

# Abstracts Materials for Tomorrow 2023 Day 1-3

## Day 1 Wednesday November 8

BEN J. BOYD

### Probing the emerging concept of the gastrointestinal biomolecular corona

#### Biography

Prof. Ben Boyd is a colloid and physical chemist with PhD from the University of Melbourne. After industry experience in the explosives and pharmaceutical industries, he commenced an academic position at Monash Institute of Pharmaceutical Sciences (MIPS) at Monash University in Australia. He has previously held an Australian Research Council Future Fellowship, and was recently awarded a Novo Nordisk Laureate Research Fellowship, based primarily at the University of Copenhagen. His research focuses on colloidal and structural aspects of lipids, lipid self-assembly and pharmaceutical systems, and his group is active in developing new synchrotron-based characterization approaches for lipid and solid-state systems. More recently he has established a new group at University of Copenhagen investigating the formation, structure and implications of the gastrointestinal biomolecular corona. He is an elected Fellow of the Controlled Release Society and the American Association of Pharmaceutical Scientists. He has held leadership positions across a range of scientific societies, most recently as President of the Controlled Release Society and President of the Australasian Colloid and Interface Society. He is also co-editor of the Journal of Colloid and Interface Science, and was Editor for Asia for Drug Delivery and Translational Research.

#### Abstract

It is now well understood that particles administered to the bloodstream adopt a biomolecular corona consisting of both proteins and lipids. The composition and structure of the corona dictates the interaction of the particles with tissues, modulating attributes such as delivery and toxicity. The analogous concept of the gastrointestinal biomolecular corona has received relatively little attention, yet is anticipated to be an important consequence of a wide range of particles, and could have positive or detrimental impact on the behaviour of the particles in the gut and their interactions with gut biology. The group has been exploring this concept in a few areas, asking questions around the structure and composition of the biomolecular corona formed on drug particles, inorganic particles such as silica particles and metal oxides, as well as lipid emulsions and structured lipid particles. The media range in complexity from simple bile salt micelles through to very complex systems such as milk. To study these we use a range of scattering (small angle X-ray and neutron scattering) and spectroscopic methods (CD, low frequency Raman scattering) and analytical separation and quantification to try to link composition of the corona to structure, and ultimately the fate of the particles. Some early findings include that the presence of the corona can impact on drug solid state behaviour, bioactive proteins can be enriched on inorganic particles upon exposure to milk, and protein denaturation at the surface can be altered through differences in gastrointestinal media composition. The early studies will act as a signpost for future investigations of how differently structured corona on particles can alter interactions with gut microbiome and mucus.

## JOHAN KARLSSON

### Nanoparticles for programming immune cells

#### Biography

I have since the beginning of my research career been active in the field of nanomedicine. As a Ph.D. student in Prof. Martin Andersson's lab at Chalmers University of Technology, we demonstrated the use of mesoporous biomaterials for inbuilt controlled release of active therapeutic agents from bone anchoring implants to promote bone integration. I later became postdoctoral fellow in the labs of Prof. Peter Searson and Prof. Jordan Green at the Johns Hopkins University, where my research focused on engineering nanoparticles for crossing biological barriers to reach cells that determines the disease progression of cancer. We demonstrated how programming of cancer cells and immune cells can be used for new and improved cancer immunotherapies. I was recently recruited to Linköping University and the Dept. of Physics, Chemistry and Biology, where my lab will focus on immunoengineering strategies using biomaterials to program immune cells for precision medicine approaches.



#### Abstract

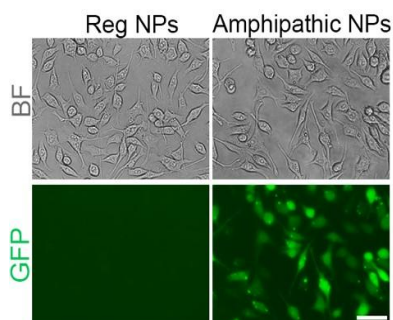


Figure 1: Optical readout using GFP to identify nanoparticles for efficient dendritic cell (DC) transfection

An approach with tremendous potential for cancer treatments is to harness the inherent capability of our immune system to attack tumor cells. Technologies that would induce signaling of tumor antigens in antigen-presenting cells (APCs); such as dendritic cells (DCs), have the potential to realize personalized cancer vaccination. Our strategy to address this technical challenge is to deliver mRNA that encodes cancer-specific antigens to instruct for antitumor immune responses. However, this approach requires intracellular delivery of mRNA to induce the expression of the encoded antigen. We have accordingly engineered polymeric nanoparticles for highly efficient intracellular delivery and preferential delivery to dendritic cells. We have carried out high-throughput *in vitro* screening for structure-functional understanding *identify*

*nanoparticles for* of cellular uptake and endosomal escape based on nanoparticle design. Furthermore, these nanoparticles were engineered for systemic administration and facilitated tissue-mediated delivery to the spleen, and preferential delivery to dendritic cells *in vivo*. The biodegradable nanoparticles delivering antigen-mRNA strongly reduced the tumor burden in *in vivo* tumor models of murine melanoma and colon adenocarcinoma.

## ANGELA B. GROMMET

### Under Confinement: Separation, Transportation, and Reactivity Modulation

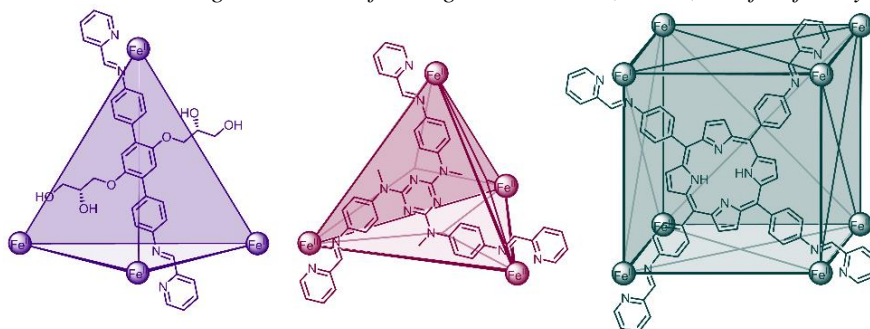
#### Biography

Angela Grommet is a newly appointed Assistant Professor within the Department of Chemistry and Chemical Engineering at Chalmers University of Technology. She was hired in 2022 under the auspices of both the Nano and the Materials Science Areas of Advance. Angela earned a BSc in Chemistry and minors in Physics and English Literature from Kansas State University in 2013. And – as you may have inferred – she’s “not in Kansas anymore”. Angela was swept over the rainbow to conduct her PhD in Chemistry at the University of Cambridge, which she completed in 2018. She then took up a Zuckerman Postdoctoral Fellowship at the Weizmann Institute of Science, and moved to the Karolinska Institute as a postdoctoral researcher in 2021. During her tenure at the Karolinska Institute, Angela was awarded a Marie Skłodowska-Curie Postdoctoral Fellowship, which she declined in favor of joining Chalmers.

#### Abstract

Coordination cages are supramolecular boxes that assemble spontaneously when the right organic ligands (L) and transition metal cations (M) are combined in solution. The size and shape of these boxes can be controlled by changing the geometry of the organic ligand, and the coordination geometry around the metal center. Furthermore, cages contain central cavities, allowing them to serve as “hosts” for encapsulating “guest” molecules. And upon confinement within coordination cages, guest molecules often behave differently than they do in solution, leading to accelerated reactivity, enhanced selectivity, or altered stability.

*Figure 1. Coordination cages assembled from ligands with two-, three-, and fourfold symmetry.*



Nevertheless, cage cavities tend to be highly symmetric, leading to poor size- and shape-complementary with prospective guest molecules, and hampering translation of laboratory observations to industrial applications. Cavity environment can be tuned by combining two or more types of ligands to create heteroleptic cages, but often requires clever design and significant synthetic effort. In the Grommet research group, however, we are pioneering methodology to streamline the preparation of heteroleptic coordination cages. By reducing the barrier to identifying the best cage for a given application, we envision that this methodology will allow us to begin using cages as porous materials, as catalysts, and as receptors.

CELINE CALVINO

## From Stimuli-Responsive System to Renewable Materials

### Biography

Céline received her MS degree from the department of Chemistry at the University of Fribourg, Switzerland, with a focus in organic synthesis, polymer chemistry, and materials science. She completed her master's thesis at Asulab, a division of The Swatch Group R&D Ltd, investigating the formation of homogeneous and resistant anchor layers on the surface of watch components, and on the introduction of the epilam (anti-spreading agent) effect using controlled polymerization processes via "grafting from" and "grafting to" methods. Céline stayed in Fribourg to pursue her PhD in polymer chemistry and materials at Adolphe Merkle Institute. Her thesis focused on the design of chromogenic systems relying on supramolecular interactions and on their incorporation into polymeric materials to create new functional mechanoresponsive materials. Céline embarked on her postdoctoral journey at the Pritzker School of Molecular Engineering, University of Chicago, supported by a SNFS Mobility Fellowship. Her research focused on the use of dynamic covalent chemistry to functionalize cellulose nanocrystals and on the development of appropriate engineering melt processes for the preparation of mechanically reinforced and sustainable nanocomposite materials. In 2021, Céline was appointed as Junior group Leader and principal investigator at the University of Freiburg, Germany, with a research interest on the design of stimuli-responsive systems to achieve renewable polymer materials.

### Abstract

Responsive materials, capable of adapting their properties in response to external stimuli (i.e. temperature, light, or mechanical force) in a predictable manner, hold great promise in enhancing sustainability and prolonging material life cycles. In this context, our research introduces innovative approaches leveraging stimuli-responsive systems to advance the sustainability of polymer materials. The first approach integrates photoswitchable chemical motifs that can form and break bonds upon exposure to distinct wavelengths of irradiation. A meticulous examination of photomediated formation and cleavage reactions enabled a near-perfect optimization of reaction yields, approaching 100%. Furthermore, the successive execution of both reactions demonstrated a remarkable level of cyclability on both molecular and macromolecular levels, underscoring the potential for future renewable polymerization and ligation mechanisms. The second approach centers on mechanically-activable encapsulated chemistries to produce versatile functional composite materials. Self-reporting materials function has been achieved by encapsulating chromophores, which, upon release, undergo physical changes and result in a visible color change in the damaged region of the material. In an alternate system, these encapsulated entities were employed to trigger the degradation of adhesives upon mechanical compression. The functionality of these composite adhesives has ultimately been harnessed to induce controlled debonding on demand. In summary, our work aims to demonstrate how stimuli-responsive systems can serve as a tool to enhance the sustainability of materials, whether by extending their lifespan or enabling their reutilization.

## MARGARITA TROBOS

### “Race for the surface” between bacteria and immune cells on biomaterials

#### Biography

Assoc. Prof. Margarita Trobos holds a PhD in Medical and Infectious Microbiology from the University of Copenhagen and the Statens Serum Institut (Denmark), and a previous MSc in Biology from Salamanca University (Spain). After working shortly as consultant for the World Health Organization, she became the leader of the Infection Control projects and coordinator of the BIOMATCELL VINN Excellence Center of Biomaterials and Cell Therapy at the Department of Biomaterials (University of Gothenburg).

Currently, Assoc. Prof. Trobos leads a research group with focus on biomaterial-associated infections, covering aspects on the pathogenesis (biofilm mechanisms and antimicrobial resistance) and evaluating novel diagnostic, preventive and therapeutic strategies. She has developed innovative models and techniques to study bacterial-host-biomaterial interactions. In collaboration with clinical partners, she evaluates new tools to improve the diagnosis and treatment of infections associated with orthopaedic implants.

#### Abstract

Gristina *et al* in 1987 suggested that the fate of a medical implant is decided in a “Race for the surface” between bacteria and host cells, where whichever is first to colonize the surface will dominate it. Bacteria can form a biofilm on an implant surface and can lead to infections difficult to treat.

Surface properties, like topography and chemistry, have been shown to influence bacterial and host cell attachment. The surface of Ti6Al4V has been modified to contain well defined hierarchical topographical features, wettability, and antimicrobial compounds.

The aim was to investigate the role of topography and chemistry on the “race for the surface” between bacterial and host immune cells.

Results from *in vitro* monocultures and cocultures of THP-1 macrophages and *Staphylococcus aureus* on Ti6Al4V-modified surfaces, performed during early and late adhesion timepoints, will be presented.

## DAN ISAKSSON

From small to big carriers.

How surface interaction helps to reduce carbon dioxide emissions in shipping.

#### Biography

I am currently working as a Senior Chemist & Laboratory Operations Manager at I-tech AB. In 2006 I received my PhD degree in organic Chemistry from Royal Institute of Technology in Stockholm. My PhD contained among other things attempted synthesis of a natural product with possible use against marine fouling. I spent 2007-2009 as a post doc in the Marine Paint project at Chalmers university of technology, looking at possible delivery systems for medetomidine in marine paints. Joined I-tech in 2009 and worked there since then.



#### Abstract

Shipping is the biggest and most efficient carrier of goods around the world. But in order to be efficient the hull of the ship need to remain clean and the frictional resistance of the ship moving thru the water should be kept to a minimum. This is accomplished using marine paints that protect the hulls from attachment and growth of marine

organisms (marine fouling). The majority of marine paints used today contain biocides that help protect the hull against fouling. Depending on the specification a marine paint is designed to last for 3-5 years with a constant slow release of biocides from coated surface. This presentation will describe how we use small inorganic particles as carriers for our biocide Selektepe and controlling its release so that it lasts for the designed lifetime of the coating system.

## LISA SKEDUNG

### Towards a PFAS-free industry

#### Biography

Lisa Skedung has a PhD in surface chemistry from KTH (2012). The research topic was psychophysics, linking human tactile perception with physicochemical properties of various surfaces and materials. She started as a researcher at RISE (then SP) directly after her PhD and has further developed the tactile perception area at RISE. Since then, she has managed and worked in many bilateral and consortium-based research projects related to human perception of all kinds of materials, material/surface characterization, tribology, human skin, cosmetics, formulation, biobased materials and chemical substitution. Lisa has worked actively since 2016 with projects promoting PFAS-free alternatives and substitution of PFAS, including POPFREE projects funded by Vinnova and partners, for which she has been the project manager for three. One of them was the POPFREE Ski goes Global project, which has paved the way for PFAS-free competitive skiing. Spreading awareness about PFAS and helping industry in their phase-out journey, is a genuine interest.



#### Abstract

Per- and polyfluoroalkyl substances (PFAS) are a broad class of chemicals (> 10 000 substances) used throughout society in consumer products, high tech applications and industrial processes. Despite widespread use, PFAS are highly persistent, and many are linked to adverse health effects. Consequently, PFAS restriction and phase-out initiatives have increased recently, culminating in the submission of a class-wide restriction proposal to the European Chemicals Agency. Although legislation is not yet at place, many companies have been motivated to phase out PFAS. Many PFAS-free alternatives and products have been developed, not least by partners in the POPFREE projects. However, there is an urgent need for new innovations, where the greatest challenge seems to be alternatives to fluoropolymers used in harsh environments. The presentation will address both uses where alternatives have been developed as well as uses that need new PFAS-free solutions (materials for tomorrow).

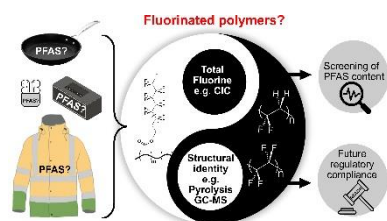


Figure 1: Screening for PFAS content in products

identification of polymeric PFAS in a wide range of consumer products. This combination of analytical methods screen for a wider range of PFAS substances and can help companies understand if they have PFAS in their products, and regulatory bodies to screen products for compliance with future regulations.

In the proposal for a broad PFAS restriction, that is now under consideration in EU, there is a requirement not to exceed 50 ppm F ( $\mu\text{g F/g}$ ), to include both polymeric and non-polymeric PFAS. Within the POPFREE Industry project, combustion ion chromatography (CIC)-based total fluorine (TF) determination together with pyrolysis-gas chromatography-mass spectrometry (Pyr-GC/MS) have successfully been used for quantification and

RUIFEI WANG

Controlling droplet properties for sustainable agriculture

#### Biography

Dr. Ruifei Wang received his PhD in Industrial Biotechnology from Chalmers University of Technology, Sweden. He joined Nouryon in 2018 and since then has been working as R&D Scientist and Project leader. He is actively involved in several projects in boosting agriculture productivity by developing novel and green adjuvants. He is also the technical lead at Nouryon on biopesticide formulation for Agricultural and Food.



#### Abstract

The characteristics of droplet are of great importance for delivering agrochemicals to plants. Surfactants and polymers, referred to adjuvants, are useful tools in manipulating properties of droplets, and their interaction with plant surfaces. Adjuvants play a critical role in enhancing efficacy of pesticides and fertilizers, and are therefore widely used in modern agriculture practices. In this presentation, the functionalities of adjuvants are reviewed. Three attributions of adjuvants are highlighted, drift control, retention and penetration enhancement. Our current understanding is shared on the physiochemical mechanisms of adjuvants in these sub-steps. Better understanding the surface science involved in agriculture is a cornerstone for innovation and advancing precision delivery system. More research and actions are needed to secure food production in a sustainable way for the generations to come.

Day 2 Thursday November 9

ROSA M. ESPINOSA-MARZAL

Long-range interactions in highly concentrated electrolytes

#### Biography

Dr. Espinosa-Marzal is a Professor at the University of Illinois at Urbana-Champaign (UIUC) in the departments of Material Science & Engineering and Environmental Engineering & Science. She has a Ph.D. in materials science & engineering from Hamburg University of Technology (Germany). After her Ph.D., she was a postdoctoral fellow at the Princeton Institute for the Science and Technology of Materials. Prior to joining Illinois, Dr. Espinosa-Marzal spent four years as senior scientist in the laboratory of surface science and technology at the ETH Zurich in Switzerland. Since 2016, she serves as member of the executive committee of the Division of Colloids and Surface Chemistry at the American Chemical Society in the role of membership secretary. Her interests include soft matter and functional interfaces, as well as biomineralization.



#### Abstract

Ionic liquids (ILs) are a highly promising class of electrolytes for myriad applications, from energy storage to solvents for reactions and lubricants. These electrolytes, in their pure form, only comprise of ions, which gives rise to a unique combination of properties, such as being non-flammable, non-

volatile, and excellent solvents, but less prone to thermal and electrochemical decomposition compared to traditional organic solvents. ILs can thus operate at higher voltages and offer reduced safety concerns. In addition to ILs, other highly concentrated electrolytes have been also found to offer advantages in energy applications, an example of which is aqueous LiTFSI. Advancing the fundamental knowledge of the electrical double layer of highly concentrated electrolytes can help establish design principles for targeted applications. In the first part of this talk, I will summarize our recent progress in understanding the electrical double layer of highly concentrated electrolytes based on measurements with a Surface Forces Apparatus, and Atomic Force Microscopy, among others.

In their pure form, ILs exhibit high viscosity and moderate ionic conductivity. Doping the IL with alkali metal salts bearing the same anion as the host IL, a concept known as salt-in-ionic liquid (SiIL), has the potential to facilitate ion dissociation, reduce viscosity, and augment the conductivity of the metal cations. This behavior opens up opportunities for harnessing the advantageous properties of IL electrolytes in battery applications. It is well known that short-range oscillatory forces in ILs originate from the overscreening provided by ion layers that accumulate close to the charged surface. In the second part of this talk, I will show how salts modify such overscreening and present new results of long-range surface forces mediated by SiILs. I will also compare experiments and theory to propose an alternative explanation of the long-range force found in highly concentrated electrolytes.

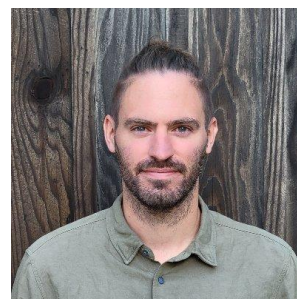
ALEXANDER GIOVANNITTI

Next-generation polymeric organic semiconductors for electrochemical transistors with applications in bioelectronics

Alexander Giovannitti, Garrett LeCroy, Camila Cendra and Alberto Salleo

Abstract

Over the last decade, significant progress has been made in developing efficient mixed-organic-ionic electronic conductors (OMIECs) for electrochemical transistors. Improvements in device performance for both transconductance and operational stability paved the way for applications of electrochemical transistors for health monitoring, neuromorphic computing, or electrochemical sensors. While the tuning of the energy levels [1] (via backbone engineering), and the local environment of the polymers [2], (via side-chain engineering) is reported to be a successful strategy for improving the electronic and ionic charge transport properties, little is known about how the short- and long-range order of polymers impacts the device performance.



In my talk, I will discuss the importance of microstructure and dynamic microstructural rearrangements of OMIECs which greatly influence the electronic charge transport properties in electrochemical transistors. By combining electrochemical and spectroelectrochemical measurements alongside electrochemical X-ray diffraction measurements, we observe that holes and anions are placed in ordered aggregates and crystallites at relatively low charge carrier densities ( $< 2 \times 10^{20} \text{ cm}^{-3}$ ) for selected OMIECs [3], explaining the large increase in transconductance at low operational voltages. Moreover, we find that the electrochemical charging of p-type polymeric OMIECs induces structural order along the polymer backbones. We interpret this structural ordering as the key factor for achieving high transconductance since percolating networks can form more easily when polymer chains are planarizing. Surprisingly, these dynamic microstructural rearrangements are highly reversible, however only when high charge carrier densities are avoided at which bipolarons



are formed. Based on these findings, I will discuss chemical design strategies for next-generation OMIECs with improved transconductance and operation stability in electrochemical transistors.

- [1] Alexander Giovannitti, Reem B. Rashid, Quentin Thiburce, et. al., *Adv. Mater.* 2020, 32, 1908047 [2] A. Giovannitti, D.-T. Sbircea, S. Inal, et. al., *Proc. Natl. Acad. Sci.* 2016, 113, 12017.  
[3] Garrett LeCroy, Camila Cendra, Tyler J. Quill, et. al., *Horiz.*, 12, 2023.

## HAINING TIAN

### The Role of Surface States of NiO in Dye-sensitized Mesoporous NiO Photocathodes: *Angel or Devil?*

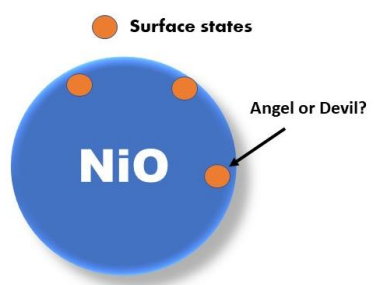
#### Biography

Haining Tian is an Associate Professor (Universitetslektor) at Uppsala University, Sweden, leading a research group of Molecular Devices for Artificial Photosynthesis. He obtained his PhD in Applied Chemistry at Dalian University of Technology (DUT) in 2009 and then moved to Royal Institute of Technology (KTH) as Postdoc and senior researcher until 2014 before he started his independent research at Uppsala University. His research interests focus on development and investigation of sustainable materials including inorganic materials, molecules and polymers for solar energy conversion and storage. He has published 100 papers cited by more than 7000 times, with H-index 47. He has been awarded Göran Gustafsson Prize for young researchers (2016, 2020), Young Investigator from European Photochemistry Association (2019) and Wallenberg Academy Fellow (2019).



#### Abstract

Nickel Oxide (NiO) as a p-type semiconductor has been used in many electronic devices such as gas sensor, solar cells and solar fuel devices. Due to the unstoichiometric composition of NiO material, many surface states, also known as defects, appear on NiO surface. When NiO is made into nanomaterials, the surface states are amplified, showing significant effect on device performance. In this talk, I will introduce our work on the role of NiO surface states in dye-sensitized NiO photocathode. Recently, we have shown that the NiO surface states are actually responsible for NiO



conductivity and participate into dye regeneration and catalytic hydrogen production in dye-sensitized NiO photocathode. It is also found that the electron hopping between NiO surface states is faster as compared to electron hopping between dyes in dye-sensitized NiO photocathode which is different from traditional dye-sensitized TiO<sub>2</sub> electrode.

Figure 2: Smooth and “bad hair day” erythrocyte

#### Ref.

1. L. Tian, R. Tyburski, C. Wen, R. Sun, M. Abdellah, J. Huang, L. D’Amario, G. Boschloo, L. Hammarström, H. Tian, *J. Am. Chem. Soc.*, 2020, 142 (43), 18668-18678
2. S. Wrede, B. Cai, A. Kumar, S. Ott, H. Tian *J. Am. Chem. Soc.*, 2023, 145 (21), 11472-11476
3. S. Wrede, L. He, G. Boschloo, L. Hammarström, L. Kloo, H. Tian *Phys. Chem. Chem. Phys.*, 2022, 24 (48), 29850-29861

## AJI P MATHEW

### Exploiting nanocellulose surface chemistry for designing functional materials

#### Biography

Aji Mathew is a Professor in Materials Chemistry with focus on Biobased functional materials since February 2017, at the Department of Materials and Environmental Chemistry, Stockholm University. She holds a PhD in Polymer chemistry (2001) and her current research have a strong focus on designing materials in nanoscale for a sustainable society. The research activities include nanocellulose and nanochitin isolation/ characterization, developing and characterising biobased membranes/filters for water purification, textile recycling, 3D printing of biobased hybrids and composites for medical applications; understanding surface chemistry and interactions of biobased materials, liquid phase atomic force microscopy and in situ SAXS. She currently also serves as director of the Stockholm University Centre for Circular and Sustainable Systems (SUCCESS) and contributes to the sustainable materials research.



#### Abstract

Nanocellulose, is one of the most promising green nanomaterial of modern times. The surface chemistry of nanocellulose can be tailored to create anionic, cationic or zwitter ionic functionalities. Water treatment is one of the emerging applications for nanocellulose, where its high surface area, versatile surface chemistry and nanostructured morphology take centre stage. Further more surface functional groups on nanocellulose acts as nucleating sites for designing highly functional biohybrids, in situ. We have shown that nanocellulose in combination with other components as metal organic frameworks (MOF), graphene oxide (GO), TiO<sub>2</sub> nanowires (NW) etc. offers charge-specific adsorption, size exclusion, antifouling, antibacterial properties, photocatalytic properties, magnetic properties and their combinations there off for advanced water treatment capabilities. The possibilities and challenges related to processing and use of nanocellulose and its hybrids for use as adsorbents, membranes, 3D printed filters etc will be discussed.

## ÅSA ÖSTLUND

### Better fibers to all

#### Biography

Åsa Östlund is the Head of R&D at Tree to Textile. Åsa is an expert in the fields of 'Sustainability in textiles and fashion' and has her field of research within 'Dissolution and regeneration of cellulose' and 'Textile recycling'. She also has experience in cross-disciplinary research and development, and has previously led larger initiatives (Mistra Future Fashion (2011-2019), the European network COST FP 1205 Innovative applications of regenerated wood cellulose fibres (2012-2016), etc, from her earlier position as researcher at RISE Research Institutes of Sweden.

Åsa has a PhD degree in Chemistry (2009) from Chalmers University Technology, with a background as a MSc in Physical Chemistry. She has 18 academic publications and a few public reports within Sustainable Textiles.



## Abstract

TreeToTextile is a potential game changer in the textile industry, with the vision Better fibers to all. We are developing a unique fiber technology that has low environmental impact and comes at a low cost. The process has low demand for chemicals, energy, and water, and is both resource and cost efficient. The technology has continuously been developed through life cycle assessments in order to significantly reduce our environmental footprint.



*Figure 3: Five jars containing samples from various process steps in the TreeToTextile process: sheets of dissolving pulp, spin-dope (dissolved cellulose), filaments, crimped fibers, cut staple fibers.*

With the target of being as resource efficient as possible from the cellulose pulp to a cellulosic staple fiber, the process is via a direct dissolution of cellulose in alkaline aqueous solvent and a wet-spinning into an alkaline spin bath followed by surface modification, drying, crimping and cutting of the prepared fiber. Going through these different stages of production implies that several surface chemistry related properties need to be taken into account and optimized. During the presentation some of these steps will be discussed/highlighted to illustrate the /complexity of the science/challenges related to process development.

## ALEKSANDRA BENKO

### Surface chemistry of carbon nanotubes governs their biomedical applications

#### Biography

Since 2017, I have been working at the Department of Biomaterials and Composites, Faculty Of Materials Science and Ceramics, AGH University of Science and Technology, Krakow, Poland. My research interest is focused on biomedical applications of carbon nanoforms, with special emphasis on chemical modifications of carbon nanotubes that grant them unique properties. I also design biofunctional solutions for dynamic in vitro cultures. I hold Bachelor's and Master's degrees in Biomedical Engineering (2011 and 2012) and a Ph.D. in Materials Science (2017), all from AGH University in Krakow, Poland. I've participated in two national and three international internships, at institutions including Alcami, Germantown, USA (2011), Webster NanoLab, Boston, USA (2019), and recently, Martin Andersson's group at Chalmers University of Technology, Gothenburg, Sweden (2023). I've participated in multiple scientific projects and lead 3: two already finished were funded by the National Science Centre (Preludium 08/2014 - 03/2017 and Sonatina 11/2017 - 11/2021), while



the third one, by the National Centre for Research and Development (03/2021 - 03/2024). The ongoing project aims to develop a set of biomaterial-based tools that would enhance the maturation of iPSCs-derived cardiomyocytes.

#### Abstract

Carbon nanotubes (CNTs) possess some properties that make them extremely interesting from a biomedical point of view. To name a few: photothermal, photodynamic and photoacoustic effects, fluorescence in the highly desired NIR-II region[1], high electrical and thermal conductivities or high mechanical strength[2]. Despite that, their application in biomedicine is still limited to the laboratory environment. Transition into the industry is being hindered by questionable cytocompatibility and some reports about possible carcinogenic effects. The controversies and unequivocal reports stem from the fact that the CNTs are often treated as a uniform material group with limited variability.[3, 4] Meanwhile, small and seemingly insignificant changes in the surface chemistry, dimensions, administration route or amount of defects, can all govern the way cells and/or pathogens react.[5, 6] Tailoring the CNTs' surface chemistry is the key to obtaining materials with strictly desired properties, including biodegradability.

Acknowledgement: I would like to acknowledge funding from the National Centre for Research and Development (Grant No: LIDER/7/0020/L-11/19/NCBR/2020) and from „Excellence initiative – research university” for AGH (funding no: 4862 501.696.7996).

#### References:

- [1]. Mandal, A.K., et al., *Scientific Reports*, 2020. 10(1): p. 5286.
- [2]. Benko, A., et al., *Cancer Drug Resistance*, 2021. 4(2): p. 264.
- [3]. Shvedova, A.A., et al., *Toxicology and Applied Pharmacology*, 2012. 261(2): p. 121.
- [4]. Ema, M., et al., *Regulatory Toxicology and Pharmacology*, 2016. 74: p. 42.
- [5]. Chatterjee, N., et al., *Carbon*, 2016. 108: p. 529.
- [6]. Kostarelos, K., *Nat Biotech*, 2008. 26(7): p. 774.

## YURY GOGOTSI

### Atomistic Design of 2D MXenes – Control of Properties via Surface Chemistry

#### Biography

Yury Gogotsi is a Distinguished University Professor and Charles T. and Ruth M. Bach Endowed Chair in the Department of Materials Science and Engineering at Drexel University (Philadelphia, USA). He also serves as Director of the A.J. Drexel Nanomaterials Institute. He received his MS (1984) and PhD (1986) from Kyiv Polytechnic and a DSc degree from the National Academy of Sciences of Ukraine in 1995. Together with his students and colleagues, he made principal contributions to the development of materials for electrochemical capacitors and other energy storage devices, discovered MXenes and polygonal nanotubes (graphite polyhedral crystals), demonstrated the tuning of structure and porosity of carbide-derived carbons, and developed new processes for the synthesis, surface modification, and purification of nanotubes and nanodiamonds. He is recognized as a Highly Cited



Researcher in Materials Science and Chemistry, and a Citations Laureate in Physics by Clarivate Analytics.

### Abstract

MXenes are a large family of two-dimensional (2D) transition metal carbides and nitrides, with a general formula of  $M_{n+1}X_nT_x$ , where M is a transition metal, X is carbon and/or nitrogen, T represents the surface terminations (O, OH, halogen, chalcogen, etc.), and  $n = 2-5$ . More than 50 MXene compositions have already been reported, but the number of possible compositions is infinite, if one considers solid solutions and combinations of surface terminations. MXenes open an era of computationally driven atomistic design of 2D materials.

MXenes have shown electronic, optical, mechanical, and electrochemical properties that clearly differentiate them from other materials. Moreover, those properties are tunable by design and can be modulated using an ionotronic approach, leading to breakthroughs in fields from optoelectronics, electromagnetic interference shielding, and communication to energy storage, catalysis, sensing, and medicine. In several applications, such as electromagnetic shielding, MXenes have outperformed all other materials. In this talk, I'll discuss the synthesis and structure of MXenes, their optoelectronic and electrochemical properties, as well as coupling between electrochemical redox processes in MXenes and their optical properties, which can be monitored in situ using spectroelectrochemistry techniques.

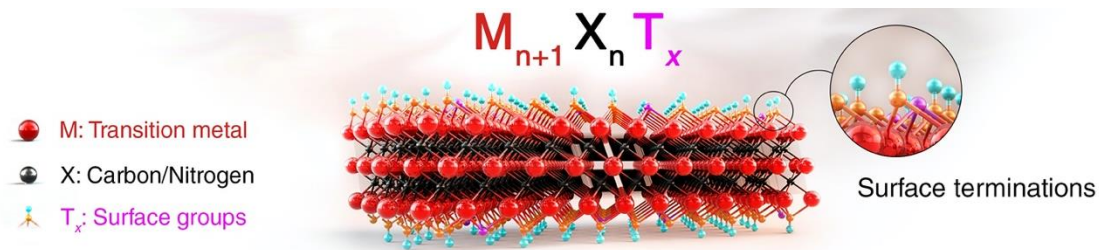


Figure 1: A representative structure of  $M_3X_2T_x$  MXene featuring its surface terminations (A. VahidMohammadi, J. Rosen, Y. Gogotsi, *Science*, 372, eabf1581, 2021)

## MATTIAS BERGLIN

### Antimicrobial peptide functionalized non-woven cellulose

#### Biography

Senior research scientist at RISE Research Institutes of Sweden, PhD in Polymer technology. Has extensive experience from interdisciplinary biomaterials research, including development of new polymers and surface functionalization in collaboration with medical scientists and industry. He has published 35+ peer-reviewed articles in the field and holds several patents.



#### Abstract

Efficient, simple antibacterial materials to combat infections are in high demand. One approach that is currently researched is the covalent attachment of antimicrobial peptide (AMP) to the material. Such technology has been heralded as an efficient strategy to lower the incidence of infection but also reduce the risk of spreading antimicrobial resistance.

Here, we will present the development of a cellulose-based solution-blown non-woven material suitable for “click on demand” attachment of functional compounds such as AMPs. This was enabled by the alkyne functionalization of the cellulose via plasma polymerization of acrylic acid followed by the EDC-coupling of propargylamine. As proof of concept, a short synthetic azide containing antimicrobial peptide (Figure 1) were designed,

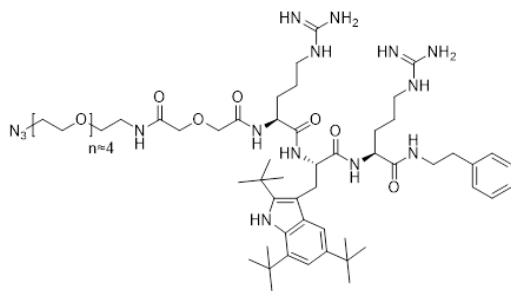


Figure 1: azide containing antimicrobial peptide

synthesized and covalently attached in a single step using copper catalysed azide-alkyne cycloaddition click chemistry. The covalent attachment of the peptide were verified by XPS and ToF-SIMS. The repelling performance of the peptide coated non-woven materials was illustrated against biofilms of *Staphylococcus epidermidis*. Our study presents the successful development of a versatile, modular, and scalable non-woven material with potential to be used in the medical field to reduce the impact of bacterial biofilms.

ANAND KUMAR RAJASEKHARAN

Amphiphilic Antimicrobial Hydrogels – A Platform Material to Enable Clinical Use of Antimicrobial Peptides in Medical Devices

Affiliation: Amferia AB

Abstract

Antimicrobial peptides are known for a long time and are a natural part of our immune system. The peptides can quickly and selectively kill bacteria, including resistant bacteria, by physically disrupting the bacterial membrane with no toxicity to the body and low risk for generating new resistance. But the clinical use of the peptides in medical device is difficult due to poor stability of the peptide which degrades in the body within a few minutes.



Amferia's patented technology, that was born out of research from Chalmers University, solved the fundamental problem of the peptide's poor stability and enables them to be used clinically as a medical device. This is achieved by permanently bonding the peptides to a solid amphiphilic hydrogel. Specifically, we take advantage of the shared property of amphiphilicity of the peptides and hydrogel (amphiphilicity is the property of a substance to like and hate water at the same time, for example like soap). This property makes the hydrogel lock the peptides in one place, protect the peptides from degradation and keeps them active and stable for 5 days (an increase in stability by 5000 times), enabling the peptides to kill bacteria in a clinical setting, safely and without leaching out of the material<sup>1</sup>!

Amferia's innovation adds further value by taking benefit from the amphiphilicity, as this allows products to be manufactured at scale using simple chemistry and existing production processes. Today the materials are used as wound dressings for infection management in human and animal wounds. The material is further being investigated for continuous development in several other areas, including sprays for deep wounds, and coatings for implants and a variety of catheters<sup>2</sup>.

The evidence behind the innovation i.e., efficacy on bacteria and safety to the body is supported through numerous scientific publications<sup>1-3</sup> (a) material characterisation (b) in-vitro microbiology and biofilm studies on bacteria including resistant bacteria in the presence of real wound fluids and (c) in-

vivo infection models in animals and (d) clinical case reports in veterinary wounds and a clinical study on human skin<sup>3</sup>.

#### References:

1. Antimicrobial Peptide-Functionalized Mesoporous Hydrogels, Atefyekta, Blomstrand et. al. published in ACS Biomaterials Science and Engineering — 2021
2. Cross-Linked Lyotropic Liquid Crystal Particles Functionalized with Antimicrobial Peptides, Blomstrand et. al. International Journal of Pharmaceutics — 2022
3. Clinical investigation of use of an antimicrobial peptide hydrogel wound dressing on intact skin, Edvin Blomstrand, Saba Atefyekta, Anand K Rajasekharan, and Martin Andersson, Journal of Wound Care —2023

## ALEXANDRA AULOVA

### Antibacterial surface: a tale of 2D filler, its orientation and the role of rheology

#### Biography

Did her PhD at University of Ljubljana on application of neural networks for modelling of viscoelastic materials and worked there at Faculty of Mechanical Engineering further on in a field of solid-state rheology, mechanical characterization of viscoelastic materials and polymer processing. In 2021 continued work on composite processing at Chalmers Technical University in a Rheology and Processing of Soft Matter group under guidance of prof. Roland Kadar. Currently working as a scientist at Nouryon Surface Chemistry, Agriculture and Food.



#### Abstract

Antimicrobial surfaces gained their importance with the rapid development of antimicrobial resistance (AMR). Surface structurization is one of the approaches efficient for fighting even resistant microbial strains. Mechanical destruction of the bacterial membrane does not allow it to develop resistivity and, therefore, is a desirable approach to design antimicrobial surfaces. One of such surfaces can be achieved by using a highly filled highly-oriented polyethylene-graphene nanoplatelet composites (PE-GnP). Materials produced by the coating of PE with GnP, batch melt mixing and extrusion through a capillary channel are slowly cut.

After chemical etching the GnP edges protruding from the surface function as blades and both prevent bacteria from attaching to

the surface and penetrate their membrane to ease their elimination. Effects of PE molecular topology and molecular weight are investigated on different levels: effect on rheological properties, on orientation and, finally, on the antibacterial properties of the prepared surfaces.

PE material with linear (HDPE) and four different branched structures (LDPEs) were utilized as matrix materials. Their molecular structure was studied by means of Gel Permeation Chromatography (GPC) and further correlated to rheological properties. Rheological characterization of GnP composites was performed using a rotational rheometer equipped with serrated plate-plate geometries to avoid slip. Extensional viscosity has been performed using a rotational rheometer accessory in order to study the

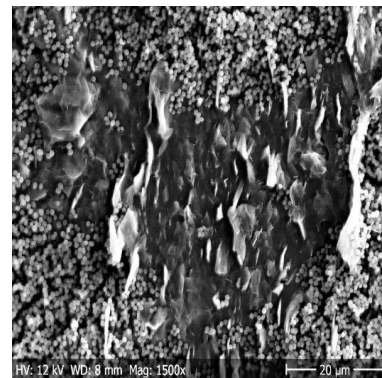


Figure 1: SEM picture demonstrating efficacy of oriented GnP against *S.aureus*

effect of branching and strain hardening factor. Small angle X-ray scattering (SAXS) was utilized to determine GnP orientation. Assessment of antibacterial properties was performed by established colony counting procedure. We discovered that molecular topology affects GnP orientation and branched PE with low molecular weight provides most favorable antibacterial properties.

*S. Pandit, et al. Precontrolled Alignment of Graphite Nanoplatelets in Polymeric Composites Prevents Bacterial Attachment, Small, vol.16 (5), 2020, [doi.org/10.1002/sml.201904756](https://doi.org/10.1002/sml.201904756)*



Day 3 Friday November 10

MATS JOHANSSON

Biobased components in organic coatings

### Biography

Professor Mats Johansson is since 2006 a full professor in polymer technology at KTH Royal Institute of Technology, Stockholm, Sweden. Between 2011 and 2023 he also acted as Head of the department. His educational background is a MSc in Chemical Engineering at KTH in 1988 and a PhD in Polymer Technology from the same university in 1992. This was followed by post-doctoral research period at EPFL in Switzerland 1992-93.



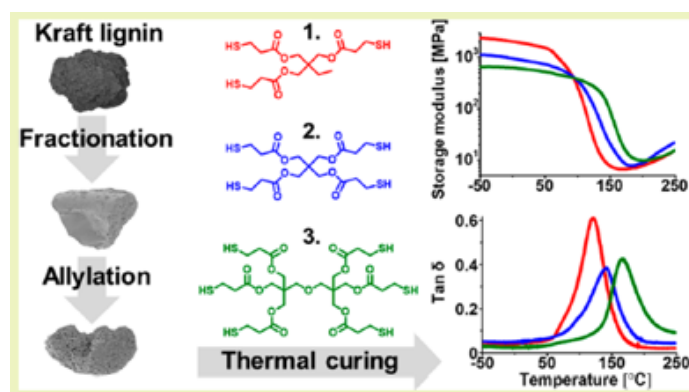
Mats Johansson has more than 30 years' experience of research in the field of polymer technology with a strong focus on synthesis and characterization of thermosets in thin film applications. Prof Johansson has published more than 165 scientific peer reviewed original research scientific publications and more than 100 conference contribution. Co-founder and member of the organizing committee for the annual conference "Coating Science International", the Netherlands from 2005 – present, acting chair for the conference 2015 – 2017. Mats Johansson is since January 2019 Editor in Chief for Progress in Organic Coatings.

### Abstract

The organic coatings industry is a large volume producer of polymer based materials used in a wide variety of applications. Significant efforts has during the last decades been made to increase the sustainability of this industry sector using various approaches ranging from replacement of organic solvents, to more energy efficient processes, and the introduction of renewable resources into the product stream.

This presentation will describe a series of different cases where research effort has been taken to address the challenge of making more sustainable coatings systems. The main focus will be on how different renewable resources can be utilized both in conventional coatings but also how the combination of new benign monomers and new crosslinking chemistries can present alternative systems.

Concrete examples are fatty acids in coil coatings, new monomers from underutilized sources e.g. bark, thiol-ene chemistry enabling use of biobased monomers in UV-curable formulations, and lignin based thermoset coatings.



ACS Sustainable Chem. Eng. 2021, 9, 1692–1702

## ROMAIN BORDES

### Cellulose-Silica composites for preventive conservation of works of art

#### Biography

Romain Bordes is leading a researcher group at the division of Applied Chemistry at Chalmers University of Technology, Gothenburg, Sweden. With a background on surfactant chemistry, he has oriented his research activities towards the fundamental and applied aspects of dispersed systems. In 2015, he started using novel surfactants and nanomaterials for the conservation of works of art, with strong emphasis on using nanocellulose and silica-based materials. This field of research continues now with preventive conservation aspects, and the development of novel adsorbents. In 2022, he co-founded the startup company Adsorbi, that has since then brought to the market the adsorbents developed within the frame of the EU project APACHE.



Romain also serves as section editor for *Current Opinion in Colloid and Interface Science* and is associate editor of *Colloids and Surfaces A: Physicochemical and Engineering Aspects*.

#### Abstract

Volatile Organic Compounds (VOCs) are a critical issue in museums and archives, as their storage spaces constitute closed or poorly ventilated areas, where VOCs can accumulate and cause irreversible degradation of works of art. This issue is more and more pressing, and the current solution is to use activated carbon as adsorbent, with its cortege of drawbacks – limited capacity, poor affinity, etc. In that context, silica and cellulose-based materials are of high interest as they are cheap, abundant, and environmentally benign. Furthermore, they can be surface functionalized to enable capturing a broad range of pollutants.



*Figure 4: Color change of the cellulose-silica adsorbents during exposure to VOCs*

In the EU project APACHE, we have developed a new family of adsorbents for small organic pollutants, i.e. formaldehyde, acetaldehyde, acetic acid and formic acid, and other atmospheric pollutants, taking advantage of the versatility offered by modifications through polyelectrolyte adsorption on silica and cellulose, along with the high specific surface of these

materials. After characterization by thermogravimetric analysis, scanning electron microscopy, Fourier transform infrared spectroscopy and nitrogen sorption, the adsorption performances have then been evaluated using gas flow reactor and Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFT), or Selected Ion Flow Tube Mass Spectrometry (SIFT-MS). VOCs maximum adsorption capacities and kinetics were also measured gravimetrically and compared with traditional adsorbents.

The developed adsorbents exhibited up to 10-fold better performance as compared to activated carbon and captured irreversibly the pollutants. We are now working on securing their production route within the spin-off company Adsorbi.

Uta Hejral

Shedding synchrotron light on model catalysts at work

### Biography

Uta studied physics at the University of Stuttgart, Germany, and at Queen's University in Kingston, Canada. After an internship at the ESRF in Grenoble, France, she moved to Hamburg, Germany, to perform her PhD studies at DESY, and obtained her PhD from the University of Hamburg. During her PhD, she pioneered the use of High Energy Surface X-Ray Diffraction for the operando investigation of model catalyst systems for gas phase catalysis.



During her postdoc times at Lund University, Sweden, and the Fritz-Haber Institute in Berlin, Germany, she combined the technique with other operando methods and applied it to the solid/liquid interface in electrocatalysis. In September 2023, Uta joined Chalmers University of Technology as Assistant Professor in the Division of Chemical Physics in the Department of Physics.

### Abstract

Catalysts are complex material systems that consist of metal nanoparticles dispersed on highly branched supports. They accelerate chemical reactions and may be key to a sustainable society, for instance by facilitating the conversion of CO<sub>2</sub> into renewable fuels or by splitting water into green hydrogen using solar and wind power. However, to improve the catalyst performance, the interplay between the atomic-scale catalyst structure, the surface chemistry and the applied conditions need to be understood under realistic reaction conditions. This means high pressures and temperatures in gas catalysis, and corrosive environments in electrolyzers.

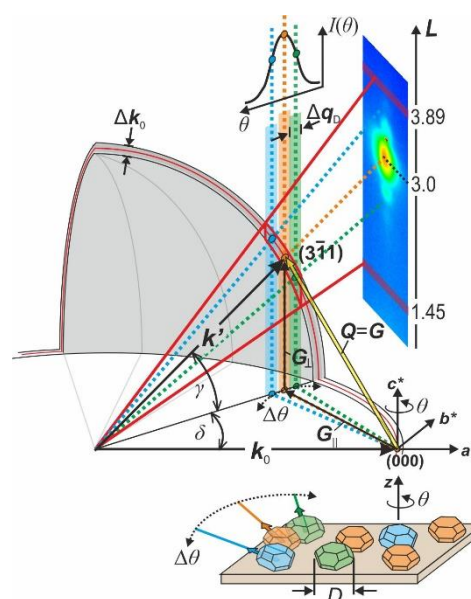


Figure 5: High-energy scattering geometry of a nanoparticle sample [2,3].

In recent years we have shown that High Energy Surface X-Ray Diffraction (HESXRD, photon energy=70-80 keV) allows a fast data acquisition for structure determination of model catalysts under reaction conditions [1-4]. Thus we could determine the atomic-scale structure of 2D surface oxides, the time-resolved tracking of transient surface phases as well as the composition-dependent size and shape-changes of alloy nanoparticle catalysts.

In this presentation I will highlight some examples of how the technique can be employed to various model catalyst systems (single crystal surfaces, nanoparticles) under harsh reaction conditions, also in combination with additional operando methods, leading to a knowledge-based tailoring of improved future catalysts.

[1] Gustafson, ..., Hejral et al., *Science* **343**, 758 (2014). [2] Hejral et al., *J. Phys.: Condens. Matter* **33**, 073001 (2021). [3] Hejral et al., *Phys. Rev. B* **96**, 195433 (2017). [4] Hejral et al., *Nat. Commun.* **7**, 1 (2016).