müller[1]

[1]Chalmers University of Technology, [2]Georgia Institute of Technology, [3]Linköping University

* jonhy@chalmers.se

The development of inter-connected small devices, so-called *Internet of Things* is increasing the demand for autonomous power sources. Heat is a plentiful and often wasted source of energy, not the least when thinking about the human metabolism and our body heat. Organic thermoelectric generators could be used to power small devices such as gas sensors or heart-rate monitors that would be solely powered by our body heat. Making use of polymers for these type of applications would increase the flexibility and lower the cost compared to inorganic thermoelectric generators.

To increase the thermoelectric efficiency the polymer is commonly doped. A dopant is a small molecule that ionizes the polymer, this leads to an increase in the electrical conductivity and therefore also an increase in the thermoelectric performance. It is also known that the solid-state structure of the polymer itself influences the electrical properties (charge mobility) of the material. However, doping tends to disrupt the solid-state order of the polymer as well as reducing the mechanical coupling between polymer chains, leading to deteriorating electrical and mechanical properties.

To investigate how the solid-state structure and doping affect the thermoelectric performance and mechanical properties we first, investigate different methods of doping and the effect on the solid-state order of poly(3-hexylthiophene) (P3HT). We find that a two-step-processing-doping-scheme (sequential doping) allows us to preserve the solid-state structure of the polymer to a larger extent than when co-processing the dopant and the polymer. Furthermore, we demonstrate that tensile drawing of the polymer combined with sequential doping lead to an enhanced thermoelectric performance of the material without affecting the mechanical properties to a larger extent.

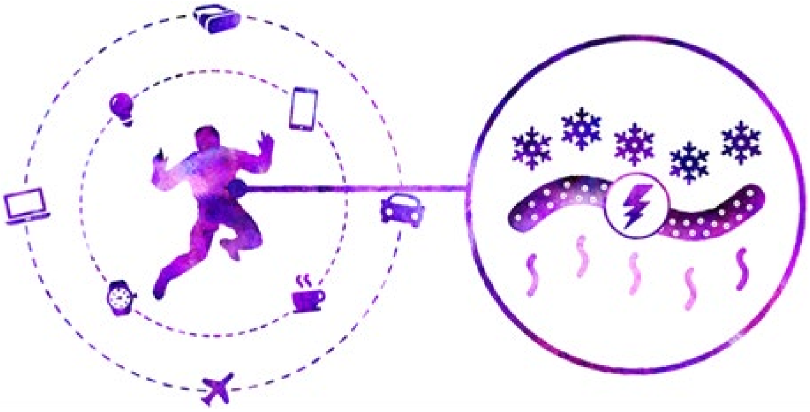


Image: Illustration of the "Internet of Things"

O5.4

Revealing Correlations of Bonding Area and Pilling Behaviour of Polypropylene Non-wovens using a Novel Objective Test Method.

Karsten Leucker[1,2], Janosch Amtmann[1], Dirk W. Schubert[1,2],etc.*

[1]Friedrich-Alexander University Erlangen-Nürnberg (FAU), Institute of Polymer Materials,
Martensstraße 7, 91058 Erlangen, Germany,
[2]Bavarian Polymer Institute, Dr.-Mack-Straße 77, 90762 Fürth, Germany

* Karsten.leucker@fau.de

Although different methods exist, it has been demonstrated that none of the existing testing methods for abrasion resistance is suitable for the testing of low basis weight polypropylene nonwovens in the range of 15 g/m² to 25 g/m². Thus, a novel test method has been developed in which the samples are scanned after certain intervals of abrasion cycles on the Martindale abrasion tester using a standard flatbed scanner. From the greyscale images generated, the total pill area and the number of pills can be determined automatically as shown in figure 1 using a simple image evaluation procedure that was optimized in this study. It was possible to objectively determine the influence of the bonded area of thermally point bonded polypropylene nonwoven on the pilling behaviour. Therefore polypropylene fibres have been calendered using bonding patterns with 8, 16 and 32 % bonding area. These nonwovens were evaluated with the novel testing method and the influencing factors on the differing pilling behaviour were examined, showing a significant influence of the bonded area onto the pilling behaviour.

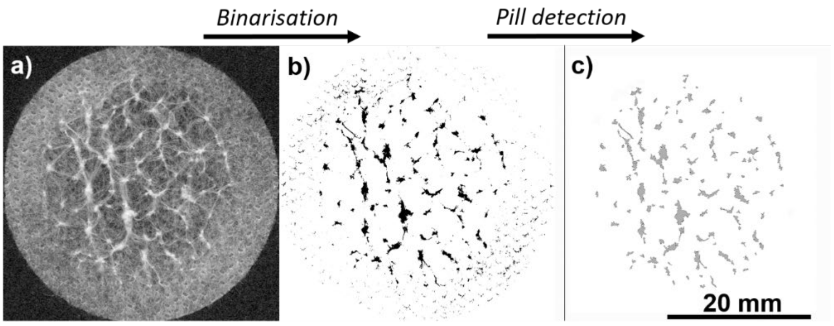


Figure1: Greyscale image of the scanned nonwoven a), the binarised image b) and all detected pills c) where the bright patches in the neat nonwoven are removed for the pill area measurements.

Acknowledgement: Funding for the abrasion tester was provided by the Bavarian Polymer Institute.

References:

Leucker, K.; Amtmann, J.; Schubert, D.W. Novel objective test method for the abrasion and pilling behaviour of low basis weight spunbond polypropylene nonwovens. *Polymer Testing,* **2018**, *69*, 175-181

O5.5

Investigating crystallization and thermal stability of polymers by fast scanning calorimetry.

*Markus Schubnell**, *Jürgen Schawe*

Mettler Toledo GmbH, Heuwinkelstrasse 3, 8606 Nänikon, Switzerland,

*markus.schubnell@mt.com

Structure formation of polymers is frequently investigated by DSC. However, the scanning rates available in conventional DSC are in many cases not sufficient to suppress reorganization processes in polymers. Also, relevant processing condition of polymers cannot be mimicked. With chip calorimeters scan rates of several 10'000 can be reached [1]. This allows studying crystallization processes and the impact of fillers and other additives on the crystallization kinetics under realistic conditions. The influence of multi-walled carbon nanotubes [2] and calcium carbonate [3] as fillers on the crystallization behavior of polypropylene (PP) was investigated by fast scanning DSC measurements. Carbon nanotubes accelerate only the α-phase formation. In the presence of a relatively high content of $CaCO_3$-based filler, an additional crystallization process is measured between mesophase formation and the heterogeneous nucleated α-phase crystallization.

At higher temperatures, polymers may undergo degradation that are not related to mass loss. With semicrystalline polymers, such processes will influence the crystallization kinetics and by this structure and mechanical properties of final products. With fast scanning calorimetry such degradation processes can be demonstrated. Also the short term thermal stability of materials can be investigated [4]. For PEEK we find significant degradation for exposure times > 4min (@ 420 °C) and 10 s (@ 380 °C). The described methodology can also be applied to analyze e.g. fast curing reactions.

References:

1. Schawe, J. E. K.; Pogartscher, S.; Concepts and praxis of material characterization using Flash DSC, in C. Schick, V. Mathot (Eds.), Fast Scanning Calorimetry, Springer, ASIN: B01HPHLZ54, **2016**
2. Schawe, J. E. K.; Pötschke, P.; Alig, I.; Nucleation efficiency of fillers in polymer crystallization studied by fast scanning calorimetry: Carbon nanotubes in polypropylene. Polymer, **2017**,116, 160 - 172
3. Schawe, J. E. K.; Vermeulen, P. A.; A new crystallization process in polypropylene highly filled with calcium carbonate. Colloid. Polym. Sci., **2015**, 293, 1607-1614
4. Schawe, J. E. K.; Ziegelmeier, S.; Determination of the thermal short time stability of polymers by fast scanning calorimetry. Thermochimica Acta, **2016**, 623, 80-85

O5.6

A novel approach for in-situ measurement of residual strain in FDM using Optical Backscatter Reflectometry.

*Shaoquan Wang [1], Kaspar Lasn [2], Christer Westum Elverum [3], Andreas T. Echtermeyer **

Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Richard Birkelands vei 2B, NO-7491 Trondheim, Norway

* andreas.echtermeyer@ntnu.no

Fused Deposition Modelling (FDM) is a promising method in the category of additive manufacturing. However, the layer-by-layer fabrication process of the FDM creates internal residual strains, which bring about a significant degradation of mechanical properties. Shape distortions may appear in the printed component. In this paper we use single mode optical fibres to measure the residual strain distribution in FDM produced polymer components for the first time. Previous measurement methods were limited to either point measurements or ex-situ measurements. An in-situ distributed strain measurement method using Optical Backscatter Reflectometry is applied along the lengthwise direction of the optical fibre sensor embedded during 3D printing. A minimum virtual gauge length of 4 mm and a spatial resolution of a 0.15 mm is experimentally demonstrated. The Optical fibre sensor is able to show variation in residual strain with different infill density. Further, it can be used to detect gaps and voids of certain size in 3D printed component

O5.7

Degradation of polyamide-based multilayer fuel line exposed to bio and petroleum diesel under “in-vehicle” conditions.

*Xinfeng Wei, Ulf W.Gedde, Mikael S. Hedenqvist**

KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE–100 44 Stockholm, Sweden

* mikaelhe@kth.se

Polymer components in motor vehicle fuel systems are exposed to elevated temperatures and fuel contact, which may lead to a deterioration in performance and serious operational problems in the vehicle, such as fuel leakage and fuel pump failure. Herein, the behaviour of polyamide (PA)-based multilayer fuel pipe was investigated in “close to real” conditions using specially-designed ageing equipment with a program designed according to the known customer driving modes and conditions (a key life test). The pipe was exposed to air on the outside and to petroleum diesel and a combination of petroleum diesel and biodiesel on the inside. It allowed for the investigation and understanding of complex ageing mechanisms, often observed in multi-layer systems with a variation in the running conditions. Particularly, ageing behaviour two types of fuel pipes with a polyamide and fluoropolymer inner layer respectively were compared. The mechanisms involved included migration of plasticizer from the PA12 outer layer to the ambient air, fuel absorption in the inner layers, oxidation, annealing, etc. The results indicated that the pipe with fluoropolymer inner layer has better resistance to fuel attack, as revealed by the small fuel uptake, the very low degree of oxidation, and the unchanged electrical conductivity, glass transition and melting behaviour, compared to the pipe with a polyamide inner layer.

References:

*1. X.-F. Wei, S. Akhlaghi, K.J. Kallio, S. Bruder, M. Bellander, U.W. Gedde, M.S. Hedenqvist, Long-term performance of polyamide-based multilayer (bio) diesel fuel lines aged under “in-vehicle” conditions, Polym. Degrad. Stab. 144 (**2017**) 100-109.*

*2. X.-F. Wei, K.J. Kallio, S. Bruder, M. Bellander, U.W. Gedde, M.S. Hedenqvist, Long-term performance of a polyamide-12-based fuel line with a thin poly (ethylene-co-tetrafluoroethylene)(ETFE) inner layer exposed to bio-and petroleum diesel, Polym. Degrad. Stab. 156 (**2018**) 170-179.*

*3. X.-F. Wei, K.J. Kallio, S. Bruder, M. Bellander, U.W. Gedde, M.S. Hedenqvist, Plasticizer migration in polyamide 12: Kinetics, prediction and its correlation with mechanical properties, Manuscript, **2019**.*

O5.8

The Effect of Extender Particle Size on the Glass Transition Temperatures of Cured Epoxies.

Muhammad Ahsan Bashir[*1], *Martin Gjerde Jakobsen* [1], *Vivian B. Farstad*[1]

[1]*Jotun Protective Coatings, Jotun A/S, 3202 Sandefjord, Norway.*

* Muhammad.bashir@jotun.no

Epoxies are extensively employed commercially in different types of protective coatings. For thermosetting epoxy coatings, various factors including the choice of curing agent, solvents, extenders, and curing conditions have a significant impact on the final (molecular and mechanical) properties of the coating. Extenders in commercial epoxy coatings are, generally, used as fillers and the impact of their physical properties (e.g., particle size and particle size distribution) on thermal properties of such coatings is not fully understood. Most of the research work done in this regard focuses on high-temperature cured epoxies related to composites technology. [1,2] Therefore, the current work represents an attempt to explore the effect of particle size of different extender particles on thermal properties (i.e., glass transition temperature (T_g)) of the fully cured epoxy coatings.

All epoxy and epoxy + Extender systems were cured at 60°C for six days prior to their analysis with Differential Scanning Calorimetry (DSC). The obtained results show that the T_g of the cured epoxy coating decreases with i) addition of inorganic extenders and ii) with decreasing the particle size of extender (see **Table-1**). These results indicate that the particles size of the used extender impacts the free volume inside the cured epoxy (keeping other parameters like curing agent, mixing ratio, curing temperature, extender loading constant) and, therefore, may have a significant effect on the mechanical properties of the coating. Relatively high surface area of small extender particles (leading to high content adsorbed species) is proposed to be the most probable reason for this depression in T_g of the cured epoxies.

Table 1*. Extender types used, D_{50} of the extenders and T_g of cured epoxy coating.*

Extender Type	D_{50} (µm)	T_g (°C)
Epoxy	-	82.9
Calcite	5.7	57.3
Feldspar	6.8	58.5
Alumina	8.0	60.5
Talc	12.9	64.6

References:

1. Yangyang, S.; Zhuqing, Z.; Kyoung-Sik, M.; Wong, C. P. Glass Transition and Relaxation Behavior of Epoxy Nanocomposites. *J. Poly. Science: Part B, Poly. Physics.***2004**, 42, 3849-3858.

2. Jae-Soon, J., Particle Size Effect on Mechanical & Thermal Properties of SiO_2 Particulate Polymer Composites. Master Thesis, *University of Delaware, Newark, Delaware, USA.* **2012**.

O6.1

Novel polymer architectures for CO_2 selective membranes.

Marius Sandru[1], Per Stenstad[1], Eugenia Sandru[1], Jing Deng[2], Liyuan Deng[2]

1) SINTEF Materials and Chemistry, Sem Sælands veg 2A, 7034 Trondheim, Norway
2) NTNU, Chemical Engineering, Sem Sælands veg 4, 7491Trondheim, Norway

marius.sandru@sintef.no

Despite the development of new polymeric materials for CO_2 capture membranes such as thermal rearranged polymers (TR), polymers with intrinsic micro porosity (PIM), hybrid polymer-nanoparticles membranes, only few membranes have arrived to testing at pilot scale. This clearly indicates the need of new strategies for membrane fabrication.

Most of these gas separation membranes are based on increasing either the CO_2 solubility or CO_2 diffusivity over N_2 by using different methods to increase the free volume of polymers and their sieving capacity. Our approach is based on modifying in precise and controlled manner polymers and polymeric membranes with CO_2 reactive groups. This represents a new approach in gas separation membranes that mitigates the risks associated with use of polymer blends, addition of various CO^2 enhancement materials (nanoparticles, etc): incompatibility between materials, poor and limited dispersion of particles, reproducibility and difficulty in preparing membranes.

In this paper, we will report novel membrane preparation by modifications of high permeable but low selective polymers such as poly(trimethylslilylproyne) (PTMSP), polydimethylsiloxane (PDMS) and polyvinyl alcohol PVA. The membranes and polymers are modified membranes with CO_2 -philic groups and will discuss the influence of various parameters on membranes structure and their separation performances. A variety of new functionalities can be integrated, for instance amino groups, by applying various modification techniques and procedures.

It was observed that uniformity of the polymer modifications plays a major role on membranes separation properties and is dependent on various factors. Excessive polymer crosslinking reduced the expected CO_2 flux for PVA membranes and needed to be further investigated and eliminated.

The structural changes of polymers (PTMSP) were confirmed by ^{1}HNMR and the amine content was estimated as well. The amine content of modified PTMSP was low, indication a small percentage of the monomer units in the polymer chains were modified.

The membranes structure is characterized by SEM pictures and FT-IR. The density of amino groups is determined by an innovative method and is correlated with the results from mixed gas permeation testing using a synthetic flue gas: 10 % CO_2 in N2, fully humidified. Depending on the polymer and modification method, significant CO_2/N_2 selectivity enhancement was documented.

Acknowledgement This work is supported by the Research Council of Norway through CLIMIT program ("POLYMEM" project, No. 254791)

O6.2

Stimuli-responsive polymers as functional materials to discriminate complex mixtures.

*Xiaomin Qian, Fabian Itel, Noga Gal, Brigitte Städler**

Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark

* bstadler@inano.au.dk

Discriminating food or environmental samples from each other is a challenging task since they are complicated mixtures consisting of thousands of different molecules. Conventional methods, such as gas chromatography-mass spectrometry (GC-MS), are usually time-consuming and require professional users. To accelerate this process, colorimetric and fluorescent sensors have emerged as a potential tool because of their high sensitivity, fast response and easy read-out on a spectrometer. In this aspect, conjugated polymers are particularly intriguing since stimulation at a single site along the backbone affects the properties of the entire system, which amplifies the output signals and results in a higher sensitivity. Polydiacetylenes (PDAs) are polymers derived from diacetylenes upon UV light irradiation that have been extensively studied as bio/chemo-sensors as a result of their unique colorimetric (blue to red) and fluorescent (non-fluorescent to fluorescent) responses upon various external stimulations, such as heat, pH, mechanical stress, metal ions, bacteria, proteins and so on[1]. We have successfully developed PDA sensors based on different diacetylenes with specifically designed head groups targeting selected small molecules in complex mixtures. Diacetylenes were mixed with different ratios prior to PDA vesicle assembly to identify compositions that yield the highest sensitivity to desired small molecules either in a single- or multi-composition solution. Finally, to determine the discriminative ability of the PDA sensors, different exemplary complex mixtures were tested. Statistical analysis of the obtained colorimetric responses were conducted to generate fingerprints of each complex mixture. Taken together, with due development, these PDA sensors provide great opportunity for the fast and cheap assessment of compositional quality and alterations in liquid samples reaching from industrial wastewater to biological fluids.

References:

1. Qian, X.; Städler, B. Recent Developments in Polydiacetylene-Based Sensors. *Chemistry of Materials,* **2019**, *31*, 1196-1222.

O6.3

Microencapsulation by complex coacervation of oil soluble vitamins.

Eugenia Sandru, Wilhelm Glomm, Le Thuy Truong, Peter Molesworth, Heidi Johnsen

SINTEF Industry, P.O. Box 4760 Torgarden, NO-7465 Trondheim, Norway

* Eugenia.Sandru@sintef.no

In the modern world the use of encapsulated ingredients in various products is widely known. Active ingredients like flavors, vitamins, omega 3 oils are sensitive to light, oxygen, heat or have poor solubility that strongly affects their bioavailability. Microencapsulation is a useful tool to preserve the beneficial properties of these ingredients and to control their release at both the right place and the right time [1, 2]. The active ingredients - the core of the microcapsule - is surrounded by a shell composed of materials including a variety of food grade polymers, carbohydrates, fats and waxes that acts as barrier against environmental stress. Multiple microencapsulation techniques have been developed to protect ingredients that are to be applied in e.g. foodstuffs, beverages, nutritional supplements, cosmetic products, pharmaceutical products or animal feed. We report here encapsulation of vitamin A and E by complex coacervation. The coacervates were then dried to obtain the dry microcapsules. The most studied polymer system by complex coacervation is the gum arabic/ gelatin [3]. The issue when using other types of materials except gelatin is the stability of the microcapsules during drying as well as preserving the morphology and stability of the microcapsules when upscaling from laboratory scale. We have encapsulated oils soluble vitamin A palmitate and vitamin E acetate using polymeric system gum-arabic/bovine albumin serum protein in 1L batch scale. Stable microcapsules were prepared by complex coacervation, and their morphology was preserved during drying. The encapsulation efficiency was checked by LC-MS analysis on both coacervates and dried microparticles.

1. Nazzaro, F., et al., Microencapsulation in food science and biotechnology. Curr. Opin Biotechnol., 2012. 23(2): p. 182-186.

2. Ballesteros, L.F., et al., Encapsulation of antioxidant phenolic compounds extracted from spent coffee grounds by freeze-drying and spray-drying using different coating materials. Food Chem., 2017. 237: p. 623-631.

3. Lemetter, C.Y.G., F.M. Meeuse, and N.J. Zuidam, Control of the morphology and the size of complex coacervate microcapsules during scale-up. AIChE J., 2009. 55(6): p. 1487-1496.

O6.4

Counterion turns poly(ionic liquid)-PEG copolymer thermoresponsive.

*Vikram Baddam, Heikki Tenhu**

Department of Chemistry
University of Helsinki

* heikki.tenhu@helsinki.fi

A block copolymer poly(ethylene glycol)-b-poly(vinylbenzyltrimethylammonium triflate), PEG-PVBTMA-OTf, and a homopolymer PVBTMA-OTf were synthesized through RAFT reactions. Studies on aqueous triflate (OTf) solutions showed the hydrophobic OTf turns the polycation thermoresponsive and it phase separates upon cooling at the UCST. In the block copolymer, the interaction between the PEG and the cationic (ionic liquid) block makes the phase separation occur in a stepwise manner. Upon cooling, transparent solutions first turn turbid at T_{cU} and then partially clear at Tc_{L}. Importantly, the Tc_{L} is not observed in a mixed solution of PVBTMA-OTf and PEG macro chain transfer agent, this showing the interaction between chemically different chains is effective when the chains are covalently bound to a block copolymer structure. The complex phase behavior may be rationalized through considering the interplay between ionic, hydrogen bonding, and hydrophobic interactions. A close look on the behavior of polymers with varying lengths of the cationic block, confirms the suggested course of aggregation upon cooling (Figure 1).

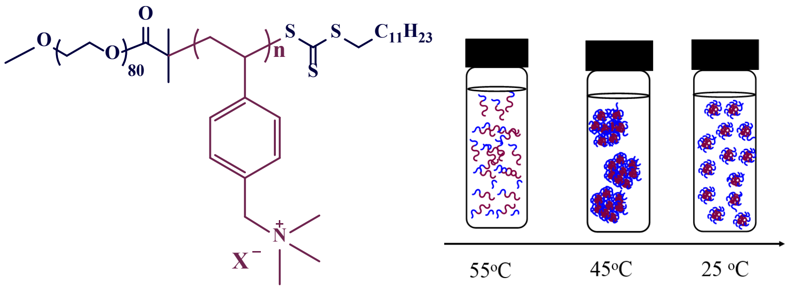


Fig. 1: *Structure of the polymer (left) and suggested course of aggregation upon cooling a triflate solution (right)*

References:

1. Baddam, V. Aseyev, S: Hietala, E. Karjalainen, H. Tenhu; Macromolecules 51(23), 2018, 9681-9691
2. J. Niskanen, H. Tenhu; Polym. Chem. 8(1), 2017, 220-232

O6.5

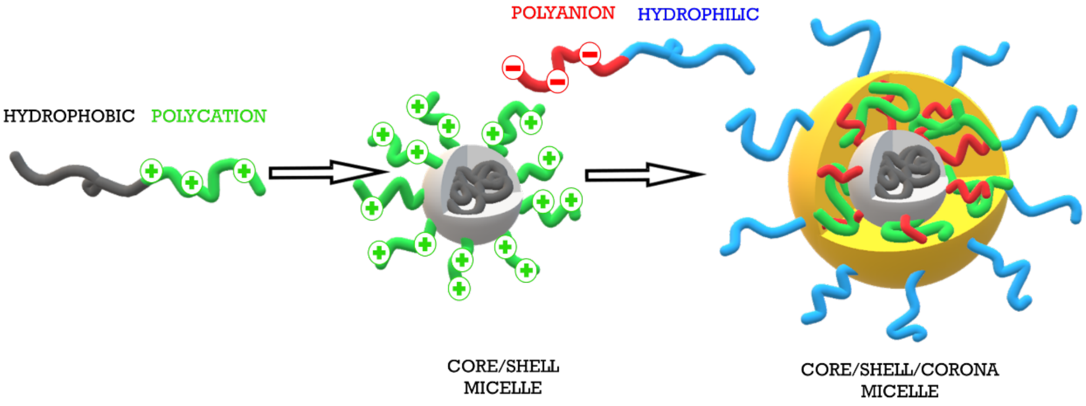
Three-layered onion micelles with soft poly(lauryl acrylate) core: co-assembly and morphological transition.

Anastasiia Murmiliuk[1]*, *Sergey K. Filippov*[2], *Zdeněk Tošner* [1], *Michael Gradzielski*[3], *Stergios Pispas*[4], *Athanasios Skandalis*[4], *Miroslav Štěpánek*[1].

[1]*Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Hlavova 8, 128 00 Praha 2, Czech Republic*
[2]*Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovsky Square 2,162 06 Prague 6, Czech Republic*
[3]*Stranski Laboratory of Physics and Theoretical Chemistry, Institute of Chemistry, Technical University of Berlin, D-10623 Berlin, Germany*
[4]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece*

* anastasiia.murmiliuk@natur.cuni.cz

Amphiphilic diblock copolymers consisting of a water-soluble and a hydrophobic block form micelles in aqueous solutions that can be used as nanocarriers in encapsulation and controlled release. The hydrophobic blocks usually form a glassy micellar core with a rigid structure that limits the applications of these polymers. We studied complexation of poly(ethylene oxide)-*block*-poly(methacrylic acid) and poly(lauryl acrylate)-*block*-poly(trimethylaminoethyl acrylate) where hydrophobic block of poly(lauryl acrylate) (PLA) forms fluid micellar cores. We followed complex formation using a combination of scattering, microscopy, calorimetry, nuclear magnetic resonance and surface tension measurements. We proved that the PLA-containing diblock polyelectrolyte forms three-layered onion (core/shell/corona) micelles with a soft ellipsoid PLA core, a middle layer of interpolyelectrolyte complex formed by oppositely charged polyelectrolyte blocks, and a hydrophilic corona formed by Gaussian chains of poly(ethylene oxide). Thanks to their unique tunable properties, core/shell/corona micelles with a soft PLA core, an interpolyelectrolyte shell and a hydrophilic corona may be used as nanocapsules with the controllable size, core shape and the middle layer charge and thickness.



O6.6

Polyoxalates for marine antifouling coatings.

Kjartan Tobias Boman, Cecilia Winander, Marit Dahling*

Jotun AS, Sandefjord, Norway

* kjartan.tobias.boman@jotun.no

Keeping a ship hull free from biofouling is important, both for the environment and for the ship's owner. Fouling organisms will settle on any unprotected surface and can cause a substantial increase in drag and fuel consumption leading to increased emissions of exhaust gases and increased fuel cost. A common way to protect the hull is to use biocidal, self-polishing coatings where the release of biocides is controlled by the degradation of the binders in the coating.

The development of polyoxalates as degradable binders for self-polishing antifouling coatings will be presented. It will be shown how the properties of the coating is affected by changes in the polymer and some of the tests a product must pass before it can be launched commercially. Controlled polishing is not the only requirement for an antifouling coating. It must also be mechanically robust to withstand the harsh conditions of the sea, be easy to apply on the hull and meet regulations from various authorities.

O6.7

Self-healing polymers for durable icephobicity.

Yizhi Zhuo[1], *Jianying He*[1]*, *Zhiliang Zhang*[1]*

[1]*Norwegian University of Science and Technology (NTNU)*

* jianying.he@ntnu.no, zhiliang.zhang@ntnu.no

Ice accretion presents a severe risk for human safety. Numerous surfaces with low ice adhesion strength (<100 kPa) have been developed to mitigate the detrimental effects.[1-4] For such icephobic surfaces, damages will usually occur during deicing and practical application. When ice formed on such damaged surfaces, mechanical interlocking will occur, thus leading to increase of ice adhesion. In order to avoid the interlocking effect, herein self-healing coatings are designed and synthesized, as shown in Fig. 1. The molecular structure, surface morphology, mechanical properties, and durable icephobicity of the coating were studied. Significantly, the coating guarantees an ultralow ice adhesion strength of 6.0±0.9 kPa, outperforming many other icephobic surfaces. The coating also exhibits an extraordinary durability, showing a very low long-term ice adhesion strength of ~12.2 kPa after 50 icing/deicing cycles. Most importantly, the coating was able to exhibit a self-healing property from mechanical damages in a sufficiently short time, which shed light on the longevity of icephobic surfaces in practical applications.

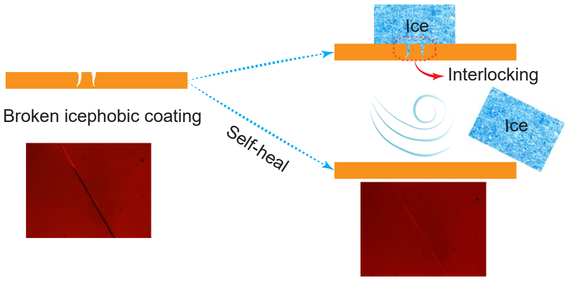


Fig. 1 Slef-healing coating with durable icephobicity.

References:

1. Zhuo, Y.; Hakonsen, V.; He, Z.; Xiao, S.; He, J.; Zhang, Z., Enhancing the Mechanical Durability of Icephobic Surfaces by Introducing Autonomous Self-Healing Function. *ACS Applied Material & Interfaces* 2018, 10 (14), 11972-11978.

2. He, Z.; Zhuo, Y.; He, J.; Zhang, Z., Design and Preparation of Sandwich-ike Polydimethylsiloxane (PDMS) Sponges with Super-low Ice Adhesion. *Soft Matter* 2018, 14 (23), 4846-4851.

3. He, Z.; Xiao, S.; Gao, H.; He, J.; Zhang, Z., Multiscale Crack Initiator Promoted Super-low Ice Adhesion Surfaces. *Soft Matter* 2017, 13 (37), 6562-6568.

4. Zhuo, Y.; Li, T. ; Wang, F.; Håkonsen, V.; Xiao, S. ; He, J.; Zhang, Z., An Ultra-durable Icephobic Coating by a Molecular Pulley. *Soft Matter* 2019, 10.1039/C9SM00162J.

O6.8

From ultrafiltration to nanofiltration by controlled pore collapse of modified polyethersulfone membranes.

*Libor Zverina, Manuel Pinelo, John M. Woodley, Anders E. Daugaard**

Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 227, 2800 Kgs. Lyngby, Denmark

* adt@kt.dtu.dk

Polyethersulfone is a widely used ultrafiltration membrane material thank to its good film-forming and membrane-forming properties, thermal stability, chemical inertness, and mechanical strength. Polyethersulfone membranes find a range of applications in food processing, biomedical field, and water-treatment technologies. To further extend the application range of these membranes, there is a strong need for control over membrane properties.

Here we demonstrate how modification of membrane surface chemistry can be used to control the extent of pore collapse and ultimately to tailor membrane properties. Commercial hollow-fiber polyethersulfone membranes were activated by a heterogeneous reaction introducing benzyl chloride functionality to the surface from which surface-initiated atom transfer radical polymerization of several monomers was conducted [1]. The polymer grafts could be used for controlling the water flux and solute retention characteristics of the membranes (Figure 1). The modified membranes were subsequently dried to facilitate pore collapse. The chemical nature of the grafted polymer is directly reflected in the water flux-to-retention ratio and the extent of pore collapse. Controlled membrane pore collapse could be exploited to obtain higher retention (Figure 1).

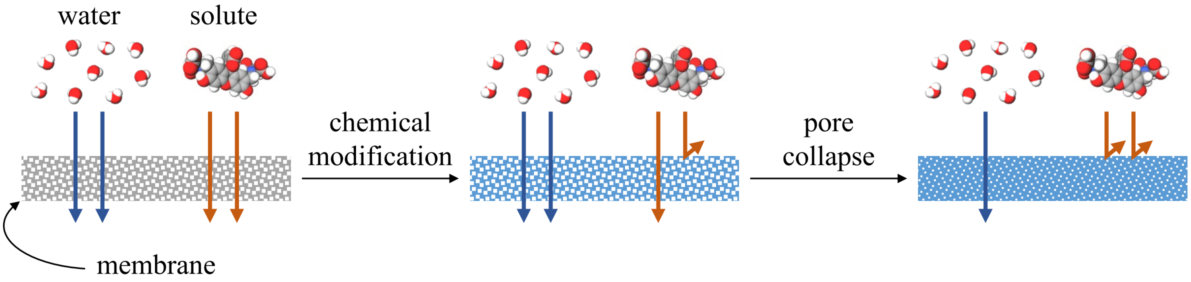


Figure 1: Increase in solute retention after surface modification and subsequent pore collapse.

References:

1. Hoffmann, C.; Silau, H.; Pinelo, M.; Woodley, J. M.; Daugaard, A. E. Surface modification of polysulfone membranes applied for a membrane reactor with immobilized alcohol dehydrogenase. *Mater. Today Commun.* **2018**, 14, 160–168

O6.9

Low-bandgap donor-acceptor polymer brushes.

Anna Gruszkiewicz[1*], Szczepan Zapotoczny[1]

[1]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

*anna.gruszkiewicz@uj.edu.pl

During last few years one can observe a significant increase in market of organic photovoltaic devices, which is strictly connected with progressive rise in energy consumption, as well as with attempt to reduce use of non-renewable deposits. Novel solar cells based on polymer materials reveal many advantages in comparison to their inorganic equivalent, such like relatively low-cost, high flexibility or easy tunability of chemical properties [1]. Nevertheless, the construction of such a device demands application of macromolecules layer on proper surface, that is why polymer brushes, which can provide high stability and directional charge transfer along single polymer chain, seem to be very promising for that purpose [2].

Here, we present designing and the way of synthesis of low-bandgap polymer brushes consist of alternating donor and acceptor molecules. The DFT calculations of energy of the HOMO-LUMO vertical transition were performed to estimate the value of the energy gap for oligomers with various acceptor units, linkages and substituents. Next, in order to obtain designed polymer brushes via organometallic reactions, appropriate initiator monolayer on the surface was deposited and proposed donor and acceptor moieties were successfully synthesized in multistep procedure. The progress of experiments was followed by IR spectroscopy, UV-Vis spectrometry, ellipsometry and contact angle measurements.

Acknowledgements:

Authors acknowledge the support from the project Diamond Grant No. K/PMI/000296 financed by the Ministry of Science and Higher Education. This research was also supported in part by PLGrid Infrastructure.

References:

1. Shrotriya, V. Polymer Power. *Nature Photonics,* **2009**, *3,* 447-449.
2. Wolski, K.; Gruszkiewicz, A.; Wytrwal-Sarna, M.; Bernasik, A.; Zapotoczny, S. The grafting density and thickness of polythiophene-based brushes determine the orientation, conjugation length and stability of the grafted chains. *Polymer Chemistry,* **2017**, *8*, 6250– 6262.

O7.1

Creep of Epoxy in Water: Time-Temperature-Concentration Superposition.

*Andrey E. Krauklis *, Anton G. Akulichev, Abedin I. Gagani ‡ and Andreas T. Echtermeyer*

Department of Mechanical and Industrial Engineering (past: Department of Engineering Design and Materials), Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway; anton.akulichev@gmail.com (A.G.A.); andreas.echtermeyer@ntnu.no (A.T.E.)

‡ Work done at NTNU, currently at Hamburg University of Technology (TUHH), Germany; abedin.gagani@tuhh.de (A.I.G.)

* Correspondence: andykrauklis@gmail.com; andrejs.krauklis@ntnu.no

Long-term creep properties and the effect of water are important for fiber reinforced polymer (FRP) composite materials used in offshore applications. Epoxies are often used as a matrix material in such composites. A typical design lifetime of offshore FRP structures is 25 or more years in direct contact with water leading to some deterioration of the material properties. Knowing and forecasting the extent of the material property deterioration in water is of great interest for designers and users of the offshore FRP structures. It has been established that the Time-Temperature Superposition Principle (TTSP) is a useful tool for estimating changes in properties of polymer materials at long times or extreme temperatures. In this work, a Time-Temperature-Concentration Superposition Principle (TTCSP) is described and used for predicting the long-term creep behavior of an epoxy compound. The studied epoxy does not degrade chemically via hydrolysis or chain scission, but is negatively affected by plasticization with water. The methodology enables prediction of the long-term viscoelastic behavior of amorphous polymers at temperatures below the glass transition (T_g) using short-term creep experimental data. The results also indicate that it is possible to estimate the creep behavior of the plasticized polymer based on the short-term creep data of the respective dry material and the difference in dry and plasticized polymer's T_g. The methodology is useful for accelerated testing aspects and for predicting the time-dependent mechanical properties of a plasticized polymer below the glass transition temperature.

Keywords: epoxy; creep; water; plasticization; viscoelastic; time-temperature superposition principle; TTSP; accelerated testing; methodology.

O7.2

Thermoplastic elastomers – Long-term mechanical properties for sealing applications.

Anna-Maria Persson[1,2,*], *Erik Andreassen*[2] , *Kristian Martinsen*[1], *Einar L. Hinrichsen*[2]

[1]*Department of Manufacturing and Civil Engineering, NTNU, NO-2821 Gjøvik*
[2] *Polymer and Composite Materials Group, SINTEF Industry, NO-0373 Oslo*

* anna-maria.persson@sintef.no

The mechanical long-term behaviour of thermoplastic elastomers (TPE) is of uttermost importance when such materials are considered for demanding sealing applications. The materials may be characterized through mechanical tests such as creep, stress relaxation and cyclic loading (Fig. 1). However, both relaxation and creep tests are time consuming, and gaining knowledge about long term behaviour from shorter cyclic tests would be attractive. This study was performed on a small selection of TPEs and rubbers. The TPEs were one thermoplastic vulcanizate (TPV) and one styrenic thermoplastic elastomer (TPS). The rubbers were EPDM and a liquid silicon rubber (LSR). Except the EPDM, these materials are intended for two-component injection moulding.

Time-dependent responses may be constitutively modelled as viscoelastic or viscoplastic, and damage may be included [1]. Although creep and relaxation are two sides of the same coin, these two responses are commonly represented by viscoplastic and viscoelastic models, respectively. Several constitutive models which can account for all the responses above have been published [2], but these models typically need extensive experimental work for calibration. Given the amount of published work on models intended for elastomers, the focus in this study is to compare the capabilities and limitations of existing modelling approaches in combination with the above-mentioned characterization methods.

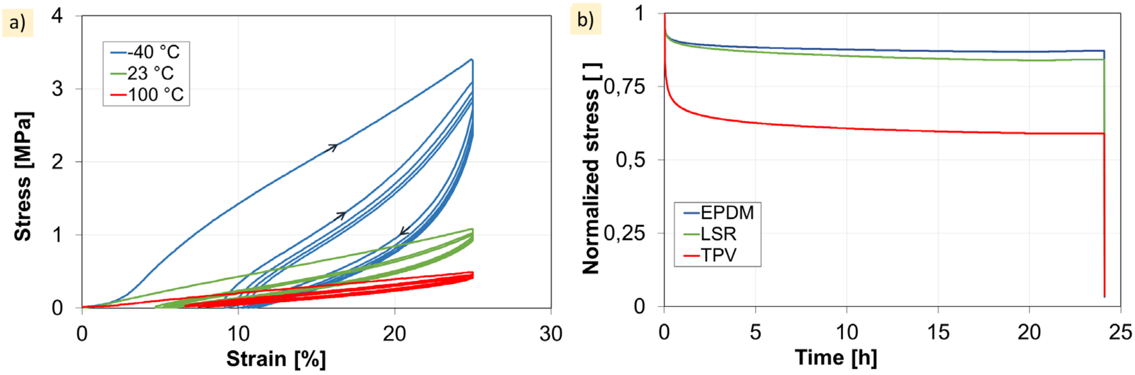


Figure 1. a) Cyclic loading of a TPV at -40 to 100 °C b) Stress relaxation of three elastomers at 60 °C.

References:

1. Holzapfel, G. A. Hyperelastic materials. In *Nonlinear Solid Mechanics.* John Wiley & Sons Ltd, Chichester, England, **2000**, 205-304

2. Bergström, J. Viscoplasticity models. In *Mechanics of Solid Polymers.* William Andrew Publishing, San Diego, USA, **2015**, 371-436

O7.3

Effect of initial thickness for the onset of buckling in hydrogel plates.

Arne Ilseng[1], Victorien Prot[1], Bjørn H. Skallerud[1], Bjørn T. Stokke[2].*

[1]Biomechanics, Department of Structural Engineering, Norwegian University of Science and Technology
[2]Biophysics and Medical Technology, Department of Physics, Norwegian University of Science and Technology

* arne.ilseng@ntnu.no

Hydrogels swelling in a constrained environment can display various buckling patterns, from global wrinkles to localized creases, due to the generation of compressive stresses. This phenomenon is an intriguing scientific problem that has generated considerable attention over the last decades. While analytical models for predicting the onset of buckling is limited to homogeneous swelling, the use of numerical modeling frameworks, like the finite element method, gives possibilities to account for transient swelling effects. Including such transient effects in the model would introduce a dependence on the length scale of the problem. In this work, we aim at quantifying the effect of initial hydrogel thickness for the onset of buckling in layered hydrogel plates with a gradient stiffness.

The constitutive equations for transient gel swelling are outlined in a finite element modeling framework and implemented as a user material routine for the finite element software Abaqus. The analogy between heat transfer and gel diffusion is utilized to obtain a relatively simple implementation as the temperature-displacement elements default in the finite element software can be used to mimic the distribution of the chemical potential through the gel. The implemented model is validated with analytical results for transient swelling of a homogeneous gel showing an excellent agreement.

With the use of the implemented model, the effect of initial dimensions on the onset of buckling is studied for layered hydrogel plates. Three different regions of plate thickness were observed. For plates thinner than 1μm, a relatively large swelling ratio at the onset of buckling was seen, while for plates thicker than 100 μm a relatively low swelling ratio was observed at the onset of buckling. At a thickness between 1μm and 100 μm, a gradual change of the swelling ratio at the onset of buckling was found as the thickness was changed. In addition, the wavelength of the resulting buckling pattern was found to be reduced as the plate thickness was increased.

The results obtained with the transient swelling framework were compared with analytical models assuming equilibrium swelling, the results showing excellent correspondence for very thin plates. Hence, the importance of including transient effects in the modeling procedure increase significantly as the initial plate thickness is increased beyond a threshold value.

O7.4

Revealing novel power laws and quantization in electrospinning considering jet splitting – towards predicting fiber diameter and its distribution.

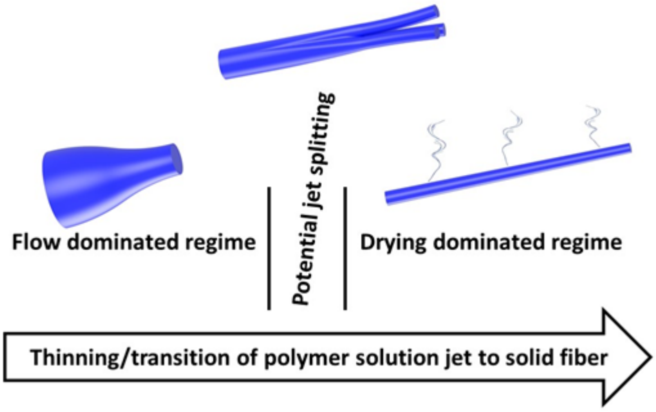
Dirk W. Schubert.

Friedrich-Alexander University Erlangen-Nürnberg (FAU), Faculty of Engineering, Department of Materials Science, Institute of Polymer Materials, Martensstraße 7, 91058 Erlangen, Germany

Bavarian Polymer Institute
Key Lab Advanced Fiber Technology
Dr.-Mack-Straße 77, 90762 Fürth, Germany

dirk.schubert@fau.de

A theory is given to predict the fiber diameter resulting from electrospinning and its distribution. In particular, scaling laws are predicted based on fundamental physics and revealing some peaks in the fiber diameter distribution are not "experimental failure", but are physical consequences of jet splitting, appearing as an indication of quantization of the fiber diameter. The key approach is the separation of electrospinning into a flow-dominated and a drying-dominated regime, where jet-splitting occurs at the transition from the one to the other regime. A clear recommendation is given for analyzing experimental data to challenge the predicted scaling laws. The work opens a door towards the design of the electrospinning fiber diameter and its distribution due to the separation of effects considering charge density, adjustable by salts, and surface tension, adjustable by surfactants, which are linked by viscosity. This work was motivated by the SFB TRR 225.



References:

D. W. Schubert, *Macromolecular Theory and Simulation*, in print, **2019**.

O7.5

Quantitative understanding of ionization of weak polyelectrolytes and weak polyampholytes: simulations vs. experiment.

Raju Lunkad, Anastasiia Murmiliuk, Milan Boublík, Pavel Dubský, Pascal Hebbeker,
*Miroslav Štěpánek, Peter Košovan**

Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czech Republic

* peter.kosovan@natur.cuni.cz

To achieve quantitative understanding of pH-responsive ionization of weak polyelectrolytes and weak polyampholytes, we combine coarse-grained simulations with various experimental techniques. We demonstrate that the ionization of a weak acid group at the end of a polyelectrolyte chain is suppressed by electrostatic repulsion with charges on the polymer chain, and that this effect diminishes by the addition of salt [1]. The simulation predictions agree well with experimental determination using fluorescence spectra of a pH-indicator attached to a poly(methacrylic acid) chain. In a more complex system, we investigate several oligopeptides which consist of aminoacids with weak acid and weak base groups in the side-chains. The presence of like-charged groups on the ampholyte suppresses the ionization of a particular group, while oppositely charged groups enhance its ionization. Therefore, the overall effect depends on the aminoacid sequence of the peptide, and on the pKa values of the ionizable groups. Our simulations of oligopeptides show significant deviations from the ideal ionization behaviour of the free aminoacids [2]. The predicted ionization of the peptides agrees well, in a broad range of pH values, with ionization determined from capillary zone electrophoresis experiments. Agreement between simulations and potentiometric titrations is attained in a narrower range of pH values. It is limited by the reliable determination of charge on the peptide from the measured pH and added volume of the titrant. Overall, our investigations show that coarse-grained models can be used to quantitatively predict the non-ideal ionization of complex polyelectrolytes and polyampholytes, where suitable analytical predictions are lacking, and experimental determination is limited by technical problems.

References:

1. A. Murmiliuk, P. Košovan, M. Janata, K. Procházka, F. Uhlík, and M. Štěpánek. Local pH and effective pK of a polyelectrolyte chain: Two names for one quantity? ACS Macro Letters, 7(10):1243–1247, 2018.
2. R. Lunkad, A. Murmiliuk, M. Boublík, P. Dubský, M. Štěpánek, P. Košovan. A simple model for quantitative prediction of pH-controlled ionization of various oligopeptide sequences. (In preparation)

O7.6

Monte Carlo simulation of halloysite nanotube and polyelectrolyte.

Hyejeong Cheon[1], *Morten Stornes*[1], *Costanza Tedesco*[2], *Rita S. Dias*[1]*

[1] *Norwegian University of Science and Technology(NTNU), Trondheim*
[2] *Visiting from University of Palermo, Palermo*

* rita.dias@ntnu.no

Enzyme immobilization for enzymatic synthesis is commonly used for stabilizing enzymes and improving their functions. A popular methodology is the physical adsorption of enzymes on nano-scaled carriers because of large surface area for high loading efficiency. Some enzymes have disordered structure(Intrinsically disordered protein, IDP), and we chose to represent it as a polyelectrolyte. A nanocarrier is represented as halloysite nanotube which is a clay mineral which possesses a tubular structure with oppositely charged surfaces [1, 2].

In this work, we have used Monte Carlo simulations and a coarse-grained model to study the adsorption of an enzyme onto a halloysite nanotube. The enzyme is described as charged beads linked by harmonic bonds (polyelectrolyte) [3]. The nanotube is depicted by two types of beads constituting a positively charged inner surface and a negatively charged outer surface where fractional charges are dependent on the pH (see figure 1). Here, we perform variation of pH and polyelectrolyte architecture.

The adsorption probability of the polyelectrolyte in the lumen shows different features from adsorption outside of the tube. Radius of gyration and end-to-end distance are analyzed by variations in pH and the charge ratio, number of blocks and charge distribution along the polyelectrolyte. The results demonstrate that the studied values of pH ranging from 2 to 8 do not affect the radius of gyration and the end-to-end distance of the polyelectrolyte, but the charge ratio, the number of blocks and the number of monomers make a significant difference on the conformation of the polyelectrolyte by statistical analysis.

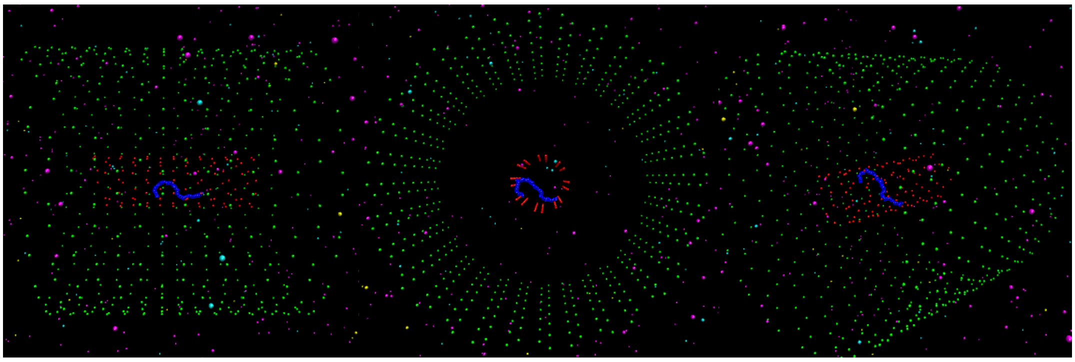


Figure 3. Representive snapshots of a polyelectrolyte adsorbed onto the lumen of a modelled halloysite nanotube.

References:

1. Dmitry G Shchukin, Gleb B Sukhorukov, Ronald R Price, and Yuri M Lvov., 1:510–513, 2005.
2. Faza Annabi-Bergaya Peng Yuan, Daoyong Tan., Applied Clay Science, 112:75–93, 2015.
3. Linse Per Rei Jurij., J Comput Chem, 6(16):1259–1274, 2015.

O7.7

Exploring mechanically-induced charge regulation in weak polyelectrolytes by computer modelling.

Pablo M. Blanco[1,*], *uís Garcés*[2], *Francesc Mas*[1] *and Sergio Madurga*[1]

[1]*University of Barcelona, Material Science and Physical Chemistry and Institute of Theoretical and Computational Chemistry (IQTC), Marti i Franquès 1, 08028 Barcelona, Spain,*
[2]*University of Lleida, Chemistry, Av. Alcalde Rovira Roure, 191, 25198 Lleida, Spain*

*pmblanco@ub.edu

Recently, the refinement of single-molecule force spectroscopic techniques, mainly Atomic Force Microscopy and optical tweezers, has led to an exponential growth in mechano-chemistry [1]. Several experiments are starting to be carried out to study mechanical response of strong polyelectrolytes, usually ss-DNA and ss-RNA, under different media conditions [2]. However, the mechanical stretching response of a weak polyelectrolyte remains a fairly unexplored area in nowadays mechano-chemistry. Weak polyelectrolytes usually have a dynamic charge which can adapt in response of external stimuli (such as changes in pH, salt concentration or by electrostatic interaction with other charged species), phenomenon known as charge regulation [3].

In this talk, a minimal model of a weak polyelectrolyte is proposed [3], which captures the fundamental aspects present in flexible weak lineal polyelectrolyte stretching. The model relies on the recently developed Site Binding Rotational Isomeric State (SBRIS) model which allows to study conformational and binding equilibria at once. The resulting scheme is used to perform semi-grand canonical Monte Carlo simulations of the mechanical stretching of two different model weak polyelectrolytes at different pH and ionic strength conditions [4]. Our results show an increase of the average degree of protonation of the macromolecule as the stretching force increase, which point out that the charge of a weak polyelectrolyte can indeed be significantly regulated by means of mechanical stretching. The physical insights here presented give relevant information for future weak polyelectrolyte stretching experiments interpretation and in the developing of new theoretical techniques able to capture the complex physics involved in these experiments.

References:

1. Giannotti, M. I.; Vancso, G. J. Interrogation of single synthetic polymer chains and polysaccharides by AFM-based force spectroscopy, *ChemPhysChem*, **2007**, 8(16), 2290–2307.
2. Saleh, O. A.; McIntosh, D. B. ; Pincus, P.; Ribeck, N. Nonlinear low-force elasticity of single-stranded DNA molecules. *Physical Review Letters*, **2009**, 102(6), 1–4.
3. Blanco, P. M.; Madurga, S.; Mas, F.; Gracés, J .L. Coupling of Charge Regulation and Conformational Equilibria in Linear Weak Polyelectrolytes: Treatment of Long-Range Interactions via Effective Short-Ranged and pH-Dependent Interaction Parameters, *Polymers*, **2018**, 10(8).
4. Blanco, P. M.; Madurga, S.; Mas, F.; Gracés, J .L., in preparation.

O8.1

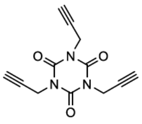
Utilizing Thiol-ene and Thiol-yne Chemistry to Create New Materials for Dental and Skeletal Repair.

*Viktor Granskog, Mathieu Arseneault, Daniel Hutchinson, Michael Malkoch**

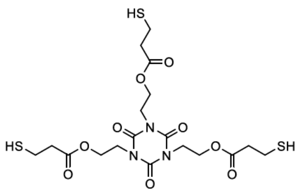
[1]*KTH Royal Institute of Technology, Department of Fibre and Polymer Technology,*

* malkoch@kth.se

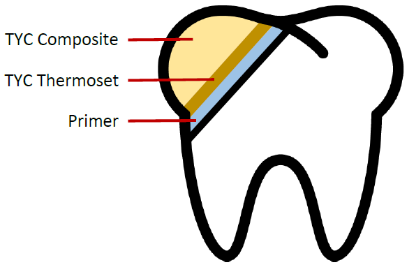
The field of dental repair is dominated by composite materials based on methacrylates. However, these polymeric systems have significant drawbacks, such as low conversion rates, which result in them leaching harmful unreacted monomers, and shrinkage upon curing, the stress from which can result in failure of the restoration. Our lab is seeking to overcome these issues through the development of high performance, methacrylate-free materials based on thiol and alkene functionalized triazine-trione (TATO) monomers. These branched monomers utilize photo-initiated thiol-ene coupling (TEC) chemistry to efficiently create highly crosslinked networks. When used with a self-etching primer, adhesives made with our TEC monomers have already demonstrated the strength and adhesion necessary for use in bone fixation. However, by replacing the alkene functions with alkynes we can harness thiol-yne coupling (TYC) reactions to further increase the crosslink density, flexural modulus and strength of our materials to such an extent that they show great promise for use as revolutionary dental adhesives. In this presentation, we will detail the chemistry, materials formulation, obtained properties and finally the performance of click based composites for dental restorations.



TATATO-alkyne monomer



TATATO-thiol monomer



References:

1. Arseneault, M.; Granskog, V.; Khosravi, S.; Heckler, I. M.; Mesa-Antunez, P.; Hult, D.; Zhang, Y.; Malkoch, M. The Dawn of Thiol-Yne Triazine Triones Thermosets as a New Material Platform Suited for Hard Tissue Repair. *Advanced Materials*, **2018**, *e1804966.*
2. Granskog, V.; García-Gallego, S.; von Kieseritzky, J.; Rosendahl, J.; Stenlund, P.; Zhang, Y.; Petronis, S.; Lyvén, B.; Arner, M.; Håkansson, J.; Malkoch, M. High-Performance Thiol-Ene Composites Unviel a New era of Adhesives Suited for Bone Repair. *Advanced Functional Materials*, **2018**, *e1800372*.

O8.2

pH responsive polyanions to aid cytosolic placement of nanoreactors.

Edit Brodszkij, Carina A. Ade, Bo Thingholm, Brigitte Stadler*

Aarhus University, iNANO

* ebk@inano.au.dk

Therapeutic cell mimicry aims to substitute for missing or lost cellular function as well as to equip cells with non-native activity. Artificial organelles (AO) are typically small single compartments, designed to perform a specific encapsulated catalytic reaction within cells. Among the challenges is to ensure the AO and their cargo to reach the cytosol i.e., their ability to escape the lysosome after endocytotic uptake. The latter aspect remains a long-standing challenge in nanomedicine in general.

We synthesized a series of anionic polymers with systematically varied length of the side chain by RAFT polymerization. We compared their pH responsiveness and the membranolytic properties of the lead polymers (e.g., poly(carboxyethyl acrylate)) was assessed using giant unilamellar and nanosized vesicles. Furthermore, the polymers were evaluated in cell cultures in terms of cytotoxicity, uptake efficiency and lysosomal escape ability.

Following on, block copolymers were synthesized consisting of poly(cholesterol methacrylate) and a membranolytic hydrophilic extension. These block copolymers were employed to assemble micellar and vesicular AO. AOs were equipped with biocatalytic activity by loading with EUK, a small organic compound that mimics catalase, and their intracellular performance was determined.

These polyanion-based AOs are a promising approach since they can be placed in the cytosol and support their host cells in defending oxidative stress.

O8.3

Improving health with monodisperse beads.

*Geir Fonnum, Pontus Lundberg**

Thermo Fisher Scientific, Svelleveien 29, 2004 Lillestrøm, Norway

* pontus.lundberg@thermofisher.com

Monodisperse polymer beads are currently used in a wide range of biomedical applications such as chromatography, immunodiagnostics, molecular diagnostics, T-cell isolation and expansion, and DNA sequencing. The technology for making monodisperse beads was invented by Ugelstad in the late 1970s [1]. He found that by first introducing a low molecular weight activation agent into small monodisperse seed particles, further swelling of monomers followed by polymerization could be achieved resulting in monodisperse beads of up to 100 µm. Furthermore, Ugelstad et al. also developed a method for making the beads superparamagnetic by introducing iron oxide nanoparticles into the polymer particles [2]. These inventions have since been commercialized, further developed and tailored for different applications by varying monomers, degree of crosslinking, porosity, size, magnetic properties, coatings and surface functional groups. For example, magnetic beads functionalized with anti-CD3 and anti-CD28 has enabled personalized CAR-T-cell therapy for treatment of acute lymphomatic leukemia in children. In another example, hydrogel beads used in next generation nucleic acid sequencers for research and diagnostics of inherited diseases, oncology, infectious diseases, reproductive genomics, human identification, and agrigenomics.

SEM image of Dynabeads interacting with T-cells (left) and a sequencing chip with an illustration of hydrogel beads in the wells (right).

References:

1. Ugelstad, US Pat 4336173, 1980
2. Ugelstad, Ellingsen, Berge, Helgee, US Pat 4654267, 1983

O8.4

Polymer particles as scaffolds for 3D cell culture systems.

Wilhelm R. Glomm[1*]*, Eugenia M. Sandru*[1]*, Peter P. Molesworth*[1]*, Hanne Haslene-Hox*[2]*, Andrea D. Hoel,*[2]
Masahiro Yasuda[3]

[1]*Polymer Particles and Surface Chemistry research group, Department of Biotechnology and Nanomedicine, SINTEF AS*
[2]*Biotechnology research group, Department of Biotechnology and Nanomedicine, SINTEF AS,*
[3]*Department of Chemical Engineering, Osaka Prefecture University*

* Wilhelm.Glomm@sintef.no

A major challenge in tissue engineering and in advanced cell culture model systems is the need for more complex functionality in three-dimensional networks, where cell-to-cell adhesions and junctions play important roles, e.g. with respect to cell differentiation and signal transduction. Previously we have shown that polymer particles made using suspension polymerization with grafted epoxy chains can be used as a three-dimensional cell cultivation system which e.g. supports the proliferation and differentiation of hematopoietic stem cells [1]. The advantage of these particles is that they are easily designed in terms of size, composition and surface functionalities [2]. Here, we present recent developments in use of polymer particles as 3D cell culture systems, including compatibility with a range of cell lines, as well as their applicability in creating an interface for a developing *in vitro* neural network with 3D topology.

References:

1. Hirabayashi, Y.; Hatta, Y.; Takeuchi, J.; Tsuboi, I.; Harada, T.; Ono, K.; Glomm, W.R.; Yasuda, M.; Aizawa, S. Novel thre-dimensional long-term bone marrow culture system using polymer particles with grafted apoxy-polymer-chains supports the proliferation and differentiation of hematopoietic stem cells. *Experimental Biology and Medicine, **2011**, 236 (11), 1342-1350.*
2. Yasuda, M.; Kunieda, H.; Ono, K.; Ogino, H.; Iwasaki, T.; Hiramoto, M.; Glomm, W.R.; Hirabayashi, Y.; Aizawa, S. Adhesive Cell Cultivation on Polymer Particles Having Grafted Epoxy Polymer Chains. *Tissue & Cell,* **2011**, *43* (2), 115-124.

P1

Electrostatic coassembly of thermoresponsive double hydrophilic block polyelectrolytes.

*Anastasiia Fanova**[1], *Miroslav Štěpánek*[1], *Stergios Pispas*[2].

[1]*Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, 12840 Prague 2, Czech Republic,*

[2]*Theoretical & Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou, 11635 Athens, Greece*

* fanovaa@natur.cuni.cz

Interpolyelectrolyte complexes (IPECs) are formed by mixing oppositely charged polyelectrolytes in solution due to both strong electrostatic interaction and gain in entropy because of release of the low molecular weight counterions. Complexation of double hydrophilic block polyelectrolytes (DHBP), which are diblock copolymers with one charged block and one neutral hydrophilic block, usually results in core-shell micellar structure formation. In this case the micellar core was formed by IPEC insoluble in water, while the micellar corona was formed by hydrophilic neutral chains, which stabilized the core in the aqueous solution. The polyelectrolytes coassembly behavior depends on numerous factors such as composition, charge-to-charge stoichiometry, ionic strength and pH among other factors [1,2]. Due to the possibility of tuning this factors, IPECs can find applications as containers for guest substances including bioactive compounds [1,2].

One of the possible ways to change and control structure of the resulting co-assemblies is the introduction of thermoresponsive fragments in the composition of interacting polyelectrolytes [3]. Thus, in the present communication we analyzed the complexation behavior of positively (Quaternized poly(2-(dimethylamino)ethylmethacrylate)-*b*-poly(*N*-isopropylacrylamide), QPDMAEMA-PNIPAm) and negatively (Poly(acrylic acid)-*b*-poly(*N*-isopropylacrylamide), PAA-PNIPAm) charged DHBPs with a thermosensitive block (PNIPAm) as a function of their charge ratios. Specifically, we followed the coassembly kinetics of these DHBPs at equivalent stoichiometry using a combination of light scattering, SAXS, time-resolved SAXS, TEM and DSC methods.

References:

1. Pergushov, D. V.; Müller, A. H. E.; Schacher, F. H. Micellar interpolyelectrolyte complexes. *Chemical Society Reviews*, **2012**, *41* (21), 6888–6901.
2. Harada, A.; Kataoka, K. Supramolecular assemblies of block copolymers in aqueous media as nanocontainers relevant to biological applications. *Progress in Polymer Science (Oxford)*, **2006**, *31*(11), 949–982.
3. Dähling, C.; Lotze, G.; Drechsler, M.; Mori, H.; Pergushov, D. V.; Plamper, F. A. Temperature-induced structure switch in thermo-responsive micellar interpolyelectrolyte complexes: Toward core-shell-corona and worm-like morphologies. *Soft Matter*, **2016**, *12*(23), 5127–5137.

P2

Influence of polymer morphology and oxygen containing species on the DC conductivity for low-density polyethylene.

Mattias Karlsson, Xiangdong Xu, Mikael Hedenqvist, Fritjof Nilsson and Richard Olsson *

KTH Royal Institute of Technology, The School of Engineering Sciences in Chemistry, Biotechnology and Health, Fibre and Polymer Technology, SE-100 44, Stockholm

* rols@kth.se

Low-density polyethylene (LDPE) is today widely used as insulation material for high voltage direct current (HVDC) cable systems for energy distribution over long distances. A key parameter for the insulation material is a high resistivity, which is characterized by measuring the leakage current of thin film samples at temperatures and electric fields similar to the operating conditions for the HVDC cables. A challenge is to understand how the conductivity is affected and can be controlled for semi-crystalline polymers where the polymer morphology can influence the conductivity as well as the amount of oxygen containing moieties, either from addition of antioxidants or generated by thermal oxidation. The influence of the supermolecular structure on the conductivity was studied for varied temperatures (25-60 °C) and electric fields (3.3-30 kV mm^{-1}) for the same LDPE material by using different sample processing techniques prior to compression moulding to thin films. Furthermore, the supermolecular structures were also studied by finite element modelling (FEM) by creating a percolating network along the boundaries between spherulites for different temperatures and electric fields.

P3

Steric Stabilisation of Liposomes in the Presence of Surface Active Peptides using End-Capped Poly(Ethylene Oxide) and PEGylated Phospholipids.

Victoria Ariel Bjørnestad[1], *Josefine Eilsø Nielsen* [1], *Reidar Lund*[1]*.

[1]*Department of Chemistry, University of Oslo*

* reidar.lund@kjemi.uio.no

Lipid vesicles, liposomes, i.e. spherical phospholipid bilayers are often used as mimics of the bacterial and mammalian membranes to study these lipid-specific interactions of surface-active molecules such as antimicrobial peptides (AMPs). Structural changes in the bilayer of the liposomes upon addition of AMP can then be characterised using X-ray scattering techniques [1]. Small angle X-ray/neutron scattering (SAXS/SANS) techniques provide the optimal tool for investigating these changes at a nanoscale. Liposomes alone, however, have been found to precipitate in the presence of AMPs, and therefore some method of stabilising the liposomes that still allows the peptide to interact with the membrane was required for their microscopic mode of action to be probed by these techniques. Two types of conjugated poly(ethylene oxide) (PEO) polymers have been tested for their potential for stabilising liposomes in the presence of surface active compounds such as the known flocculant and transfection agent poly(ethylene imine) (PEI) and the antimicrobial peptide indolicidin [2]. The two stabilised liposomal systems were studied in terms of their kinetic stability, structure and microscopic interactions with the peptides. One system consisted of adding free n-alkyl-poly(ethylene oxides) (Cn-PEO) to the liposomes after they had been formed. For the other system, poly(ethylene oxide)-modified phospholipids (”PEGylated” lipids) were incorporated into the liposomal bilayer during their formation. Both methods efficiently stabilise the liposomes through steric repulsions. Although addition of n-alkyl- poly(ethylene oxide) makes the system more versatile and simpler in terms of preparation, the n-alkyl-poly(ethylene oxide) was found to interact and modify the membranes to a great extent. At 37 °C the Cn-PEO likely partially dissolved the bilayers and formed mixed micelles with the lipids. In addition, it interacted with the AMP itself forming mixed ill-defined aggregates. The multitude of interactions yields results that are difficult to interpret. This suggested that the better approach was to use the PEGylated phospholipids for stabilisation. The PEGylation stabilised the liposomes against aggregation without modifying the bilayer significantly, and the attached polymer did not prevent the interaction of AMPs with the membrane either.

References:

1. Nielsen, J. E.; Bjørnestad, V. A.; Lund, R..; Resolving the structural interactions between antimicrobial peptides and lipid membranes using small-angle scattering methods: the case of indolicidin. *Soft Matter*, **2018,** *14*, 8750– 8763.
2. Bjørnestad, V.A.; Liposomer Som Modellsystem for Studier Av Overflateaktive Peptider. (2018)

P4

Challenges in extrusion of nanocellulose reinforced thermoplastics.

Abhijit Venkatesh[1]*, Johannes Thunberg*[1]*, Karin Sahlin-Sjövold*[2]*, Roland Kádár*[1]*, Christian Muller*[2]*,*
Gunnar Westman[2]*, Mikael Rigdahl*[1]*, Antal Boldizar*[1]

[1] *Chalmers University of Technology, Department of Industrial and Materials Science,*
[2] *Chalmers University of Technology, Department of Chemistry and Chemical Engineering,*
SE-412 96 Gothenburg, Sweden

* abhijit.venkatesh@chalmers.se

The commercialization of nanocellulose has rekindled the possibilities to utilize this as reinforcement in polymers. Nanocellulose comes from a sustainable source and possesses excellent mechanical properties, low thermal expansion and high aspect ratio. However, to realize the potential of nanocellulose as reinforcements in thermoplastics one needs to address the challenges involved in melt processing of these composites. Unfortunately, nanocellulose tend to have problems during melt processing with thermoplastic and show issues like poorly dispersion, incompatibility with the matrix (poor fibre-matrix adhesion) and formation of agglomerates at higher concentrations, all of which lead to poor mechanical and functional properties.

In this work, the challenges encountered in the processing of nanocellulose has been discussed. A master-batch of poly(ethylene-co-acrylic acid) (EAA15) and nanocellulose was obtained via water-assisted mixing and compounded along with a different grade of poly(ethylene-co-acrylic acid) pellets (EAA7). The mechanical properties of the extruded 20 vol.% nanocellulose composites was analysed along with their behaviour in melt.

Even though the dispersion at melt compounding remains challenging, the results still show an improvement in strength and stiffness when compared to the matrix with an increasing number of passes and mixing time.

P5

Revealing the Interfacial Tension between Polypropylene and an Ethylene−Norbornene Copolymer via Palierne's Emulsion Model.

*Alessandro Amella[1], Siegfried Werner[1], Joachim Kaschta[1], Dirk W. Schubert[1,2] **

[1] Institute for Polymer Materials, Martensstraße 7, 91058 Erlangen, Germany
[2] Bavarian Polymer Institute (BPI), Keylab "Advanced Fiber Technologies", Dr.-Mack-Str. 77, 90762 Fürth, Germany

*dirk.schubert@fau.de

Previous studies have shown that Polypropylene (PP) is not miscible with Ethylene-Norbornene Copolymers (ENC) with different comonomer ratios, which leads to a phase separation on a microscopic scale [1,2]. The visco-elastic behaviour under shear of such immiscible blends can be described by Palierne's emulsion model [3]. It is based on the visco-elastic behaviour of the blend components, the blend composition, and the properties of the blend morphology, i. e. the radius of the discontinuously dispersed spherical minor phase and the interfacial tension between the two phases. The latter can be determined by fitting the model's theoretical values for the blend to experimental data.

In the present work, four blends made of PP and ENC (comonomer ratio 1:1) with ENC contents up to 30 wt% were mixed in a kneader and both their rheological properties and their morphology were characterized. With increasing ENC content in the blend, the radius of the spherical ENC particles increased and the particle size distribution became broader as a result of increasing coalescence. Furthermore, the secondary plateau of the blends' storage modulus, which is directly related to the relaxation process of the deformed ENC particles during the measurement, became more pronounced with higher ENC contents since larger particles contribute longer relaxation times. By fitting the experimental data of the storage modulus to the model predictions, the interfacial tension between the two polymers at 240 °C was revealed to be 5,4 ± 0,9 mN/m and 6,0 ± 1,2 mN/m, taking into account all measured radii and their volume average, respectively. Additionally, it was investigated how the blend morphology can be altered within the rheometer at 240 °C. By using a plate-plate geometry, a shear rate gradient from the edge (shear rate at the maximum) to the center (no shear rate) of the disk shaped specimens was created, leading to a fibrillar morphology at the edge of the specimen while the shperical morphology in the center was preserved. Quenching experiments showed that the fibrillar morphology returned to its spherical equilibrium state after 30 s to 60 s post-shearing.

References:

1. Slouf, M.; Kolarik, J.; Fambri, L. Phase morphology of PP/COC blends. Journal of Applied Polymer Science, **2004**, 91 (1), 253–259.
2. Ebrahimi, M.; Nazockdast, H.; Mehranpour, M. Morphology of PP/COC composites: Effects of shear rate and organoclay partitioning. arXiv preprint arXiv:1701.02077, **2017.**
3. Palierne, J. F. Linear rheology of viscoelastic emulsions with interfacial tension. Rheologica Acta, **1990**, 29 (3), 204–214.

P6

Sustainable pathway towards large scale melt processing of cellulose-polyamide composites.

*Bashar Haseeb, Antal Boldizar, Giada Lo Re**

Department of Industrial and Materials Science - Chalmers University of Technology

* giadal@chalmers.se

For sustainable polymer composites, cellulosic reinforcements have been of considerable interest for several decades. The main favorable features of cellulose reinforcements have been their interesting mechanical properties, their renewability and availability. However, the process structuring and shaping of cellulose reinforced polymer composites has been shown to be quite challenging, such as for large-scale melt processing by extrusion. One of the major difficulties encountered is the relatively low thermal stability of cellulose, as compared to common processing temperatures used for conventional thermoplastics such as polyamides. The method of water-assisted melt compounding is presented here as an alternative to alleviate cellulose degradation [1–5]. An additional benefit is being able to use never-dried cellulose materials, thus circumventing agglomeration and hornification issues associated with drying cellulosic materials. Furthermore, the use of water as a plasticizer for polyamide materials may take advantage of cryoscopic effects, further decreasing required melt-compounding temperatures including T_g [6,7]. Bio-sourced polyamide 11 composites reinforced with cellulosic materials have been produced via conventional as well as water-assisted melt processing. Mechanical properties and molecular mass reduction due to potential hydrothermal hydrolysis have been evaluated to assess the feasibility of a wet fed approach for polyamide 11, enabling novel polyamide processing approaches for a new generation of sustainable cellulose nanocomposites.

References:

[1] C. Clemons, Comparison of compounding approaches for wood-derived cellulose nanocrystals and polyamide 6, in: Annu. Tech. Conf. - ANTEC, Conf. Proc., 2015: pp. 430–434.

[2] J. Peng, P.J. Walsh, R.C. Sabo, L.-S. Turng, C.M. Clemons, Water-assisted compounding of cellulose nanocrystals into polyamide 6 for use as a nucleating agent for microcellular foaming, Polymer (Guildf). 84 (2016) 158–166.

[3] G. Lo Re, V. Sessini, Wet feeding approach for cellulosic materials/PCL Biocomposites, ACS Symp. Ser. 1304 (2018) 209–226.

[4] G. Lo Re, S. Spinella, A. Boujemaoui, F. Vilaseca, P.T. Larsson, F. Adås, L.A. Berglund, Poly(ϵ-caprolactone) Biocomposites Based on Acetylated Cellulose Fibers and Wet Compounding for Improved Mechanical Performance, ACS Sustain. Chem. Eng. 6 (2018) 6753–6760.

[5] G. Lo Re, J. Engström, Q. Wu, E. Malmström, U.W. Gedde, R.T. Olsson, L. Berglund, Improved Cellulose Nanofibril Dispersion in Melt-Processed Polycaprolactone Nanocomposites by a Latex-Mediated Interphase and Wet Feeding as LDPE Alternative, ACS Appl. Nano Mater. 1 (2018) 2669–2677.

[6] J. Karger-Kocsis, Á. Kmetty, L. Lendvai, S.X. Drakopoulos, T. Bárány, Water-assisted production of thermoplastic nanocomposites: A review, Materials (Basel). 8 (2015) 72–95.

[7] K. Charlet, V. Mathot, J. Devaux, Crystallization and dissolution behaviour of polyamide 6-water systems under pressure, Polym. Int. 60 (2011) 119–125. doi:10.1002/pi.2920.

P7

Advanced rheological characterization of cellulose based systems.

Sylwia Wojno[1,2]*, *Roland Kádár*[1,2]

[1]*Chalmers University of Technology, Department of Industrial and Materials Science, Division of Engineering Materials, SE-412-96 Gothenburg, Sweden*
[2]*Wallenberg Wood Science Centre, Chalmers, Gothenburg, Sweden*

* wojno@chalmers.se

Cellulose nanocrystals (CNC) extracted from abundant, renewable natural polymer cellulose, show huge potential for a number of applications, either as material on its own or as renewable reinforcement in polymers. In this context, surface modification of CNC is essential to enhance properties and seek new applications. Flow structuring of suspensions, multiphase systems and composites requires large / fast deformations. Therefore, it is highly relevant to implement proper and precise analyzing methods sufficiently sensitive to detect changes in the microstructure. In the case of CNC suspensions, most of the research in the scientific literature focuses on linear viscoelastic material parameters. In contrast, non-linear material response is the effect of microstructural changes due to the applied flow field.

In this framework, the project focuses on investigating the relevance of nonlinear material rheological parameters on flow-field CNC interactions. Thus, the response characteristic in the nonlinear viscoelastic regime is highly relevant. To start with, the non-linear analysis is performed in the framework of Fourier-Transform Rheology and Tshcebyshev polynomial decomposition. The PhD project outlined is a part of the Wallenberg Wood Science Centre.

P8

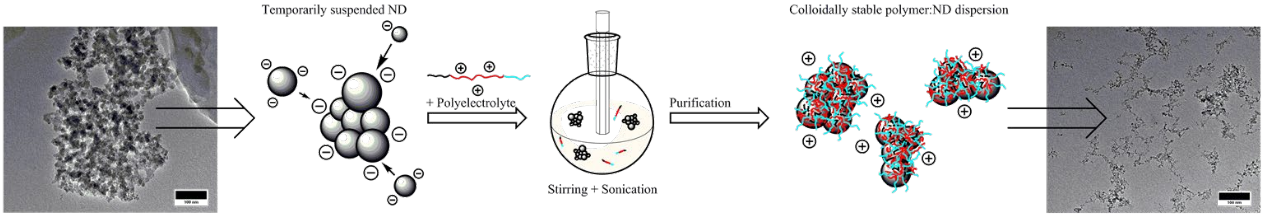
Polyelectrolyte-Nanodiamond Hybrids.

Tony Tiainen[1]*, Teemu T.T. Myllymäki*[2]*, Timo Hatanpää*[1]*, Heikki Tenhu*[1]*, Sami Hietala*[1]

[1]*University of Helsinki, Finland*
[2]*Aalto University, Finland*

Nanodiamonds (ND) are point-like carbon nanoallotropes [1]. These particles have the mechanical- and chemical properties of a macrodiamond in nanometer scale with the added benefit of a functionalizable surface. NDs have multiple applications: materials fabrication [2,3], medicine formulations, and bio-labelling [4,5] being popular in research today [6,7]. However, ND products can be difficult to work with; in particular applications requiring dispersibility and product stability. Particularly the primary- and secondary aggregation of NDs in solutions is a problem for proper control and quality of products. In our study, we aim to control and inhibit this aggregation with polymers that stabilize and add functionalities to the NDs at the same time.

We efficiently dispersed and stabilized negatively charged detonation nanodiamond powder (ND) in water by complexation with double hydrophilic block copolymers. We found that a suitable mixing ratio combined with ultra-sonication and stirring produced homogenous, long-term stable dispersions of polymer coated NDs. These particles are temperature sensitive. Furthermore, re-dispersion of dried dispersion is possible.



References:

[1] V. Georgakilas, J.A. Perman, J. Tucek, R. Zboril, Broad Family of Carbon Nanoallotropes: Classification, Chemistry, and Applications of Fullerenes, Carbon Dots, Nanotubes, Graphene, Nanodiamonds, and Combined Superstructures, Chem. Rev. 115 (2015) 4744-4822.

[2] I. Neitzel, V.N. Mochalin, Y. Gogotsi, Nanodiamonds in composites: Polymer chemistry and tribology, 6th ed., Elsevier Inc., 2017.

[3] V.N. Mochalin, Y. Gogotsi, Nanodiamond-polymer composites, Diam. Relat. Mater. 58 (2015) 161–171.

[4] J. Neburkova, J. Vavra, P. Cigler, Coating nanodiamonds with biocompatible shells for applications in biology and medicine, Curr. Opin. Solid State Mater. Sci. 21 (2017) 43–53.

[5] K. Turcheniuk, V.N. Mochalin, Biomedical applications of nanodiamond (Review), Nanotechnology. 28 (2017) 1–28.

[6] JC. Arnaut, Nanodiamonds: Advanced Material Analysis, Properties and Applications, 6th ed., Elsevier Inc., 2017.

[7] A. Vul, O. Shenderova, Detonation Nanodiamonds: Science and Applications, Taylor & Francis, 2014.

P9

Mechanical properties and lifetime prediction of recycled High-Density Polyethylene.

Ole Vidar Lyngstad [1, 3, *], Eline Gridset [2], Andrea Pettersen Helåsen[2], Hannah Thorunn Monsø [2], Runar Stenerud [3]

[1]SINTEF Manufacturing AS, Pb. 163, N-2830 Raufoss, Norway
[2]NTNU, N-7491 Trondheim, Norway

[3]Plasto AS, N-6300 Åndalsnes, Norway

* ole.vidar.lyngstad@sintef.no

To extend the use of recycled polymer materials and keep the materials within the value chain of its origin, a better understanding of how they will perform compared to virgin materials is needed. Four different High-Density Polyethylene(HDPE) from commercial sources and Post-consumer Recycled from fish farming have been evaluated by tensile and impact tests of both aged and unaged recycled HDPE samples. Mechanical properties of materials have been evaluated by testing according to ISO 527-2, and ISO 179-1, as compared to an injection molded virgin PE80 material.

To take into account ageing and weathering of polymers in practical use, samples have been exposed to artificial laboratory light sources according to ISO 4892-3. Two different exposure times have been used to evaluate material samples. The aged samples were then compared to unexposed reference samples.

P10

Cross-linking of TEMPO-CNF with Willow Bark Extract.

Lohtander T.[1,2]*, *Arola S.*[2], *Laaksonen P.*[3]

[1] *Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University, Espoo, Finland*
[2] *VTT Technical Research Center of Finland Ltd., Biomass Processing and Products, Espoo, Finland*
[3] *Häme University of Applied Sciences, Hämeenlinna, Finland*

* E-mail: tia.lohtander@aalto.fi

Biopolymer-based hydrogels are attractive materials for broad range of applications due to their biodegradable and renewable nature. TEMPO oxidized nanocellulose (TEMPO-CNF) made from wood pulp via oxidation with (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) and mechanical homogenization has good colloidal stability and uniform nanoscale fibril size distribution, which enables formation of viscous gels at quite low solid contents [1]. Combining T-CNF with cross-linker materials enables formation of hydrogels even at lower solid contents and improves material efficiency.

We have demonstrated that phenolic mixture extracted from bark of Karin willow hybrid can be used as cross-linker to obtain gel-like material at relatively low TEMPO-CNF concentration. This certain willow bark extract contains three phenolic compounds, i.e. (+)-catechin, picein and triandin, and monosugars [2]. Phenols, like catechin, oxidizes and polymerizes upon exposure to enzymes, UV, atmospheric oxygen and/or heat [3]. In catechins, the active moiety behind phenomena is catechol, which, for example, is playing important role in adhesive proteins secreted by mussels [4]. Non-covalent interaction forces dominate the binding of polyphenols to cellulose and the main driving forces are hydrogen bonding and hydrophobic interactions [5].

The cross-linking of 0.2 % [w/v] TEMPO-CNF was studied with 0.4% [w/v] willow bark extract and neat catechol with rheological experiments. The oxidation and polymerization was conducted both as bulk reaction and as surface reaction with laccase enzyme and UVC treatment, respectively. Cross-linking with catechol yielded strongest gel-like material, where as pure TEMPO-CNF showed very weak gel-like behaviour. Results also prove the effectiveness of bulk polymerization compared to surface sensitive UV method in formation of hydrogel.

We also demonstrated that cellulose nanofiber-based paste is applicable for printing patterns on cellulose fabric. We developed a method that can improve the fastness properties of color produced with willow bark extract. Contrary to most natural dyes, the color deepens when the method is applied. In addition, the treated pattern retains its color after wash better than untreated pattern due to the formation of crosslinks between active parts of the dye molecules and cellulose.

References:

1. Saito T., Kimura S., Nishiyama Y., and Isogai A. *Biomacromolecules*, **2007**, *8(8)*, 2485–249.
2. Dou J., *et al. ACS Sustainable Chem. Eng.,* **2018**, *6(4)*, 5566–5573.
3. Mitra S. *Ind. J. of Chem.*, **2014**, *53B*, 1255–1262.
4. Yang J., Cohen Stuart M.,and Kamperman M. *Chem. Soc. Rev.*, **2014**, *43*, 8271–8298.
5. Anh Dao T. Phan *et al. Food Chemistry*, **2015**, *17*, 388–396.

P11

Nano-cellulose coatings for antifouling and mechanical enhanced polyethersulfone (PES) membranes.

Andrea Aguilar-Sánchez[1], Blanca Jalvo[1], Aji P. Mathew[1]

[1] *Division of Materials and Environmental Chemistry, Stockholm University, SE-10691 Stockholm, Sweden*

* andrea.aguilar@mmk.su.se

Membrane technology is commonly used for filtration processes of industrial wastewater. Using membranes for water filtration is a safe and energy efficient solution. One of the main problems that arises during the usage of membranes is the fouling effects. Fouling increases the membrane separation resistance, reduces productivity due to a flux decline and affect membrane selectivity. These effects can be avoid by modifying the surface of the membranes using bio-based materials such as nano-cellulose. Nano-cellulose is a great example of a material obtained from renewable resources, which provides high reinforcement and antifouling properties to membranes.

The aim of this work was the development of coatings with cellulose nano-crystals (CNC) and Tempo-oxidized cellulose nano-fribrils (T-CNF) using polyvinyl-alcohol (PVOH), as binding phase to enhance mechanical and antifouling properties over pure commercial PES membranes. The coatings were chemically crosslinked to increase mechanical properties and to improve stability of the coating and avoid swelling. It is expected that by avoiding swelling, permeability remains stable through time. All coating formulations remained stable after 10 hours of crossflow filtration. Mechanical properties of the coated membranes were improved in both dry and wet conditions, showing higher values of tensile strenght and E modulus compared to the uncoated ones. In addition, coated membranes showed high hydrophilicity and low adherence of bovine serum albumin (BSA).

The coatings developed showed stability over PES membranes and provide them with a nanostructured surface which showed an extended durability in use. The modified surface membranes presented good mechanical properties in dry and wet conditions, high flux, high hydrophilicity, resistance to BSA fouling and to different pH environments. Moreover, these modified membranes showed promising results for fast upscaling at industrial level due to the simplicity of the coating process and the availability of the materials in the market.

Acknowledgements:

This project has received funding from the European Union's Horizon 2020 research and innovation programme under H2020 Pilot, Nanotextsurf ; Grant No 760601.

P12

Lignin-based hybrid nanocapsules for phase-change materials.

Alexander Henn[1]*, Mika Sipponen*[1]**, Monika Österberg*[1]***

[1] *Department of Bioproducts and Biosystems, Aalto University, School of Chemical Engineering,*

* mika.sipponen@aalto.fi; monika.osterberg@aalto.fi

Colloidal lignin particles (CLPs) have shown great potential in various fields due to their many useful properties.[1] CLPs have been evaluated as drug delivery vector,[2] wound healing adhesive,[3] co-polymer in bio-composites,[4] and more. Here we extend the application range of CLPs towards thermal heat storage by fabricating lignin-based phase-change materials. Co-precipitation of lignin and fatty acids formed core-shell nanocapsules, whose structure could be confirmed by TEM analysis. Thermoporometry-DSC was used to characterize the intraparticle porosities that showed distinctly different size distributions for CLPs and hybrid nanocapsules in comparison to those of bare kraft lignin aggregates. Additionally, DLS and AFM measurements indicated good stability in aqueous dispersions and uniform and predictable particle size distribution. DSC measurements showed that the hybrid capsules possess excellent conservation of latent heat storage capacity after multiple thermal cycles compared to free lauric acid, whose melting and solidification peaks were unstable. Overall, our results provide new information of the nanoscaled porosities of CLP and hybrid capsules and pave the way to these renewable and natural materials in energy storage applications.

References:

(1) Lievonen, M.; Valle-Delgado, J. J.; Mattinen, M. L.; Hult, E. L.; Lintinen, K.; Kostiainen, M. A.; Paananen, A.; Szilvay, G. R.; Setälä, H.; Österberg, M. A Simple Process for Lignin Nanoparticle Preparation. *Green Chem.* **2016,** *18*, 1416 - 1422.

(2) Sipponen, M.H., Lange, H., Ago, M., Crestini, C. Understanding Lignin Aggregation Processes. A Case Study: Budesonide Entrapment and Stimuli Controlled Release from Lignin Nanoparticles. *ACS Sustainable Chem. Eng.* **2018**, *6* (7), 9342−9351.

(3) Mattinen, M.-L.; Riviere, G.; Henn, A.; Nugroho, R. W. N.; Leskinen, T.; Nivala, O.; Valle-Delgado, J. J.; Kostiainen, M. A.; Österberg, M. Colloidal Lignin Particles as Adhesives for Soft Materials. *Nanomaterials* **2018**, *8* (12), 1001.

(4) Farooq, M.; Zou, T.; Riviere, G.; Sipponen, M. H.; Österberg, M. Strong, Ductile, and Waterproof Cellulose Nanofibril Composite Films with Colloidal Lignin Particles. *Biomacromolecules* **2018,** *20* (2), 693–704.

P13

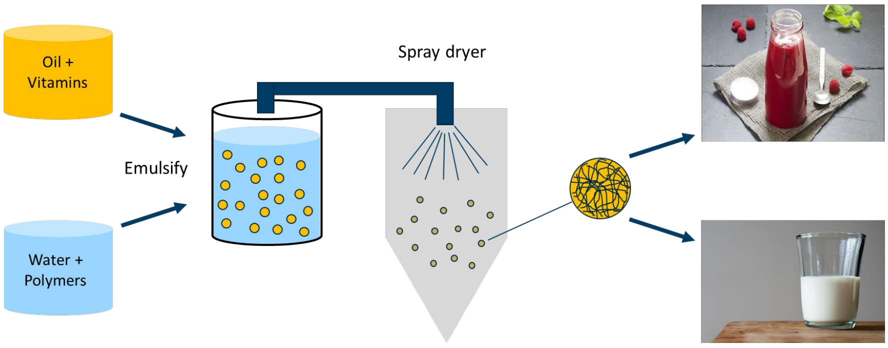
Microencapsulation of Vitamin A Palmitate and E from Oil to Powder by Spray Drying.

Le Thuy Truong, Eugenia Sandru, Peter Molesworth, Wilhelm Glomm, Heidi Johnsen

SINTEF Industry, P.O. Box 4760 Torgarden, NO-7465 Trondheim, Norway

* E-mail address of corresponding author: LeThuy.Truong@sintef.no

For numerous applications, there is a need for encapsulation and controlled release of active substances, owing to e.g. the need for protection of the active substance, poor solubility of the active compounds, or a release profile suited to the lifetime of the material [1, 2]. Here, we report the microencapsulation of Vitamin A and E by oil-in-water emulsions by spray drying, using a small library of polymer matrix materials like gum acacia (GA), gelatin, whey protein isolate (WPI), maltodextrin (MALT) and bovine serum albumin (BSA), as well as the characteristics and stability of the resulting microcapsules. Different combinations of wall materials and different wall/oil ratios have been investigated to elucidate optimal conditions. The feed rate of the emulsion, the inlet temperature and the outlet temperature were varied systematically. We were able to encapsulate oils at higher ratios than previously reported reducing the wall material used by up to 50%. Oil encapsulation efficiency, particle surface oil and moisture content, powder morphology and particle size were analysed. Yields of spray dried material were consistently in the range of 30-40% and surface oil (from 0-8%) varied with wall material but typically this increased significantly as wall material to oil ratio was reduced. Vitamin encapsulation efficiency and capsule stability will also be discussed.



Schematic of process undertaken: Formulation, emulsification, spray drying and redispersion

References:

1. Ray, S., U. Raychaudhuri, and R. Chakraborty, *An overview of encapsulation of active compounds used in food products by drying technology.* Food Bioscience, 2016. **13**: p. 76-83.
2. Gharsallaoui, A., et al., *Applications of spray-drying in microencapsulation of food ingredients: An overview.* Food Research International, 2007. **40**(9): p. 1107-1121.

P14

Protein/protein Nanocomposite Based on Whey Protein Nanofibrils in a Whey Protein Matrix.

Xinchen Ye[1], *Kristina Junel*[2], *Mikael Gällstedt*[3], *Maud Langton*[4], *Xin-Feng Wei*[1], *Christofer Lendel*[1]*, *Mikael S. Hedenqvist*[1]*.

[1]*KTH Royal Institute of Technology,*
[2]*RISE Bioeconomy Innventia AB*
[3]*SIG Combibloc*
[4]*Rice SLU Swedish Agricultural University*

* lendel@kth.se; mikaelhe@kth.se

Improving the competitiveness of bioplastics compared with fossil-based materials is a major topic for the development of a more sustainable society. In this effort, nanotechnology provides the opportunity to improve the material properties of bioplastics. One important way is the development of nanofibrils-reinforced composites. This method could be more interesting if both the matrix and nanofibrils (PNFs) come from similar sources, which weakens the incompatibility between the two parts. In this project, whey protein, a side product from cheese factory, was chosen as the raw material to explore the possibility of improving the mechanical properties of a glycerol-plasticized protein films using whey PNFs. The results showed modified mechanical, optical properties and protein structures with the addition of whey PNFs. Tensile tests on the composite films indicate an increased elastic modulus and a decreased extensibility with increasing content of PNFs, although the films are still ductile at the maximum PNF content (15 wt %).

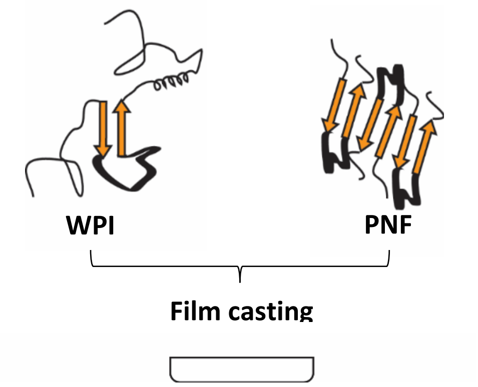


Fig. 1 *Whey PNFs were added into whey protein matrix then casted into films*

P15

Novel Absorbent Materials obtained from Plant Proteins.

Antonio Capezza,[a, b*] *William Newson,*[a] *Richard Olsson,*[b] *Mikael Hedenqvist,*[b] *Eva Johansson*[a]

[a]*SLU Swedish University of Agricultural Sciences, Department of Plant Breeding, , Box 101, SE-230 53 Alnarp, Sweden*

[b]*KTH Royal Institute of Technology, Fiber and Polymer Technology, School of Chemical Science, Biotechnology and Health, SE-100 44 Stockholm, Sweden.*

*ajcv@kth.se, antonio.capezza@slu.se

Superabsorbent polymers (SAPs) are the core raw materials used in many daily-care applications such as diapers and sanitary pads. The exponentially grow of the world population and/or people's needs are therefore increasing the demand for such SAPs, which are currently dominated by petroleum-based polyacrylic acid polymers. It is indeed forecasted that the market for SAPs will account for more than ca. 11 million dollars by 2023 and will also expand to other areas such as the agricultural industry for yield increase.[1] Despite their low cost and high efficiency, these SAPs materials lack sustainability and thus emerging technologies with less environmental footprint are needed. The potential use of natural-based polymers having high liquid uptake capacity may provide a sustainable alternative to already existing petroleum-based SAPs.[2] Wheat gluten based foams (obtained by both lyophilisation and physical mixing processes) have shown the potential to perform as water-absorbent materials. 30 grams of water per gram of dry material (g/g) and a high non-polar liquid uptake have been achieved in these gluten porous structures, together with a previously unreported sponge effect.[3,4] Here, chemical functionalization has been herein carried-out for ensuring a high liquid retention within the material's structure simultaneously as producing solid particles, thus being able to compete with synthetic SAPs. The protein-based materials developed increased their weights ca. 5 times in water as compared to untreated proteins. The results indicate that the modification of these materials may lead to that those obtained from renewable resources can replace fossil-based absorbing materials in the future.

References:

1. Research, R. M. (2015). Global SAP (Superabsorbent Polymers) Market Driven by Top 6 Companies at 80% SAP Manufacturing Capacity. Retrieved from http://www.prnewswire.com/news-releases/global-sap-superabsorbent-polymers-market-driven-by-top-6-companies-at-80-sap-manufacturing-capacity-520573382.html

2. A. J. Capezza, W. R. Newson, R. T. Olsson, M. S. Hedenqvist, and E. Johansson. Advances in the Use of Protein-Based Materials: Toward Sustainable Naturally Sourced Absorbent Materials, 2019, ACS Sustainable Chemistry & Engineering. DOI: 10.1021/acssuschemeng.8b05400

3. B. Alander, A.J. Capezza, Q. Wu, E. Johansson, R.T. Olsson, M.S. Hedenqvist. A facile way of making inexpensive rigid and soft protein biofoams with rapid liquid absorption. Industrial Crops and Products, 2018, 41-48.

4. Wu et al., Highly Absorbing Antimicrobial Biofoams Based on Wheat Gluten and its Biohybrids. 2016, ACS Sustainable Chemistry and Engineering, 2395-2404.

P16

High precision monitoring of ionic strength dependent swelling of cationic hydrogels: A basis for finite element modelling.

Nataša Žuržul [1], Arne Ilseng [2], Victorien E. Prot [2], Bjørn T. Stokke [1], Bjørn H. Skallerud [2]*

[1] *Department of Physics, The Norwegian University of Science and Technology, Norway,*
[2] *Department of Structural Engineering, The Norwegian University of Science and Technology, Norway*

* natasa.zurzul@ntnu.no

Hydrogel materials have received considerable attention due to their versatility, high water content, nontoxicity and the possibility of tuning their behavior. By tailoring their structure, hydrogels can interact with environmental changes [1]. To improve understanding of the process of hydrogel swelling and predict the hydrogel response, swelling behavior of the cationic hydrogels is measured by high-resolution interferometry. The technique provides a resolution of 2 nm change in the optical length within a nearly hemispherical hydrogel of 50 μm radius [2]. Acrylamide-based hydrogels functionalized with various mol fractions of the cationic monomer are exposed to varying ionic strength of the solution. Addition of cationic monomer with quaternary amine groups (ATMA) ensures stability over possible pH fluctuations and eliminates its influence on the experimental results [3]. The interferometric readout platform allows determination of swelling kinetics with the 1 Hz temporal sampling. Such high-resolution experimental swelling data represent an improved basis for benchmarking the quantitative modelling by means of an inverse finite element method.

References:

1. Hendrickson, G.R.; Lyon, L.A. Bioresponsive Hydrogels for Sensing Applications. *Soft Matter* **2009**, *5*, 29–35.
2. Tierney, S.; Hjelme, D.R.; Stokke, B.T. Determination of Swelling of Responsive Gels with Nanometer Resolution. Fiber-Optic Based Platform for Hydrogels as Signal Transducers. *Anal. Chem.* **2008**, *80*, 5086–5093.
3. Palermo, E.F.; Lee, D.-K.; Ramamoorthy, A.; Kuroda, K. The Role of Cationic Group Structure in Membrane Binding and Disruption by Amphiphilic Copolymers. *J Phys Chem B.* **2011**, *115*, 366–375.

P17

Molecular structure influence on bending behavior of polyester-filaments examined using a modified cantilever bending test.

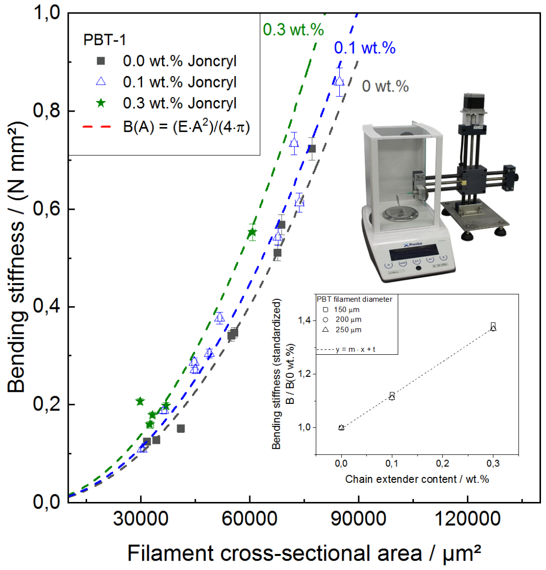
Tim Höhnemann[1], Marcus Himmler[1,2] and Dirk Wolfram Schubert[1,2]*

[1] Institute of Polymer Materials, Friedrich-Alexander University Erlangen-Nuremberg, Martensstr. 7, 91058 Erlangen, Germany
[2] Bavarian Polymer Institute, Dr.-Mack-Str. 77, 90762 Fürth, Germany

* tim.hoehnemann@fau.de

An experimental set-up used to measure the bending stiffness of polymer filaments, motivated by the need for a test method, delivering reliable bending stiffness results directly from a simple kept experimental set-up, combined with easy sample preparation and controlled influence of machine, sample and test conditions is presented. Further the set-up and procedure is used for a study on filaments of poly(butylene terephthalate) (PBT).

As a polymer, synthesized by polycondensation, PBT intrinsically shows a low melt strength, limiting the use for several processes.[1] To overcome this, the use of chain extenders, additives of low molar mass which are known to increase the molecular weight of polymers and broaden the molar mass distribution is frequently reported. [1,2] Also the effect of molar mass to improve several mechanical properties, like toughness or tensile strength is known. [1]



In our work, we reveal a positive effect of the discussed polymer modification by chain extension on the bending stiffness of filaments. Therefore PBT is modified with Joncryl, a commercial multifunctional chain extender via reactive kneading in a pre-step as also executed in former studies on PET. [2] The modified materials are additionally analyzed by size exclusion chromatography with coupled light-scattering and shear rheological measurements to quantify the chain extension-effect at a molecular level and to detect critical chain extender amounts.

References:

1. Guo, B.; Chan, C.-M.; Chain Extension of Poly(butylene terephthalate) by Reactive Extrusion. *Journal of Applied Polymer Science, **1999**, 71 (11), 1827-1834*
2. Härth, M.; Kaschta, J.; Schubert, D.W.; Shear and Elongational Flow Properties of Long-Chain Branched Poly(ethylene terephthalates) and Correlations to Their Molecular Structure. *Macromolecules,* **2014**, 47 (13), 4471-4478

P18

Precipitation of ZnO in presence of cellulose.

Billy Hoogendoorn, Björn Birdsong, Mattias Karlsson, Richard T Olsson*

Royal institute of technology (KTH), Stockholm, Sweden

* Billyho@kth.se

Zinc oxide as an inorganic material has gathered a lot of interest during the past decades due to its use in applications such as solar panels and sun screens. This zinc oxide can be conveniently synthesized via environmentally friendly aqueous procedures. However, even with seemingly similar protocols, major differences in the crystal zinc oxide morphology often show due to small variations in the synthesis parameters.

During the formation of zinc oxide, several interesting phenomena occurs as related to the used salt type, allowing for ZnO particles with morphologies ranging from rod- to star-shaped particles. The synthesis parameters can also significantly affect the crystallization process in terms of sizes, which thereby affect several of the properties of zinc oxide [1,2,3,4].

Furthermore it has been reported that it is possible to produce hybrid materials containing various other metallic oxides by including polymer particles or cellulose, which in turn has been shown to have a significant effect on the crystals that are formed during the synthesis [5,6]. The inclusion of cellulose in the synthesis of ZnO-crystals could thereby provide a promising alternative to control the crystallization process by using a renewable raw material.

The goal of this study is to investigate how the introduction of cellulose crystals affect the formation of ZnO-crystals during the aqueous synthesis of ZnO-rods. The morphology of the ZnO grown in the presence of cellulose crystals was studied for different fibre concentrations and compared to the ZnO-morphologies reached without the presence cellulose during the synthesis.

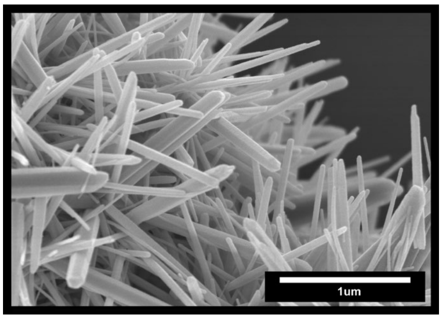


Image 1: SEM-image showing the morphology of the synthesized ZnO-rods

1: M. E. Karlsson, Y. C Mamie, Calamida, J. M. Gardner, V. Ström, A. M Pourrahimi, R. T. Olsson. Langmuir (2018). 34 (17). 5079-5087.
2: J Zhang, L Sun, J Yin, H Su, C Liao, C Yan. Chemistry of Materials (2002). 14 (10). 4172-4177.
3: R. Sivakumar, K. Punitha, C. Sanjeeviraja, R Gopalakrishnan. Materials letters (2014). 121. 141-144.
4: J.L. Castro-Mayorga, M.J. Fabra, A.M. Pourrahimi, R.T. Olsson, J.M. Lagaron. Food and Bioproducts processing (2017). 101. 32-44.
5: V. Fischer, I. Lieberwirth, G. Jakob, K. Landfester, R. Munoz-Espi. Advanced functional materials (2013). 23 (4). 451-465
6: J. Ma, Z. Sun, Z. Wang, X Zhou. Cellulose (2016). 23 (6). 3703-3715.

P19

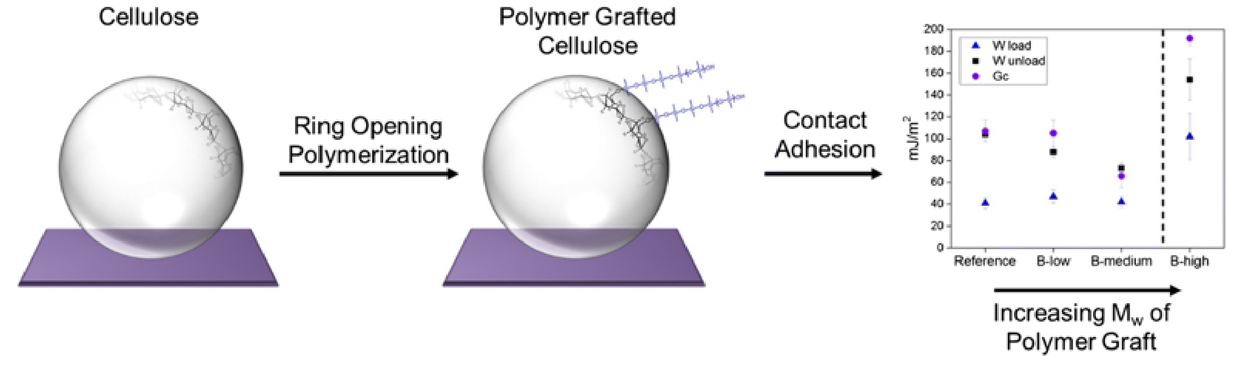
Macroscopic cellulose probes for the measurement of polymer grafted surfaces.

Andrea Träger[1], Gregor Klein[1], Christopher Carrick[1], Torbjörn Pettersson[1,2], Mats Johansson[1], Lars Wågberg[1,2], Samuel A. Pendergraph[1,3], Anna Carlmark[1,3]*

[1]Department of Fibre and Polymer Technology, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH Royal Institute of Technology, Stockholm, Sweden
[2]School of Engineering Sciences in Chemistry, Biotechnology and Health, Wallenberg Wood Science Center, WWSC, KTH Royal Institute of Technology, Stockholm, Sweden

* spender@kth.se

A synthesis protocol was identified to produce covalent grafting of poly(dimethyl siloxane) from cellulose, based on prior studies of analogous ring opening polymerizations. Following this polymer modification of cellulose, the contact adhesion was anticipated to be modified and varied as a function of the polymer molecular mass. The synthetic details were optimized for a filter paper surface before grafting the polymer from bulk cellulose spheres. The adhesion of the unmodified and grafted, bulk cellulose spheres were evaluated using the Johnson–Kendall–Roberts (JKR) theory with a custom build contact adhesion testing setup. We report the first example of grafting poly(dimethyl siloxane) directly from bulk cellulose using ring opening polymerization. For short grafting lengths, both the JKR work of adhesion and the adhesion energy at the critical energy release rate (G_c) were comparable to unmodified cellulose beads. When polymer grafting lengths were extended sufficiently where chain entanglements occur, both the JKR work of adhesion and G_c were increased by as much as 190%. Given the multitude of options available to graft polymers from cellulose, this study shows the potential to use this type of cellulose spheres to study the interaction between different polymer surfaces in a controlled manner.



P20

Comparison of natural and accelerated aged DH pipes.

Alberto Vega[1*], Nazdaneh Yarahmadi[1], Ignacy Jakubowicz[1]

[1]RISE Research Institutes of Sweden

* alberto.vega@ri.se

District heating (DH) networks are the predominant heating systems in Scandinavia because of its effectiveness and positive environmental impact using heat sources that would otherwise be wasted. Only in Sweden, more than 50 % of housings are connected to DH networks, which have been installed since 1950 [1].

The introduction of polymers in DH pipes in the form of rigid polyurethane foam (PUR) for insulation and high-density polyethene (HDPE) for protection helped to impulse the use of DH networks. Many interesting challenges and questions arose from this development. One of them was: what is the technical lifetime of the current DH generation?

Some studies have tried to find a method to establish the status of the current DH networks and predict their technical lifetime. However, there are many factors that affect the deterioration of DH pipes, especially for PUR, as shown in [2], which make it very complex to find a prediction model. Models based on linear Arrhenius relationship seems to be incomplete [3].

For this study, DH pipes from different places in Sweden and Norway were collected. The pipes have been in service for more than 30 years, which means several temperature variations. The aim was to study the impact of natural ageing on the mechanical adhesion and chemical structure of the polyurethane (PUR), which will affect the pipe's performance. The SP plug method was used to study the adhesion between PUR and the steel service pipe. Also, Fourier transforms infrared spectroscopy (FTIR) was implemented to observe any changes in the chemical structure.

The obtained results were compared with previous results from accelerated aged DH pipes. This will help us to gain a better comprehension of the deterioration of the current generation of DH networks and to improve the accelerated methods used today to predict the technical lifetime of DH pipes.

[1] S. Werner, "District heating and cooling in Sweden," *Energy,* pp. 419-429, 2017.

[2] Y. Nazdaneh, A. Vega och I. Jakubowicz, "Accelerated ageing and degradation characteristics of rigid polyurethane foam," *Polymer Degradation and Stability,* pp. 192-200, 12 March 2017.

[3] A. Vega, N. Yarahmadi och I. Jakubowicz, "Determination of the long-term performance of district heating pipes through accelerated ageing," *Polymer Degradation and Stability,* pp. 15-22, 5 April 2018.

P21

Synthesis and characterization of surface-grafted conductive polymer brushes.

Gabriela Grześ[1*], Karol Wolski[1], Szczepan Zapotoczny[1]

[1]*Jagiellonian University, Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry,*
Gronostajowa 2, 30-387 Cracow, Poland

zajacg@chemia.uj.edu.pl

Conductive polymer brushes are structures composed of densely packed conductive polymer chains which have stretched conformation and are attached with one end to a substrate. These structures are very promising in many applications including e.g. nanoelectronics because that could serve as versatile macromolecular platforms with enhanced directional transport of electrons. The new class of conjugated polymer brushes are expected to be used in next generation polymer solar cells, organic light emitting diodes (OLEDs) or field-effect transistors.

In our work, we have presented formation of conductive polymer brushes from proDOT-based monomer (3,4-(2-dimethylpropylenedioxy)thiophene methacrylate) which may exhibit unique electrical and optical properties. Firstly a two-step synthesis of the new bifunctional monomer has been carried out and optimized. This monomer has blocked positions of β-carbons, which may bring benefits in the form of improved stability and in the formation of longer conjugated chains in polymer brushes duo to stiffen conformation. Then the monomer was used to obtain homopolymer brushes using surface initiated atom transfer radical polymerization (SI-ATRP). In the last step, the brushes with pendant proDOT groups were subjected to the oxidative polymerization with $FeCl_3$. Oxidative polymerization of the neighboring proDOT groups in the brushes enabled formation of conjugated polymer chains. The obtained materials were characterized using atomic force microscopy (AFM). Differences between surface properties before and after oxidative polymerization was determined by grazing angle FTIR spectroscopy and UV-Vis spectroscopy. Moreover, images of this material were captured by confocal microscopy.

The authors would like to acknowledge TEAM project (2016-1/9, financed by the Foundation for Polish Science (Smart Growth Operational Program 2014-2020)) for the financial support.

P22

Optimization of self-templating polymerization towards a facile and efficient synthesis of polythiophene-based brushes.

Joanna Rokita[1*], *Anna Gruszkiewicz*[1], *Karol Wolski*[1], *Szczepan Zapotoczny*[1]

[1]*Jagiellonian University, Faculty of Chemistry,*
Department of Physical Chemistry and Electrochemistry,
Gronostajowa 2, 30-387 Kraków, Poland

* joanna.rokita4@gmail.com

Alternative sources of energy gain more and more interest, due to lessening of natural resources and growing environmental pollution. Organic photovoltaic solar cells are promising solution thanks to inexpensive production costs and flexibility. However, the greatest challenge for scientists is to develop a stable material with satisfactory electrical properties to form efficient solar cells. Well-ordered structure of conjugated polymer brush allows to directional transport of the charge carrier what makes them suitable for photovoltaic applications.

Inspired by these needs in our studies we have focused on optimization of conjugated polymer brush synthesis. We present here the synthetic route to conjugated poly(3-methylthienyl methacrylate) (PMTM) brushes (grafted on indium tin oxide) that utilizes surface-initiated ATRP followed by oxidative template polymerization. Oxidation of pendant thiophene groups in the parent brushes by means of FeCl3 allows connection between adjacent thiophene rings and forming a system of conjugated bonds. The various conditions of this process were investigated and followed by FTIR semi-quantitative measurements, UV-VIS spectroscopy, AFM and confocal microscopy.

Acknowledgements:

The authors would like to acknowledge TEAM project (2016-1/9, financed by the Foundation for Polish Science (Smart Growth Operational Program 2014-2020)) for the financial support.

References:

1. Wolski, K.; Gruszkiewicz, A.; Wytrwal-Sarna, M.; Bernasik A.; Zapotoczny, S.; *The grafting density and thickness of polythiophene-based brushes determine the orientation, conjugation length and stability of the grafted chains*, Polymer Chemistry, 8, 6250-6262, **2017.**

P23

Understanding migration behaviour of non-ionic surfactants in polypropylene.

Khushdeep Sharma[1], *Franz Lanyi*[1], *Dirk W. Schubert*[1,2]*

[1]*Institute for Polymer Materials , Martensstraße 7, 91058 Erlangen, Germany*
[2]*Bavarian Polymer Institute (BPI), Keylab "Advanced Fiber Technologies", Dr.-Mack-Str. 77, 90762 Fürth, Germany*

* dirk.schubert@fau.de

Isotactic polypropylene (iPP) is a semi-crystalline polymer, which is generally hydrophobic in nature. There are only very few studies available in the scientific literature on the migration behavior of non-ionic surfactants in polyolefins and consequent surface modification. The surfactant molecules have tendency to bloom or migrate through amorphous regions of the iPP to the top layer of the surface in adequate concentration to provide prolonged hydrophilic surface. In this study, the iPP surface has been modified by melt blending of non-ionic surfactant. The aim of the study was focused on the influence of processing, surface crystallinity and morphology on the additive migration behaviour of a non-ionic surfactant. The migration behaviour of a non-ionic surfactant was studied in injection moulded plates, cast extruded films, annealed and uniaxially stretched films, fibres and non-wovens to understand influence of processing and post treatment methods. The surface crystallinity of iPP and surface concentration of additive on the iPP surface was measured through the Attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR). It was concluded that alteration of the surface properties of iPP and migration behaviour is highly dependent on the processing method used, percentage of surface crystallinity, type of morphology and crystal phase in the iPP samples.

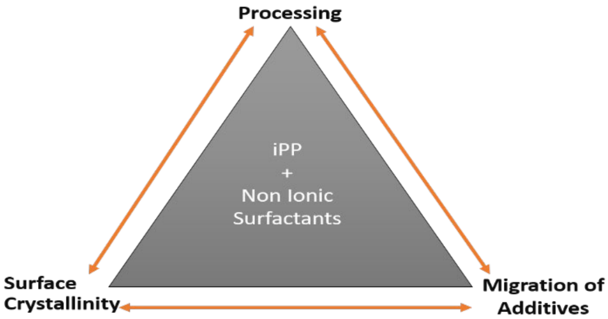


Figure: Motivation of the current study

References:

1. V.M. Datla, E. Shim, B. Pourdeyhimi, Polypropylene surface modification with stearyl alcohol ethoxylates to enhance wettability, J. Appl. Polym. Sci. 121 (2011) 1335–1347.
2. K. Lee, K. Cho, I. Park, B.H. Lee, D. Rana, S. Choe, Migration phenomena of surfactants in polyethylene film, J. Polym. Sci. B Polym. Phys. 37 (1999) 1387–1395.

P24

Thermoresponsive polymers for kinetic gas hydrate inhibition.

*Erik Gisle Dirdal and Malcolm A. Kelland**

Department of Chemistry, Bioscience and Environmental Engineering, Faculty of Science and Technology, University of Stavanger, N-4036 Stavanger, Norway.

* malcolm.kelland@uis.no

Pipeline blockage due to gas hydrate formation is the number one problem to overcome in transporting oil and gas in deep water subsea flowlines. Kinetic hydrate inhibitors (KHIs) are water-soluble polymers that have been used by the oil and gas industry for 25 years as one method to prevent gas hydrates from forming. Interestingly, the most effective polymers used as KHIs show thermoresponsive behaviour in aqueous solution. This means they exhibit a phase change at the cloud point temperature (Tcl) when the solution is heated. The polymer cloud point is often low and not far above the equilibrium temperature for gas hydrate formation (about 15-25 °C). Examples of such commercial KHIs polymers include poly(N-vinyl caprolactam) (Tcl = 30-40 °C), poly(N-isopropylmethacrylamide) (Tcl = 35-45 °C) and hyperbranched poly(ester amide)s (30-40 °C).

We report our work on these and many other classes of water-soluble polymers to determine if there is a correlation between cloud point and KHI performance. In our own laboratories and in collaboration with other research groups worldwide, we have synthesised and tested a wide variety of low cloud point polymers with a variety of different shapes, molecular weights, functional groups and sizes of pendant hydrophobic groups. Our main conclusion is that low cloud point for a polymer, near the hydrate formation temperature, appears to be useful for high KHI efficacy, but only if certain criteria for the polymer are met. These include low molecular weight, pendant hydrophobic groups of an optimal size, and the correct hydrophilic functional groups. Possible theories as to why low cloud point for a KHI polymer can be beneficial are discussed.

References

Sloan, E. D., Jr.; Koh, C. A. *Clathrate Hydrates of Natural Gases*, 3rd ed.; CRC Press (Taylor & Francis Group): Boca Raton, FL, 2008.

Kelland, M. A. A Review of Kinetic Hydrate Inhibitors - Tailor-Made Water-Soluble Polymers for Oil and Gas Industry Applications. In *Advances in Materials Science Research*; Wytherst, M. C., Ed.; Nova Science Publishers, Inc.: New York, **2011**; Vol. 8, Chapter 5.

P25

Phase behaviour of poly(2-propyl-2-oxazoline)s.

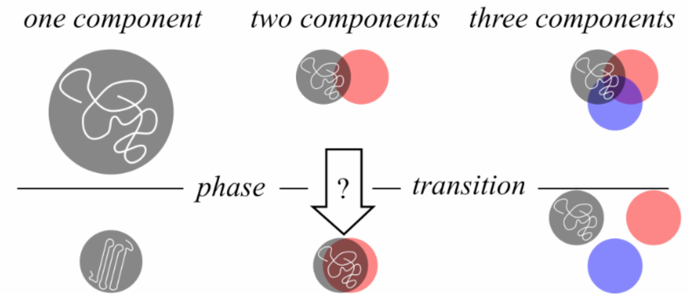
Fabian Pooch[1]*, *Francoise M. Winnik*[1], *Heikki Tenhu*[1]

[1]*University of Helsinki, Department of Chemistry, P.O. Box 55, 00014 Helsingin Yliopisto, Finland*

* fabian.pooch@helsinki.fi

Macroscopic properties and molecular conformation are intimately linked. Every macroscopic phase transition originates from a molecular reorganization process. Such processes include the crystallization/melting of a polymer in the solid state, the mixing/separation of two or more chemically different polymers or the thermos-responsiveness of a polymer in solution. In order to predict and control the macroscopic properties for specific applications it is necessary to understand the processes of organization on the molecular level.

Poly(2-propyl-2-oxazoline)s are chemically versatile and exhibit a rich phase behaviour which makes them popular candidates for various applications. In this presentation, I will showcase the diversity of poly(2-propyl-2-oxazoline) phase transitions observed in various molecular environments. These span from single component to three component systems. The more complex systems exhibit rather uncommon and unexpected behaviours. Their molecular origins are uncovered in this presentation.



Scheme: One-, two-, and three-component systems consisting of at least one is a polymeric component undergo phase transitions. These may be crystallization, mixing or phase separation.

References:

1. Fabian Pooch, Marjolein Sliepen, Kenneth D. Knudsen, Bo Nyström, Heikki Tenhu, and Françoise M. Winnik, Poly(2-isopropyl-2-oxazoline)-b-poly(lactide) (PiPOx-b-PLA) Nanoparticles in Water: Interblock van der Waals Attraction Opposes Amphiphilic Phase Separation. *Macromolecules,* **2019**, 52 (3), 1317-1326
2. Fabian Pooch, Marjolein Sliepen, Kirsi J. Svedström, Antti Korpi, Françoise M. Winnik and Heikki Tenhu, Inversion of crystallization rates in miscible block copolymers of poly(lactide)-block-poly(2-isopropyl-2-oxazoline). *Polymer Chemistry,* **2018**, 9, 1848-1856

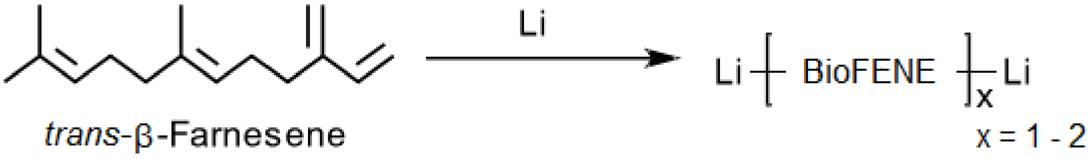
P26

BioFENE™ based initiator for the anionic polymerizations of bi-functional butadiene homo- and co-polymers.

Pleska Alexander[1], Chao Herbert[2], Pytela Jindřich[1], Trnka Tomáš[1].

[1]*Cray Valley Czech, Kralupy nad Vltavou (CZ),*
[2]*Total Cray Valley, Exton (USA).*

Dilithio initiators for anionic polymerization produced from lithium and dienes are known for decades. However, their commercial use is rather limited due to their poor solubility in organic solvents. Recently, new dilithio initiators for polymerization of butadiene homo- and co-polymers have been developed from BioFENE™ (*trans*-β-farnesene) in our labs. Thanks to bulky structure of BioFENE™ molecule, a good solubility of the initiators is achieved. Prepared initiator is not only soluble in polar solvents but also in non-polar ones. Reduction of polar solvents in the initiator solution results in greater control over butadiene homo- or co-polymer microstructure thus the polymers and oligomers with low vinyl incorporation can be prepared. Lab experiments were not only focused on the synthesis process but also on the study of stability of the new bi-functional initiators. Effectiveness of initiators was proved by preparation of bi-functional low molecular weight as well as the high molecular weight polymers.



References:

1. Pleska, A. Dilithium initiators (2016) **US9732179B2**.

P27

UCST-Type Nanogels for Enzymatic Catalysis.

Dong Yang[1], *Sami Hietala*[2]*

[1,2]*Department of Chemistry, University of Helsinki, FIN-00014HU*

sami.hietala@helsinki.fi

Stimuli-responsive nanogels are soft crosslinked colloidal particles exhibiting volume phase transitions. They can be employed in enzymatic catalysis utilizing the so called single enzyme encapsulation approach, where a thin polymer layer is built around the enzyme stabilizing its structure and shielding the catalytic activity, see Figure 1.

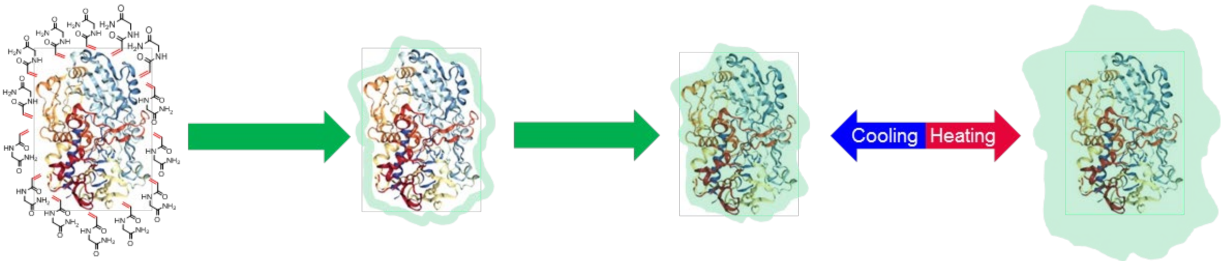


Figure 1. Single enzyme encapsulation of PNAGA and thermal response.

Poly(N-acryloylglycinamide) (PNAGA) is a non-ionic polymer showing upper critical solution temperature (UCST)-type behavior in water. For PNAGA nanogels the phase transition leads it to swell upon heating and shrink upon cooling.[1] This reversible thermal phase transition behavior makes PNAGA nanogels interesting for the stabilization of enzymes under harsh conditions simultaneously allowing control over the activity as well as a possibility for recycling the enzymes.

References:

1. D. Yang, M. Viitasuo, F. Pooch, H. Tenhu, S. Hietala, Polymer Chemistry, 9 (2018) 517-524.

P28

Prediction of Plasticization Mechanisms for Starch based Plastics: Experimental and Molecular Dynamics Approach.

Hüsamettin D. Özeren, Fritjof Nilsson, Richard Olsson and Mikael S. Hedenqvist*

Department of Fiber and Polymer Technology, School of Engineering Sciences in Chemistry, Biotechnology and Health, Royal Institute of Technology, SE-100 44 Stockholm, Sweden

* ozeren@kth.se

The field of bio-based plastics has developed significantly in the last decades and there is increasing concern on industries to shift existing materials production from petrochemicals to renewable resources. Bio-based plastics are offering competitive mechanical properties and getting more popular in a cost-effective manner. Starch based plastics is considered to be important for use in biodegradable plastic products. Nevertheless, a major drawback associated with starch-based polymers is their brittleness, which is related to the glucosic chain rigidity in the backbone. Therefore, effective-compatible plasticizers are needed. The widely used plasticizer in research is glycerol, due to its effectiveness, stability and low price. The purpose of this study is to understand plasticization mechanism and plasticizer interactions of amorphous starch (amylopectin) with glycerol and/or other similar structure based plasticizers such as polyols. In addition, the second aim is to improve the plasticization mechanism and of polar polymers and compatibility, in general manner. A combined experimental and molecular dynamics (MD) approach is used to obtain mechanical and thermal properties of the starch based plastic. Several techniques are used to determine experimentally the properties of the casted starch films, including DSC, DMA and tensile testing. MD simulations are performed on 3-10 polymer chains (1176 atoms/chain) using the several combined force fields. The glass transition temperatures (T_g) and Young's modulus were obtained by volume change at different temperature [1] and uniaxial deformation simulations [2]. The results show that the thermal and mechanical properties computed from MD simulations are in good agreement with experimental data on systems with a plasticizer content of 0-40 wt.% and the model is promising to investigate also plasticization mechanism of other polar polymers.

References:

1. Han, J.; Gee, R. H.; Boyd, R. H., *Macromolecules* **1994,** *27*, 7781-7784.
2. Hossain, D.; Tschopp, M. A.; Ward, D. K.; Bouvard, J. L.; Wang, P.; Horstemeyer, M. F., *Polymer* **2010,** *51* (25), 6071-6083.

P29

Revealing critical model parameters for predicting the bioprintability of hydrogel systems.

Stefan Schrüfer[1,2], Dirk W. Schubert[1,2].

[1] *Friedrich-Alexander-University Erlangen-Nürnberg, Institute of polymer materials, Martensstr. 7, 91058 Erlangen, Germany*

[2] *Friedrich-Alexander-University Erlangen-Nürnberg, Bavarian polymer Institute, Keylab of advanced fiber technologies, Dr.-Mack-Str. 77, 90762 Fürth, Germany*

stefan.schruefer@fau.de

Bioprinting has become an important approach for creating customized tissue replacements, used either for healing or replacing damaged human tissue and cartilage [1, 2]. One of the crucial factors in 3D biofabrication is cell proliferation, which is highly influenced by the shear stresses occurring during the printing process [3]. Not only the cell proliferation but also the printability of hydrogels, which is defined by shape fidelity and printing resolution, is dependent on the rheological properties of the used bio ink.

In order to characterize their behavior, shear rheological measurements are the method of choice. Nevertheless, an adequate characterization of hydrogels can be challenging yet insufficient in order to not only describe, but predict printability. Therefore, this work does not only aim to give advice in order to generate artifact free measurement data, but also reveals a simple approach, that can be used to evaluate a wide range of rheological model systems.

These model systems, consisting of simple springs and dashpots, are applicable for the description of complex, viscoelastic material properties that can be observed for polymer solutions. A direct correlation of the calculated model parameters to 3D printing processes leads to possible critical threshold values that can be used for the prediction of printability for different hydrogel systems.

References:

1. B. Duan, State-of-the-Art Review of 3D Bioprinting for Cardiovascular Tissue Engineering, Annals of biomedical engineering 45 (1), 2017, 195–209.

2. J.M. Lee et al., Design and Printing Strategies in 3D Bioprinting of Cell-Hydrogels: A Review, Advanced healthcare materials 5 (22), 2016, 2856–2865.

3. A. Blaeser et al. Controlling Shear Stress in 3D Bioprinting is a Key Factor to Balance Printing Resolution and Stem Cell Integrity, Advanced healthcare materials 5 (3), 2016, 326–333.

P30

Revealing novel power laws and quantization in electro-spinning considering jet splitting – Experimental.

Vincent Allen[1], Ursula Gunselmann, Dirk W. Schubert[1].

[1] *Friedrich-Alexander-University Erlangen-Nürnberg, Institute of polymer materials,*
Martensstr. 7, 91058 Erlangen, Germany

Vincent.allen@fau.de

Electrospinning is a process which reliably produces fibers tens of nanometers to tens of micrometers in diameter with the use of simple laboratory equipment by pushing a polymer liquid through a nozzle with an applied electric field. A new, purely theoretical model by Schubert considers applied voltage, viscosity, charge density, surface tension and jet splitting for predicting fiber diameter and the corresponding distribution for solution electrospinning [1]. Using suggestions provided in [1] an experimental investigation of changes in fiber diameter dependent on viscosity and concentration was performed using standard solution electrospinning equipment. Blend ratios of poly-ε-caprolactone (PCL) with two different molar masses (Mn = 10 kg/mol and Mn = 80 kg/mol) were deliberately varied to change viscosity almost independent of total polymer concentration in a Chloroform-Ethanol (7:3) solvent solution.

SEM and image analytical software were utilized for the determination of fiber diameter. Results revealed the existence of mono- and bi-modal fiber diameter distributions due to the occurrence of jet splitting. Theoretical predicted power laws for the fiber diameter considering an un-split base mode and a split mode were validated by analyzing systematically a large experimental space for the first time. Additionally, the prediction of an upper limit of standard deviation in relation to the average fiber diameter could be revealed, further validating the theoretical predictions. These validations of jet splitting and quantization with respect to fiber diameter distribution opens an entirely new door for predicting and modelling fiber diameters in solution electrospinning.

References:

1. Schubert, D. W., Revealing novel power laws and quantization in electrospinning considering jet splitting – towards predicting fiber diameter and its distribution. *Macromolecular Theory and Simulation,* **2019**, *in press*

P31

Using Monte Carlo simulation to probe gel-nanoparticle interfaces with restricted polymers to mimic surface topologies.

Nicholas Christiansen[1]*, *Rita S. Dias*[2]

[1]*Department of Neuromedicine and Movement Science, NTNU – Norwegian University of Science and Technology, Norway*
[2]*Department of Physics, NTNU – Norwegian University of Science and Technology, Norway*

* nicholas.christiansen@ntnu.no

The use of nanoparticles (NPs) for medical purposes has increased over the past decades, with a wide variety of applications ranging from contrast agents for medical imaging, to targeted drug and gene delivery. Recently, silica (SiO_2) NPs has been show to mediate gluing of gels and medical devices to tissue, as well as wound closure in rats [1, 2]. The adhesion was shown to be gel specific with SiO_2 NPs gluing two slabs of poly(dimethylacrylamide) gels but failing to do so with polyacrylamide gels. Besides possessing a much milder application, the NP solution showed a better rate of wound healing compared to traditional suturing methods, as well as good hemostatic capabilities.

In this work we have investigated the interaction between a single NP and a polymer network interface. The latter is simplified by using a simple chain system with varying degrees of restrictions. Restricting one end of the polymer mimics a loose chain on the surface of a gel, while restricting two ends refers to a polymer chain belonging to the gel network. The strength of the attraction between the NP and the polymer chains was varied throughout the work. Chains with one fixed end showed a similar interaction with the NP as expected from a free chain, while chains with both ends restricted showed a richer behavior that depend on node separation, where node separation mimicked the swelling of the hydrogel.

References:

1. Rose, S., Prevoteau, A., Elzière, P., Hourdet, D., Marcellan, A., & Leibler, L. (2014). *Nature*, *505*, 382.
2. Meddahi-Pellé, A., Legrand, A., Marcellan, A., Louedec, L., Letourneur, D., & Leibler, L. (2014). *Angew. Chem.*, *53*, 6369.

P32

Tuning the interactions of oligopeptides with star-like polyelectrolytes by means of charge regulation.

Raju Lunkad, Anastasiia Murmiliuk, Milan Boublík, Pavel Dubský, Mariusz Uchman,
*Pascal Hebbeker, Miroslav Štěpánek, Peter Košovan**

Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czech Republic

* peter.kosovan@natur.cuni.cz

Using a combination of experiments and computer simulations we show that variable ionization of weak acid and base groups on oligopeptides can be used to tune their interaction with polyelectrolytes. We choose oligopeptides as a model system because they can be easily prepared with a well defined sequence of various acid and base groups in the side-chains. However, the observed effect is generic and applicable to any weak ampholytes. Using molecular simulations in the constant pH ensemble we show that under suitable conditions the peptides can adsorb on polyelectrolytes on the “wrong side of the isoelectric point”, i.e. when the peptide charge in the bulk has the same sign as that of the polymer. Upon interaction with the polyelectrolyte, the weak acid and base side-chains of the peptide adopt their ionization state to the local environment. In such case, a positively charged peptide in the bulk coexists with its negatively charged form adsorbed on the polycation. The adsorption can be tuned not only by pH, but also by varying the sequence of acid and base groups on the peptide, and by their pKa and pKb. This provides new possibilities for the rational design of short peptide sequences which adsorb on polyelectrolytes and on charged surfaces at desired conditions.

P33

Soft alginate hydrogels modified with bioactive peptides as extracellular matrices for 3D fibroblast culture.

Daria Zaytseva-Zotova[1*], *R. Ruohola*[1], *W.I. Strand*[1], *A. Akbarzadeh*[1], *H. Haslene-Hox*[2], *Ø. Arlov*[2], *A. Vikenes*[2], *A.D. Hoel*[2], *G. Klinkenberg*[2], *Finn L. Aachmann*[1], *H. Sletta*[2], *Berit L. Strand*[1]

[1]*Department of Biotechnology and Food Science, NTNU N-7491 Trondheim, Norway,*
[2]*Department of Biotechnology and Nanomedicine, SINTEF Industry, Postboks 4760 Torgarden, 7465 Trondheim, Norway*

* daria.zaytseva-zotova@ntnu.no

A natural linear polysaccharide alginate is attractive material for creation of soft hydrogels that resemble three-dimensional microenvironment essential for normal functioning of fibroblasts. Alginate hydrogels have been shown to have outstanding biocompatibility, tunable physical and mechanical properties, and they can be fabricated under physiological conditions allowing gentle entrapment of living cells. But alginates do not contain any specific binding sites for cell attachment [1].

This work was aimed at development of alginate hydrogels with mechanical and biological properties tailored to the specific needs of fibroblasts. Alginates from *Laminaria hyperborea* stipe (F_G 0.68 and M_W 240-300 kDa) were periodate oxidized and then grafted with peptides, that mimic cell binding motives of laminin and fibronectin (GRGDSP, IKVAV and YIGSR), by reductive amination as described before [2]. Degree of grafting and molecular weight of the produced materials were characterized by ^{1}H-NMR and SEC-MALLS. Soft hydrogels were formed by mixing aqueous solutions of the polymers, buffer, $CaCO_3$ nanoparticles and glucono-δ-lactone. Gelation kinetics was studied using oscillatory rheometry. Viability of human lung fibroblasts IMR90 on the surface and within the hydrogels was examined *in vitro* using optical microscopy. It was shown that viability of the fibroblast depends on mechanical and biological properties of the hydrogels: IMR90 cells favoured softer gels that contained GRGDSP sequences.

This research work is a part of 3DLife project within Center of Digital Life Norway and is financed by the Research Council of Norway (project 269273).

References:

1. Andersen, T.; Strand, B. L.; Formo, K.; Alsberg, E.; Christensen, B. E. Alginates as biomaterials in tissue engineering. In *Carbohydrate Chemistry*, 1st ed.; Rauter, A. P., Lindhorst, T., Eds.; Royal Society of Chemistry: Cambridge, UK, 2012; Volume 37, pp. 227-258.
2. Dalheim, M. Ø.; Vanacker, J.; Najmi, M. A.; Aachmann, F. L.; Strand, B. L.; Christensen, B. E. Efficient functionalization of alginate biomaterials. *Biomaterials*, **2016**, *80*, 146-156.

P34

Polysaccharide-based Liquid-Core Nanocapsules as Perfluorocarbons Delivery Systems.

Małgorzata Janik[1]*, *Katarzyna Sobolewska*[1], *Szczepan Zapotoczny*[1]

[1]*Jagiellonian University, Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry,*
Gronostajowa 2 30-387 Cracow, Poland

* mal.janik@uj.edu.pl

Magnetic resonance imaging (MRI) is a powerful method based on nuclear magnetic resonance (NMR) studied from early 1970s. There are many issues connected with ^{1}H MRI and contrast agents (CAs), eg. low sensitivity, the signal from water background and intrinsic sources of contrast in tissues, requirement of the use of high concentrations of CAs resulting in toxicity, *etc.* [1]. The most interesting strategy to overcome them is the development of a "second colour" imaging using heteronuclear atoms, eg. ^{31}P, ^{23}Na, ^{19}F or ^{13}C in addition to ^{1}H [2]. According to the chemical characterization, the ^{19}F seems to be the most promising atom. It has 100% natural abundance, spin ½, the value of gyromagnetic ratio close to ^{1}H (40.08 and 42.58 MHz/T, respectively) and it has sensitivity equal to 83% of hydrogen sensitivity[3].

Perfluorinated compounds, especially perfluorocarbons (PFCs), have some limitations in biomedical use. One of the most challenging is their hydrophobicity. To overcome this problem the use of delivery system is needed. Herein, research is focused on nanocapsules as PFCs delivery system for potential ^{19}F MRI-based diagnosis. The aim of the work was to obtain polysaccharide-based nanocapsules templated on liquid perfluorinated cores by using ultrasound-assisted emulsification. The hydrophobically modified polysaccharide was used to stabilize emulsion by anchoring perfluorinated hydrophobic arms in an PFCs droplet without the need of using low molecular weight surfactants.

The encapsulation of 1-bromoperfluorooctane (PFOB), perfluorononane (PFN) and perfluoro-15-crown-5-ether (PFCE) is reported. The physicochemical characterization including morphology, sizes and stability is described. Moreover, the encapsulation efficiency on the basis of ^{19}F NMR measurements of emulsions was calculated and values for different PFCs are between 81-98%. ^{19}F NMR spectra let observe that the structure of PFCs is not changed after encapsulation.

References:

1. Atanasijevic, T.; Shusteff, M.; Fam, P.; Jasanoff, A. Calcium-sensitive MRI contrast agents based on superparamagnetic iron oxide nanoparticles and calmodulin. *Proc. Natl. Acad. Sci. U.S.A.,* **2006**, *70*, 274.
2. Shan, L.; Chopra, A.; Leung, K.; Eckelman, W.C.; Menkens, A.E. Characterization of nanoparticle-based contrast agents for molecular magnetic resonance imaging. *J. Nanopart. Res.*, **2012**, *14*, 1122.
3. Knight, J.C.; Edwards, P.G.; Paisey, S.J. Fluorinated contrast agents for magnetic resonance imaging; A review of recent developments. *RSC Adv.*, **2011**, 1*, 1415.*

Acknowledgment. M. J. gratefully acknowledges the financial support of the Polish Ministry of Science and Higher Education within the "Diamentowy Grant" Programme, grant agreement no. 0154/DIA/2016/45.

P35

Electrospun PCL-Collagen nanofiber membranes as substitutes for posterior lamellar keratoplasty.

*<u>Marcus Himmler</u>[1,2] *, Fabian Garreis[3], Friedrich Paulsen[3], Dirk W. Schubert[2], Thomas A. Fuchsluger[1]*

[1]Department of Ophthalmology, University Medical Center Rostock, Rostock, Germany,
[2]Institute of Polymer Materials, Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany
[3]Institute of Functional and Clinical Anatomy, Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany

*marcus.himmler@fau.de

Purpose:
Posterior lamellar keratoplasty (DSAEK, DMEK) currently is the gold standard for treating patients with a corneal endothelial cell pathologies resulting in functional impairment. This surgical approach depends on the availability of human donor corneas. An artificial biomimetic graft carrying human corneal endothelium could minimize this dependency giving access of this surgical method to larger numbers of patients. Thus, waiting lists could be reduced. In this study, electrospun polycaprolactone (PCL)-collagen nanofibers were tissue-engineered with corneal endothelial cells (HCEC) and analysed with regard to their potential application as artificial posterior lamellar grafts.

Methods:
Membranes were produced from nanofibers obtained by electrospinning of a polymeric solution: A blend of PCL (80 kDa) and purified collagen type I from bovine skin was dissolved in diluted acetic acid (90 % AcOH, ratio of 2:1, final concentration of 0,12 g/ml). Nanofibers were electrospun with a voltage of 15 kV and a flow rate of 1 ml/h (distance needle tip counter electrode: 15 cm). The fabricated membranes were characterized regarding fiber diameter and fiber orientation. Human corneal endothelial cells (HCEC-12) were seeded on the membranes in culture medium F99 with an initial cell count of 20.000 cells per well in 24 well plates and cultivated for 5 days. Suitability check for the nanofiber membranes as posterior lamellar graft was done using microscopic methods and focusing on cell morphology and cell-cell interface. For light microscope imaging cells were stained with haematoxylin and eosin (HE staining). Expression on the tight junction associated protein zonula occludens-1 (ZO-1) was analysed by immunostaining of HCECs.

Results:
Electrospinning of PCL-Collagen blends provided membranes in a non-woven, fibrous structure with a random fiber orientation and fiber diameter of 288 (±96) nm. With a spinning time of 5 minutes membranes with an average thickness of 10 µm were obtained, a thickness similarly to a Descemet's membrane. HCECs grown on the PCL-collagen membrane expressed ZO-1, typically for the corneal endothelium to perform as barrier between the cornea and the anterior chamber. Further imaging shows well-spread cells grown on the nanofiber membranes.

Conclusions: Randomly electrospun PCL-collagen nanofibers offer an interesting opportunity to overcome the shortage of posterior lamellar grafts. Further studies are needed to evaluate functional performance in both ex vivo and in vivo settings.

Sponsors

The Research Council of Norway

TRONDHEIM KOMMUNE

NKS

ThermoFisher SCIENTIFIC

www.thermofisher.com

Thermo Fisher Scientific is the world leader in serving science. Our mission is to enable our customers to make the world healthier, cleaner and safer. We help our customers accelerate life sciences research, solve complex analytical challenges, improve patient diagnostics, deliver medicines to market and increase laboratory productivity. Through our premier brands – Thermo Scientific, Applied Biosystems, Invitrogen, Fisher Scientific and Unity Lab Services – we offer an unmatched combination of innovative technologies, purchasing convenience and comprehensive services.

polymers

www.mdpi.com/journal/polymers

Polymers published by MDPI is an international, open access journal of polymer science that provides an interdisciplinary forum for publishing advances in in the fields of polymer synthesis and analysis, polymer physics, polymer theory and simulation,polymer processing and performance, and polymer applications. Polymers is collaborating with Nordic Polymer Days 2019 in the preparation of a Special Issue and by presenting awards to outstanding young researchers presenting their work at this conference.

BioMACROMOLECULES

pubs.acs.org/journal/bomaf6

Biomacromolecules published by the American Chemical Society, is a leading peer-reviewed scientific journals publishing leading edge research at the intersection between biology and polymer science. Biomacromolecules is reaching out to Nordic Polymer Days 2019 by presenting awards to outstanding young researchers presenting their work at this conference.

Exhibitors

TA Instruments

www.tainstruments.com

TA Instruments designs and manufactures the world's highest performing Thermal, Rheology, Microcalorimetry & Thermophysical Properties solutions by focusing on four fundamental measurements: temperature, weight, displacement, and force. TA's analytical instruments span a myriad of material types for characterization R&D/QC and applications. Innovative, accurate, easy-to-use, and reliable are words that describe a TA Instruments product. Each designed with the customer in mind, and delivers outstanding performance and is backed by superior customer support. TA Instruments are manufactured in the USA (New Castle, DE/Lindon, UT/Saugus, MA/Eden Prairie, MN) and in Hüllhorst, Germany.

matriks KJEMISK TEKNOLOGI

www.matriks.no

Matriks AS offers laboratory solutions, instruments and services in Norway. Our largest supplier is Agilent Technologies, but we also represent other suppliers including Elementar, Rigaku, Recipe, Inorganic Ventures, LabLogic, LCTech. Matriks AS is the market leader in chromatography, mass spectrometry and spectroscopy. Our main products are in liquid- and gas-chromatography, mass spectrometry, spectroscopy and systems for protein and DNA/RNA analysis. Our goal is to maintain continuous development of our team and portfolio in order to offer the best solutions and services to our customers today and in the future.

www.nmas.no/

Nerliens Meszansky was first founded in 1917 and owners are the Norwegian company Vind. Our office, application lab, service workshop and warehouse are based in Oslo, and we are today 53 employers. We are also certificates in accordance with QA system ISO 9001:2015, certified 1995 and Environmental system ISO 14001:2015, certified 2018. Among out suppliers we can mention the following: Thermo Fisher Scientific, Beckman Coulter, Promega, Foss, Gilson, Elga, AMETEK Brookfield, Büchi Glas Uster, Büchi Glas Uster, Molecular Devices, Precisa, Copan, Nuair, VKI, LGC Standards, Spex CertiPrep, Hack Lange, Pyrolab, Frontier Lab, Markes International, Macherey Nagel and PyroLab. Nerliens Meszansky is the official distributor for Thermo Fisher Scientific instruments in Norway and among the instruments we work with we can mention the following: FT-IR, Raman, UV-VIS, NIR, NMR, AAS, ICP-OES, ICP-MS, GC, GC-MS, LC/HPLC, LC-MS, IC, IC-MS, extruders and compounding, XPS and rheology.

www.mt.com/no/no/home.html

METTLER TOLEDO is a leading global manufacturer of precision instruments and services for use in laboratories and manufacturing. We offer weighing, analytical and inspection solutions along our customers' value chain. We manufacture high-end products including industrial scales, laboratory balances, Rainin pipettes and process analytics equipment. We provide Process Analytical Technology to optimize crystallization, catalyzed reactions, polymerization reactions, and other processes.

www.netzsch.com/ta

Our analytical instruments serve to characterize thermal effects and determine materials data such as the melting/crystallization of thermoplastics, glass transition temperature, thermal stability, composition of rubber mixtures, curing behavior of thermosetting materials, and E modulus values of anisotropic composites. Polymers can generally be divided into three main groups: thermoplastics, elastomers and thermosets. Their thermal properties can be determined with our thermoanalytical measuring systems in the areas of product development, quality assurance, failure analysis and process optimization.

List of participants

Sl. No.	First Name	Last Name	University / Research Institution
1	Andrea	Aguilar Sanchez	Stockholm University
2	Vincent	Allen	Lehrstuhl für Polymerwerkstoffe Universität Erlangen-Nürnberg
3	Alessandro	Amella	Friedrich–Alexander University Erlangen–Nürnberg
4	Christian	Andersen	Danish Polymer Centre, DTU Chemical Engineering
5	Erik	Andreassen	SINTEF
6	Marte	Arntsen	RESMAN
7	Sulalit	Bandyopadhyay	NTNU
8	Muhammad Ahsan	Bashir	Jotun AS
9	Linn	Berglund	Luleå university of technology
10	Victoria Ariel	Bjørnestad	University of Oslo
11	Pablo M.	Blanco	University of Barcelona
12	Kjartan Tobias	Boman	Jotun AS
13	Dag Werner	Breiby	NTNU
14	Edit	Brodszkij	Aarhus University
15	Antonio	Capezza	KTH/SLU
16	Hyejeong	Cheon	NTNU
17	Ravindra Reddy	Chowreddy	Norner Research AS
18	Nicholas	Christiansen	NTNU - Norwegian University of Science and Technology
19	Arild Holm	Clausen	NTNU
20	Corinna	Dannert	NTNU
21	Rita	Dias	NTNU Norwegian University of Science and Technology
22	Andreas	Echtermeyer	NTNU
23	Ulrica	Edlund	KTH Royal Institute of Technology
24	Anastasiia	Fanova	Charles University
25	Muhammad	Farooq	Aalto University
26	Vivian	Farstad	Jotun A/S
27	Betsy	Feng	Polymers, MDPI
28	Ekkehard	Füglein	NETZSCH-Gerätebau GmbH

29	Karolina	Gaska	Chalmers University of Technology
30	Shiyu	Geng	Luleå University Of Technology
31	Wilhelm	Glomm	Sintef As
32	Anna	Gruszkiewicz	Jagiellonian University
33	Gabriela	Grześ	Jagiellonian University
34	Stephanie	Haider	Johannes Kepler University
35	Finn Knut	Hansen	University of Oslo
36	Bashar	Haseeb	Chalmers University of Technology
37	Andrea Pettersen	Helåsen	Ntnu
38	Karl Alexander	Henn	Aalto University
39	Sami	Hietala	University of Helsinki
40	Hilde	Hindbjørgmo	RESMAN
41	Tim	Höhnemann	Lehrstuhl für Polymerwerkstoffe, Universität Erlangen-Nürnberg
42	Billy	Hoogendoorn	Kth, Royal Institute Of Technology
43	Daniel	Hutchinson	Kungliga Tekniska Högskolan
44	Søren	Hvilsted	Hvilsted Consult
45	Jonna	Hynynen	Chalmers University of Technology
46	Arne	Ilseng	NTNU
47	Susie	Jahren	SINTEF
48	Małgorzata	Janik	Jagiellonian University
49	Heidi	Johnsen	Sintef Industry
50	Helena	Jönsson	Pyrol AB/Exhibitor Representative for Nerliens Meszansky
51	Helena	Jönsson	Pyrol AB
52	Roland	Kádár	Chalmers University of Technology
53	Fuad	Karimov	SINTEF
54	Christian	Karl	SINTEF AS
55	Mattias	Karlsson	KTH Royal Institue of Technology
56	Malcolm	Kelland	University of Stavanger
57	Kenneth	Knudsen	IFE
58	Peter	Kosovan	Charles University
59	Andrey	Krauklis	NTNU
60	Claus	Larsen	TA Instruments
61	Petter	Lassen	Matriks AS
62	Karsten	Leucker	Institute Of Polymer Materials

63	Thor	Lichtenthaler	Matriks AS
64	Giada	Lo Re	Chalmers University Of Technology
65	Tia	Lohtander	Aalto University
66	Mikael	Lund	Lund University
67	Reidar	Lund	University of Oslo
68	Anja	Lund	Chalmers University of Technology
69	Pontus	Lundberg	Thermo Fisher Scientific
70	Ole Vidar	Lyngstad	SINTEF Manufacturing
71	Sina	Lystvet	Jotun
72	Michael	Malkoch	KTH Royal Institute of Technology
73	Vickram	Mangru	NETZSCH-Gerätebau GmbH
74	Hannah Thorunn	Monsø	NTNU
75	Kell	Mortensen	University of Copenhagen
76	Anastasiia	Murmiliuk	Charles University
77	Josefine Eilsø	Nielsen	University of Oslo
78	Fritjof	Nilsson	KTH
79	Kristiina	Oksman	Luleå University of Technology
80	Erfan	Oliaei	RISE Bioeconomy, KTH
81	Richard	Olsson	KTH Royal Institute of Technology
82	Sindre Nordmark	Olufsen	NTNU
83	Monika	Österberg	Aalto University
84	Sebastian	Östlund	Mettler Toledo
85	Vegar	Ottesen	NTNU
86	Yingwei	Ouyang	Chalmers
87	Hüsamettin Deniz	Özeren	KTH
88	Arun Kumar	Panneer Selvam	IFE
89	Eleonora	Parelius Jonasova	NTNU
90	Kristofer	Paso	NTNU
91	Anna-Maria	Persson	Ntnu / Sintef Industry
92	Fabian	Pooch	University of Helsinki
93	Xiaomin	Qian	Aarhus University
94	Laila Klemetsen	Rogstad	Nerliens Meszansky
95	Torhild	Røiseng	Interwell Norway
96	Joanna	Rokita	Jagiellonian University
97	Eugenia Mariana	Sandru	SINTEF Industry

98	Marius	Sandru	SINTEF Indutry
99	Markus	Schnubell	Mettler Toledo
100	Stefan	Schrüfer	FAU LSP
101	Dirk W.	Schubert	University Erlangen-Nuremberg
102	Marit	Seim	Jotun AS
103	Khushdeep	Sharma	Friedrich-Alexander-Universität Erlangen-Nürnberg
104	Anuvansh	Sharma	NTNU
105	Mika	Sipponen	Aalto University
106	Anne Ladegaard	Skov	DTU
107	Kerstin	Steyrl	Transfercenter für Kunststofftechnik
108	Bjørn Torger	Stokke	The Norwegian University of Science and Technology
109	Mihaela	Tanase-Opedal	RISE PFI AS
110	Heikki	Tenhu	University of Helsinki
111	Tony	Tiainen	University of Helsinki
112	Andrea	Träger	KTH Royal institute of technology
113	Johnny	Tran	Matriks AS
114	Tomáš	Trnka	Cray Valley Czech
115	Le Thuy	Truong	SINTEF AS
116	Alberto	Vega	RISE
117	Abhijit	Venkatesh	Chalmers University of Technology
118	Els	Verdonck	TA-Instruments
119	Elin-Melina	Visur	Nerliens Meszansky/Thermo Fisher Scientific
120	shaoquan	Wang	NTNU
121	Jiayuan	Wei	Lulea University of Technology
122	Xinfeng	Wei	Fiber and Polymer Technology, KTH Royal Institute of Technology
123	Sylwia	Wojno	Chalmers University
124	DONG	YANG	University of Helsinki
125	Xinchen	Ye	KTH Royal Institute of Technology
126	Daria	Zaytseva-Zotova	NTNU
127	Yizhi	Zhuo	Norwegian University of Science and Technology
128	Nataša	Žuržul	NTNU
129	Libor	Zverina	Danish Polymer Centre, DTU