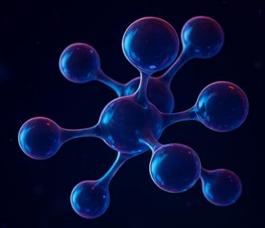
Shaping the future of material science & engineering!



## **Book of Abstracts**



**NextMatCon** 

October 17, 2025 Embuild, Hasselt, Belgium

#### Scope

This conference brings together leading researchers, industry professionals and academic experts to explore the latest advances in materials science, engineering innovation and applied technologies. This multidisciplinary conference provides a dynamic platform for cutting-edge research talks, fostering collaboration and discussing future trends across various sectors, including biomaterials, energy storage and transition and materials for smart (opto)electronics. The participants will have the opportunity to engage with keynote speakers, present their findings via interactive poster sessions and networking opportunities designed to spark innovation and drive progress in both fundamental research and industrial vision.

Join us as we shape the future of material science and engineering!

#### **Topics**

#### **Energy storage and transition:**

- Advanced solar cell technologies (e.g., Thinfilms, Solar cells (Tandem perovskites & hybrid))
- Materials enabling energy harvesting, conversion, and storage

#### **Materials for smart (opto)electronics:**

- Interconnections, device integration and printing technologies for flexible stretchable electronics
- (Organic) Light-emitting and light-detecting devices (Molecular level to device approaches)
- Optoelectronic materials and devices using hetero-structures and nanostructures

#### (Bio)materials for advanced applications:

- (Nano)materials for therapeutics and diagnostics
- Biofabrication and regenerative materials
- Innovative materials and models in toxicology

#### **Invited speakers**



Dr. Constantin d'Ydewalle (J&J Innovation Medicine) Senior Scientific Manager



**Prof. Koen Vandewal** (Hasselt university), Professor-group leader



**Dr. Gert-Jan Wetzelaer** (Max Planck Institute for Polymer Research, Mainz, Germany) Group leader

#### **Debate**

#### Dr. Sudhanshu Shukla

Researcher (IMEC, Energy Ville, Belgium)

#### Prof dr. Ken Haenen

Vicerector Research, Valorisation and internationalisation Hasselt University
Group leader Wide Band gap materials (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Prof dr. Marlies Van Bael

**Director IMO-IMOMEC** 

Responsible Design & Synthesis of Inorganic Materials (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Prof dr. Bart Vermang

Responsible Engineering Materials and Applications (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Prof. dr. ir. Wim Deferme

Engineering Materials and Applications (FME) research group (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Dr. Rozita Rouzbahani Bayatani

Senior process engineer (ASM, Belgium)

#### Prof. dr. Anitha Ethirajan

Group leader Nanobiophysics & Soft matter Interfaces (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Dr. Constantin d'Ydewalle

Senior Scientific Manager (J&J Innovation Medicine)

#### Dr. Marijke Gielen

Lab Services Manager (InvoX, Belgium)

#### Prof. dr. Koen Vandewal

Organic optoelectronics (OOE) research group (IMO-IMOMEC, Hasselt University, IMEC, Belgium)

#### Dr. Gert-Jan Wetzelaer

Group leader (Max Planck Institute for Polymer Research, Mainz, Germany)

#### Organising committee

Nele Debusschere Shabnam Ahadzadeh

Suresh Ajmeera Daniely Reis Santos

Hendrik Jeuris Marnix Persy

Alevtina Shmakova

#### MRS/E-MRS joint chapter

#### The Materials Research Societies (MRS & E-MRS)

Materials science—the pursuit of understanding, improving, and creating new materials—is essential for human progress, driving everything from technology to global sustainability. The Materials Research Society (MRS), established in 1973, and the European Materials Research Society (E-MRS), established in 1983, were founded to create an advanced, interdisciplinary platform broader than single-discipline societies.

Today, MRS/E-MRS is a member-driven global organization uniting over **20,000 materials researchers** from academia, industry, and government across more than 90 countries. Its core mission is to promote **collaboration** and an open exchange of ideas across all scientific fields (STEM), targeting projects that advance materials for the betterment of society and the promotion of **global sustainability** (e.g., clean energy and water). This international activity is showcased annually at the preeminent **bi-annual Fall- and Spring Meetings** held in the U.S. and Europe, where cutting-edge research takes center stage.

#### MRS/E-MRS Joint Chapter of Hasselt University

As part of their commitment to developing the next generation of researchers, MRS/E-MRS initiated a **University Chapter Program**. The **UHasselt MRS/E-MRS joint Chapter**, founded in **Fall 2015**, is a leading success story. It is the **first chapter in the BENELUX region** and ranks among the top five chapters in the European Union. Recognized by both the MRS and E-MRS Foundations, it effectively bridges both society communities for students and researchers.

The chapter's goal is to create a local platform for knowledge exchange and **academia-industry collaboration**. Its activities focus on **scientific outreach**, including education and popular science communication, while also addressing technological challenges impacting the Limburg region. Since its founding, the chapter has regularly held **scientific lectures** with local and international academic and industrial speakers, organized **industry visits**, and ensured student participation in the main annual MRS and E-MRS society meetings.



#### **Sponsors**

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#### Program

Time	Agenda Item	Speaker(s)
08:15 09:00	Reception	
09:00 09:15	Opening	
09:15 10:00	Lecture 1	(Bio)materials for advanced applications Dr. Constantin d'Ydewalle (J&J Innovation Medicine), Senior Scientific Manager
10:00 10:15	Coffee break	
10:15 11:00	Lecture 2	Energy storage and transition Prof. Koen Vandewal (Hasselt university), Professor, Group leader
11:00 12:15	Poster Session 1	P1-13
12:15 13:15	Lunch	
13:15 14:00	Lecture 3	Theme: Materials for smart (opto)electronics Dr. Gert-Jan Wetzelaer (Max Planck Institute for Polymer Research, Mainz, Germany), Group leader
14:00 15:15	Poster Session 2	P14-24
15:15 16:15	Debate	Chair: Dr. Shudanshu Shukla Panel: Prof. dr. Ken Haenen, Prof. dr. Marlies Van Bael, Prof. dr. Bart Vermang, Prof. dr. ir. Wim Deferme, Dr. Rozita Rouzbahani Bayatani, Prof. dr. Anitha Ethirajan, Dr. Constantin d'Ydewalle, Dr. Marijke Gielen
16:15 17:15	Pitch competition	
17:15 17:45	- Closing session and awards	

#### Lecture 1

#### Bridging Discoveries: Translational Neuroscience in Academia & in Industry

#### Constantin d'Ydewalle

Senior Scientific manager Neuroscience Discovery, Johnson & Johnson Innovative Medicine

This talk recounts a personal journey into the transformative world of translational neuroscience, where scientific discoveries gradually turned into real hope for patients suffering from neurological disorders.

I will present real-world and personal contributions from the past 15 years to illustrate how you can grow from a graduate student and academic postdoctoral fellow to a senior scientific project leader in a global pharmaceutical company. Throughout this process, I have come to appreciate and understand the vital role of interdisciplinary collaboration - between academia and industry – in transforming scientific insights into therapies that truly make a difference. My personal journey (so far) has shown me how integrating knowledge at the genetic, cellular and molecular level can unlock new possibilities for treating complex neurological conditions and ultimately improve patient lives.

In sharing this personal experience, I aim to fuel your passion for, and ambition to be part of, the exciting evolution of translational neuroscience – where discovery and innovation intersect to turn hope into reality.

#### Lecture 2

#### Organic opto-electronics for energy conversion

#### Koen Vandewal

imec, imo-imomec, Wetenschapspark 1, Diepenbeek, B-3590 Belgium Institute for Materials Research (imo-imomec), Organic Opto-Electronics (OOE), Hasselt University, Martelarenlaan 42, Hasselt, B-3500 Belgium

Organic opto-electronics has seen tremendous progress in the past decades: Organic light emitting diodes (OLEDs) are a commercial product which can be found in smart-phones and TV screens, while organic photovoltaic devices currently under development now reach power conversion efficiencies over 20% in the lab. [1]

Such solar cells would allow for an easy, light-weight, low-cost and almost invisible integration into buildings and vehicles. This presentation will give a brief overview of the relevant basic photo-physical processes occurring in organic solar cells and OLEDs. Based on our current understanding of charge carrier photo-generation, recombination, and charge transport, we will link molecular and microstructural properties to device performance parameters and limitations. [2] Based on this understanding we will further discuss recent work on new device architectures for photovoltaics [3] and photon energy up-conversion.

- 1. C. Li et al. Nat. Mater. 24, 433 (2025)
- 2. S. Ullbrich, K. Vandewalet al. Nat.Mater. 18, 459 (2019)
- 3. A. Mischok, K. Vandewal, M. Gather et al. Nat Commun 15, 10529 (2024)

#### Lecture 3.

#### Efficient and stable single-layer organic light-emitting diodes

Gert-Jan A.H. Wetzelaer<sup>1</sup>

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<sup>1</sup> Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

It is generally accepted that for organic light-emitting diodes (OLEDs) a multilayer architecture is essential for obtaining a high efficiency for the conversion of current into light. A typical multilayer OLED consists of 5 or more organic layers, which serve to transport electrical charges to the emissive layer, in which charges and excitons are confined by additional blocking layers. As such, it is ensured that electrical charges are converted into photons as efficiently as possible, which are additionally generated in the optically optimal position inside the layer stack for efficient light outcoupling. This concept has proven to be paramount for achieving high efficiency OLEDs over the last decades.

However, such a complex multilayer architecture has several drawbacks from a design and fabrication perspective. Therefore, we here aim to develop efficient single-layer OLEDs, in which charges are directly injected from the contacts into the emissive layer, without any surrounding charge-transport or blocking layers. It is first demonstrated how efficient injecting contacts can be made, to avoid losses due to injection barriers. Subsequently, charge transport in organic semiconductors is discussed from an energy-level perspective, in order to achieve balanced electron and hole transport inside the emissive layer. Combining the knowledge on charge injection and transport, efficient single-layer OLEDs are demonstrated, rivalling the performance of complex multilayer stacks. Finally, pureblue single-layer OLEDs are demonstrated, with state-of-the-art operational stability for blue OLEDs based on triplet-harvesting emitters.

## [P1] Impact of Organic Semiconductors and Device Architecture on the Efficiency and Stability of Photoelectrochemical Water Splitting

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The electrode materials, device architecture and interfacial engineering critically influence the efficiency and stability of photoelectrochemical (PEC) cells for water splitting. Organic semiconductors such as donor-acceptor polymer blends have emerged as promising materials for PEC water splitting due to their tunable optoelectronic properties and cost-effective fabrication<sup>(1)</sup>. However, their performance is often limited by some factors such as charge recombination, limited stability in an aqueous environment and charge carrier mobility<sup>(2,3)</sup>. In this study, we systematically investigate the impact of different electrode materials, surface modifications and device configurations on PEC performance. We focus on the optical and electrochemical properties of donor-acceptor polymer blends with an emphasis on the PM6 and Y6 organic materials. We employ advanced spectroscopic and electrochemical techniques such as UV-Vis absorption, Electrochemical Impedance Spectroscopy (EIS), Cyclic Voltammetry, Linear Sweep Voltammetry, and Photoluminescence to investigate charge generation, separation and their dynamics. Moreover, the analysis of catalytic materials such as Pt and Ru for Hydrogen and Oxygen evolution reactions, respectively, with protective coating is explored to enhance the stability and efficiency. The role of interfacial engineering and substrate selection i.e. ZnO/ITO is explored to enhance the performance of the system. By optimizing material and device design, this research will provide valuable insight into evolving nextgeneration PEC cells with improved photocurrent response, long-term durability and enhanced watersplitting capabilities.

- 1. Lee TH, Hillman SAJ, Gonzalez-Carrero S, Difilippo A, Durrant JR. Advanced Energy Materials. 2023;13(28).
- 2. Lee TH, Rao RR, Pacalaj RA, Wilson AA, Durrant JR. 2022;12(18).
- 3. Abe T, Nagai K, Kabutomori S, Kaneko M, Tajiri A, Norimatsu T. Angew Chem Int Ed Engl. 2006;45(17):2778-81.

#### [P2] Wearable Printed Strain—Temperature Sensor for Erectile Dysfunction Monitoring

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This work presents a wearable strain—temperature sensing system that combines a stretchable strain sensor with a temperature sensor to monitor penile erection events and improve the objectivity of Erectile Dysfunction (ED) assessment. ED is often evaluated with questionnaires or mechanical rigidity tools, which offer limited physiological detail and make it difficult to distinguish between vascular and neurogenic causes<sup>1</sup>. By measuring both deformation and temperature at the same location, our approach aims to provide a more informative signal.

The sensor patch is made on a biocompatible Flexdym substrate by screen-printing conductive silver inks. This process yields a thin, flexible structure that can be integrated into future wearable systems. The strain sensor measures axial stretch of the penile shaft through resistance changes during elongation. The temperature sensor tracks skin temperature changes linked to blood flow during erection. Prior reports indicate that penile skin temperature can rise by about 0.5-2.5 °C during erection with an average rise of ~1.5°C in healthy subjects<sup>2</sup>. To detect such changes reliably, our temperature channel provides  $\pm 0.07$  °C resolution with a response time under 10 seconds.

We calibrated the strain channel under controlled uniaxial loading and evaluated linearity, hysteresis, and repeatability. We also characterized the temperature channel against a precision reference to determine accuracy and response time. Separate characterizations confirm accurate strain detection during programmed elongation and sub-degree thermal resolution with fast response. Because the device measures both deformation and perfusion in a single, thin, flexible patch, it offers a clear path to skin-conformal use and future integration with wireless readout and data-fusion methods for objective, non-invasive ED assessment.

- 1. Leslie SW, Sooriyamoorthy T. Erectile Dysfunction. [Updated 2024 Jan 9]. In: StatPearls [Internet].

  Treasure Island (FL): StatPearls Publishing; 2025 Jan-. Available from: <a href="https://www.ncbi.nlm.nih.gov/books/NBK562253/">https://www.ncbi.nlm.nih.gov/books/NBK562253/</a>
- 2. Torenvlied, Hille & Trip, Evelien & Olthuis, Wouter & Segerink, Loes & Beck, Jack. (2024). 'Staying Hot': Investigating the influence of overnight conditions on the penile skin temperature during male sexual arousal—A novel methodology for nocturnal erection detection. BJUI Compass. 5. 439-446. 10.1002/bco2.328.

## [P3] Characterization of carbon nanotubes doped by endohedral filling for nextgeneration nanoelectronics applications

Cristian Borja-Peña<sup>1,2</sup>, Wim Wenseleers<sup>2</sup>, Sofie Cambré<sup>1</sup>

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Filling carbon nanotubes with electron-donor or electron-acceptor molecules has emerged as a promising strategy to tune their electronic properties in a controlled and stable manner<sup>1</sup>. This stability arises from the encapsulation of dopant species within the hollow core of the nanotube, protecting the molecule from environmental interactions. These hybrid systems can find potential applications in transparent conductive films, sensors, and nanoelectronic devices<sup>1</sup>.

Despite previous reports demonstrating both p- and n-type doping of carbon nanotubes, a clear and consistent spectroscopic characterization of doping remains elusive. In particular, the changes observed in the characteristic Raman features of the nanotubes vary widely across the literature, with no consensus on how doping impacts those vibrational modes. This ambiguity arises not only from the variability of the effects across different carbon nanotube diameter regimes but also from the lack of a well-defined undoped reference, as carbon nanotubes are commonly found to be slightly p-doped due to oxygen adsorption.

Additional complexity arises from the diverse forms in which carbon nanotubes are studied—powders, dispersions, or films—each of which introduces differences in the Raman and absorption spectra. Effects such as bundling, strain, environmental interactions with water or oxygen compete and affect spectral features such as shifts of the vibrational G-band in a similar manner, thereby making the assessment of doping ambiguous<sup>2,3</sup>.

To address these challenges, we have conducted a combination of spectroscopic techniques on filled nanotube samples, benchmarking their behavior compared to a neutral reference sample. These efforts aim to provide clearer insights into the spectroscopic signatures of doping and advance a more consistent framework for the characterization of doped carbon nanotubes. We then employ this characterization platform to investigate the efficiency of different filling methods, including liquid- and vapour-phase filling methods.

- 1. Allard, et al. Chem. Soc. Rev. 53 (2024) 8457–8512.
- 2. Alvarez, et al. J. Phys. Chem. C, 115 (2011) 11898-905.
- 3. Wang, et al. ACS Nano, 18 (2024) 9917–28.

<sup>&</sup>lt;sup>2</sup> Nanostructured and organic optical and electronical materials (NANOrOPT), Physics Department, University of Antwerp, Universiteitsplein 1, Wilrijk, Belgium

## [P4] Engineered In Vitro Models for ALS: Micro- and Biofabrication Tools for HumanRelevant Disease Insights

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Amyotrophic Lateral Sclerosis (ALS) is a progressive neurodegenerative disease characterized by the gradual loss of both upper and lower motor neurons. This results in muscle weakness, paralysis, and ultimately death, typically within three to five years of symptom onset. Despite extensive research, the underlying mechanisms driving motor neuron degeneration in ALS remain poorly understood. ALS pathology is shaped by multicellular interactions involving neurons, glial cells and immune components, which are difficult to accurately model using conventional 2D or 3D cell culture systems. A major limitation in ALS translational research is the poor predictive validity of preclinical models, contributing to the high failure rate of therapeutic candidates in clinical trials<sup>1</sup>.

Recent advances in microfabrication and biofabrication technologies offer powerful tools to better understand these disorders by enabling the creation of controlled, physiologically relevant in vitro systems<sup>2</sup>. This review-based poster explores how microfabrication techniques such as microfluidic chips, compartmentalized neuron-glia co-culture system, and gradient-generating platforms have advanced our understanding of key ALS-related processes, including axonal degeneration, neuromuscular junction disruption<sup>3,4</sup>. In parallel, biofabrication strategies, including 3D bioprinting and hydrogel-based scaffolds, are discussed in the context of reconstructing neural tissue architecture and mimicking extracellular matrix conditions<sup>5</sup>. The use of patient-derived iPSCs, organ-on-chip platforms, and bioengineered neural models are highlighted to demonstrate the translational impact of these approaches<sup>6</sup>. The poster concludes by discussing current challenges such as scalability, reproducibility, and sustainability, and proposes future integration strategies for accelerating biomarker discovery and therapeutic development <sup>7</sup>.

- 1. Talbot K *et al.* Guiding principles for drug discovery and development in amyotrophic lateral sclerosis. MND Association and My Name'5 Doddle Foundation: 2023.
- 2. Zhang, H. *et al.* Brain organoids-on-chip for neural diseases modeling: History, challenges and trends. *Journal of Pharmaceutical Analysis* **2025**.
- 3. Arjmand, B. *et al.* Organ on a Chip: A Novel in vitro Biomimetic Strategy in Amyotrophic Lateral Sclerosis (ALS) Modeling. *Front Neurol* **2021**, *12*, 788462.
- 4. Yu Yong, C. H., and Christopher Deppmann. A Microfluidic Culture platform to Acess Axon Degeneration. In *Axon Degeneration Methods and Protocols*, Babetto, E. Ed.; Methods in Molecular Biology, Vol. 2143; 2020; pp 83-96.
- 5. Knowlton, S. et al. Bioprinting for Neural Tissue Engineering. Trends Neurosci 2018, 41 (1), 31-46.
- 6. Osaki, T. *et al.* On-chip 3D neuromuscular model for drug screening and precision medicine in neuromuscular disease. *Nat Protoc* **2020**, *15* (2), 421-449.
- 7. Filippi, M. et al. Sustainable biofabrication: from bioprinting to AI-driven predictive methods. *Trends Biotechnol* **2025**, *43* (2), 290-303.

## [P5] Carbon nanotubes as ideal near-infrared emitters for various applications: a spectroscopist perspective

Aina Fitó-Parera<sup>1,\*</sup>, Alejandro De Sousa<sup>1</sup>, Sofie Cambré<sup>1</sup>

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Carbon nanotubes (CNTs) are among the most studied of all nanomaterials due to their exceptional mechanical, electrical, thermal, and optical properties that depend on their diameter, making them ideal candidates for a wide range of applications<sup>1</sup>. Their properties are probed by: optical absorption (in the near-infrared – visible – UV range); resonant Raman spectroscopy (RRS), to study vibrational modes; photo-luminescence excitation (PLE), to study their fluorescence emission; and, optically-detected magnetic resonance (ODMR), to investigate triplet states trapped in defects on the CNTs (see **Figure 1**). The intrinsic properties of CNTs are drastically influenced by interactions with their immediate environment, making them highly sensitive to their inner and outer suroundings<sup>2</sup>.

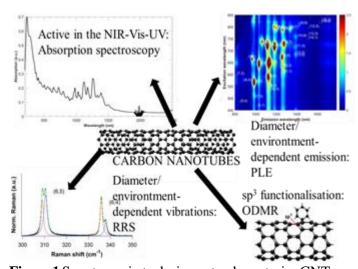


Figure 1 Spectroscoio techniques to characterise CNTs.

One excellent example is when water molecules enter the inner core of CNTs. In this case, the water molecules alter the vibrational and electronic properties in comparison to empty CNTs.3 For example, vibration modes of water-filled CNTs are shifted due to an additional restoring force exerted on the CNT by the encapsulated molecules. Also, the PL of CNTs significantly is red-shifted, broadened and drastically quenched<sup>4</sup>. We have used these

effects on the electronic and optical properties of the CNTs to investigate phase transitions of water confined to nanoscale dimensions. The 1D hollow core of CNTs also allows for unique nanohybrid structures that can tune the CNT properties for certain applications. For example, by filling SWCNTs with dye molecules a very efficient energy transfer can be achieved which of interest for solar cells<sup>5</sup>. Finally, by introducing well-controlled defects inside the SWCNT structure through functionalization, CNTs can be used as ideal nanoprobes for quantum sensing through optically-detected magnetic resonance<sup>6</sup>.

- 1. Reich S. et al., Wiley, Berlin 2003.
- 2. Allard C. et al., Chem. Soc. Rev. 2024, 53, 8457-8512.
- 3. Cambré S. et al., Phys. Rev. Lett. 2010, 104, 207401.
- 4. Cambré S. et al., ACS Nano 2012, 6, 2649-2655.
- 5. Forel S. et al., Nanoscale 2022, 14, 8385–8397.
- 6. Sudakov I. et al., ACS Nano 2023, 17, 2190–2204.

## [P6] Monitoring stagnated droplets for orchard management using flexible, printed sensors.

Asad Ullah<sup>1,2,\*</sup>, Dieter Reenaers<sup>1,2</sup>, Thijs Vandenryt<sup>1,2</sup> Ronald Thoelen<sup>1,2</sup>, Wim Deferme<sup>1,2</sup>

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<sup>2</sup>IMEC vzw, Division IMOIMEC, Wetenschapspark 1, 3590 Diepenbeek, Belgium \*Corresponding author & presenter: asad.ullah@uhasselt.be

Every year, up to 40% of crops worldwide are lost because of pests and diseases, accounting for \$220 billion in losses [1]. One major cause of these pest and disease outbreaks is the presence of stagnated water droplets remaining on leaf surfaces for extended periods, fostering a moist environment where fungal spores and pest eggs can develop [2]. This study presents the development of a printed and flexible capacitive sensor for early detection of stagnated droplets in the range of 50-500 µm for precision farming. The work includes finite element method (FEM) simulations to optimize sensor design and predict responses to droplet presence. Two sensing geometries were investigated, interdigitated electrodes (IDE) and fractal geometry-based electrodes with a dimension of 33×33 mm, initially with an electrode width of 500 µm, a gap between the electrodes of 250 µm, using electrostatic physics modelling with and without droplets. The fractal-based design demonstrates higher sensitivity due to its increased effective surface areas. The sensor was fabricated using screen printing of carbon ink on a PET substrate, enabling low cost and scalable production. Experimental characterization and sensor response measurements are planned as future work. By providing early warnings about stagnated droplets this work has the potential to reduce the use of pesticides and fungicides to prevent pest and disease outbreaks, leading to improved and sustainable crop management.

- 1. https://www.downtoearth.org.in/agriculture/at-least-40-global-crops-lost-to-pests-everyyear-fao-77252.
- 2. Dixon, G.R., 2015. Water, irrigation and plant diseases. CABI Reviews, (2015), pp.1-18.

## [P7] Impact of Cu particle size and loading on the catalytic performance of Cu/ZnO in the light-powered conversion of CO<sub>2</sub> to CH<sub>3</sub>OH

Esmee Roman<sup>1</sup>, Ken Elen<sup>1,2</sup>, Marcel A. Verheijen<sup>4,5</sup>, Daniel Mann<sup>1,3</sup>, An Hardy<sup>1,2</sup>, Pascal Buskens<sup>1,3</sup>, Marlies K. Van Bael<sup>1,2</sup>

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Achieving climate neutrality in the chemical industry requires a shift from fossil resources to sustainable energy sources and renewable feedstocks. One promising strategy is the catalytic conversion of carbon dioxide (CO<sub>2</sub>) into value-added fuels and chemicals, effectively closing the carbon cycle. Methanol (CH<sub>3</sub>OH), a key platform chemical used in the production of formaldehyde, acetic acid, olefins, and fuel derivatives, represents a highly relevant target molecule. Currently, copper-based catalysts, particularly Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> (CZA), are most widely used in the industry for the thermocatalytic conversion of CO<sub>2</sub> to methanol because of their high efficiency and stability.<sup>1,2</sup> However, these processes require elevated temperatures and pressures, typically supplied by fossil-derived heat, which limits their environmental sustainability. Therefore, photocatalytic CO2-to-methanol conversion using sunlight offers a sustainable, off-grid solution to meet rising methanol demand while reducing CO<sub>2</sub> emissions and supporting both climate and economic goals. Zinc oxide (ZnO) is a highly effective n-type semiconductor photocatalyst because of outstanding oxidation capacity, adjustable size, high chemical stability, low toxicity, and ease of preparation.<sup>3</sup> However, the limited light absorption and fast recombination of charge carriers in ZnO hinder its efficiency. Enhancements through plasmonic metal decoration (e.g., Cu nanoparticles) aim to overcome these limitations. <sup>4,5</sup> To improve catalytic performance, a more detailed investigation of the influence of Cu nanoparticle size and loading on plasmonic Cu/ZnO catalysts for solar-driven CO<sub>2</sub>-to-methanol conversion is required. In this work, we focus on the precision synthesis of Cu/ZnO catalysts, enabling systematic variation of Cu nanoparticle size (≤5 nm to ≥20 nm) and loading (1–5 wt%). By exploring the influence of Cu NP size and loading on the optical characteristics and catalytic performance of Cu/ZnO, insights into the structure-property relationships are obtained. These insights will support the rational design of efficient plasmonic photocatalysts for sustainable CO2 utilization.

This work has received financial support from the European Fund for Regional Development through the Interreg Vlaanderen-Nederland project U-SAVE, co-funded by the VLAIO network "Flanders Innovation & Entrepreneurship".

- 1. B.J. Bruna, et al. Fuel 375 (2024), 132533.
- 2. N. Barrow, et al. Sci. Adv. 10 (2024), 2081.
- 3. Y. Sun, et al. Adv. Sens. Energy Mater. 2 (2023), 100069.
- 4. F. Wang, et al. Chem. Eur. J. 29 (2023), e202202716.
- 5. J. Volders, et al. Catal. Sci. Technol. 15 (2025), 486.

#### [P8] Enhancing Water Oxidation Performance of Carbon Nitride Photoanode by Regulating Film Growth and Self-Engineered Z-Scheme Heterojunctions

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Photoelectrochemical (PEC) solar energy conversion is a promising technology to address the growing global energy demand, which is projected to exceed 30 TW by 2050, approximately twice the current supply. This approach enables the replacement of polluting and nonrenewable energy sources with clean, sustainable, and cost-effective energy harvested directly from sunlight. Carbon nitride (CN) has emerged as a promising inorganic and environmentally friendly semiconductor for driving photoelectrochemical reactions, owing to its excellent chemical and thermal stability, low cost, and favorable optical and electronic properties. However, its practical implementation is hindered by low photoactivity compared to inorganic photoanodes due to low conductivity, high charge recombination rates, and sluggish charge transfer. Here, we report CN photoanodes with photoelectrochemical water splitting performance comparable to state-of-the-art materials. The CN photoanodes were prepared by a facile and direct method by depositing carbon nitride monomers from a hot thiourea solution onto FTO substrates, followed by calcination at 500°C with different powder precursors melamine, thiourea, and urea. Incorporating powder precursors during the thermal polymerization led to favorable morphological modifications, improved structural ordering, and reduced charge transfer resistance. The powder-assisted growth using thiourea significantly enhances the PEC performance, with a threefold increase in photocurrent density. Further optimizing the thickness by tuning the concentration of the thiourea solution enhanced the overall PEC properties. These enhancements are attributed to improved charge separation and charge transfer efficiencies, as well as the formation of a Z-scheme heterojunction between the CN and SnS<sub>2</sub> layers on the FTO substrate, which facilitates more efficient charge carrier dynamics. The optimum CN photoanode achieved an excellent charge extraction efficiency and a benchmark photocurrent density of 2 mA cm<sup>-2</sup> for water oxidation and 2.7 mA cm<sup>-2</sup> for H<sub>2</sub>O<sub>2</sub> oxidation at 1.23 V vs. RHE in a neutral 0.1 M Na<sub>2</sub>SO<sub>4</sub> aqueous solution. This strategy advances the understanding of carbon nitride in fundamental photoelectrochemical studies and emphasizes its potential in practical solar-driven watersplitting applications.

## [P9] Electrical stress on metallic nanoring based networks for flexible transparent electrodes

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Transparent conductive electrodes (TCEs) are essential materials for a wide range of nextgeneration electronic and optoelectronic devices such as touch panels, displays and solar cells<sup>1</sup>. The most commonly used TCEs are based on indium tin oxide (ITO), which is not only rare, expensive and not eco-friendly to extract, but also extremely brittle, making it unsuitable for flexible devices. Therefore, there is a strong demand for alternative TCEs that are not only transparent and conductive, but also flexible and low-cost. Networks of metallic nanowires (NWs) are considered as one of the most promising alternatives to ITO.

While most of the scientific literature focusses on straight NWs (so-called nanorods), nanowires can also be manufactured in a circular shape (so-called nanorings)<sup>2</sup>. Due to their different geometry, nanorings have no dead ends in the percolation network. This could not only result in improved conductive properties but also reduce the occurrence of hot spots, leading to more durable electrodes<sup>3</sup>.

In this work, we investigate the durability of an in silico network of nanorings (like in figure 1) by subjecting them to electrical stress, which seems to be one of the most important factors influencing their durability<sup>4</sup>. The model for electrical stress is simple yet effective, as it is able to reproduce the main response features of an experimental sample under electrical stress. We also compare our results with those of a network of straight nanorods from<sup>4</sup>, who used the same stress model. We inspected the effect of the nanoring radius and density on the electrical durability of the networks.

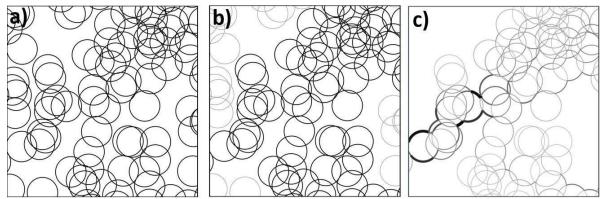


Figure 1 - An example of a nanoring network a) and its percolating cluster b). A voltage difference is placed between the vertical terminals, which results in current flowing through the percolating cluster. These currents are illustrated in c), where thicker and darker lines indicate a higher current.

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#### [P10] Organic-Inorganic Hybrid Eutectogels for Sodium-Ion Batteries

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Deep eutectic solvents (DESs), deep eutectic solvents (DESs) are ionic liquid-like mixtures formed by combining two components, creating a liquid with a much lower melting point than the individual substances. The ones based on N-methylacetamide (NMA) are gaining attention as safe, non-flammable, and cost-effective alternatives to conventional electrolytes in sodiumion batteries (SIBs), in which sodium ion(Na+) is responsible for carrying charge. However, their electrochemical stability, particularly in contact with sodium metal, as a more economical anode than lithium metal, is a critical challenge most of the time. In this study, DESs were prepared by dissolving sodium bis(fluorosulfonyl)imide (NaFSI) in NMA in two different molar ratios: a superconcentrated composition reported to improve stability, and a lower concentration aimed at balancing stability with ionic conductivity. To overcome the drawbacks associated with liquid-electrolyte batteries, such as leakage and limited mechanical robustness, these DESs were embedded into hybrid organic-inorganic silica-based matrices modified with phenyltrimethoxysilane (PhTMS) and diphenyldimethoxysilane (DPhDMS) in different ratios, resulting in mechanically more pliable eutectogels for better contact with electrodes. These modifications are intended to enhance structural resilience while retaining desirable ionic transport properties. By systematically evaluating the influence of salt concentration and matrix composition on electrochemical stability, mechanical integrity, and thermal performance, this work aims to identify optimal electrolyte formulations. The outcomes may accelerate the development of safe, efficient, and commercially viable SIBs, supporting future sustainable energy storage technologies.

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#### [P11] Structural Control of Short-Range Order in Disordered Rock Salts by a Novel Low-Temperature Solution-Based Synthesis Method

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Disordered rock salts (DRX) have the potential to replace current Ni and Co-based cathode materials, given their high energy density as well as the cheap and abundant source of precursors, enhancing sustainability in lithium-ion batteries (LIB). Its commercialization is impeded by detrimental short-range order (SRO) at the atomic level, which disrupts lithium percolation channels and decreases performance in batteries. SRO is promoted by high-temperature synthesis, which also limits F substitution. Here, we present a novel solution-based synthesis protocol to make Ti-Mn-based DRXs at low temperatures, allowing fluoride doping and opening the door for more sustainable DRX positive electrode materials for LIB. The phase purity of the product obtained from this low-temperature synthesis has been confirmed by XRD, ICP, and EDX techniques. Furthermore, the particle size and morphology have been optimized during the synthesis process to enhance the electrochemical properties of the material and the high energy densities promised by DRX materials.

## [P12] Materiomics: Training students to become future-proof materials scientists

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In 2022–2023, Hasselt University launched the Master of Materiomics<sup>1</sup>, a pioneering program dedicated to the design, development, and application of advanced materials. Rooted in materials science, the program prepares students to design sustainable and innovative materials intersection of chemistry and physics, through a combination theoretical/computational modelling and experimental techniques<sup>2</sup>. The master's program offers four specialization domains: Innovative materials for energy generation, storage, and efficiency, Sustainable materials for circular processes, Advanced materials for innovative health care, and High-tech materials for quantum technologies. Emphasizing interdisciplinary knowledge and collaboration, the curriculum bridges chemistry and physics to train materials scientists capable of addressing complex, real-world challenges. The demand for such highly skilled profiles is growing across industry and academia, including in strategic initiatives such as the Einstein Telescope. Graduates are equipped to tackle critical issues at the materials level, contributing to societal transitions such as the need for biomaterials, climate action, sustainable energy systems, high-tech health care, strong cybersecurity, and advanced space technologies. With this contribution, we aim to connect to both industry and academia to foster collaborations between the master's program and both domains.

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#### [P13] SUBLIME: Stretchable & Ubiquitous Liquid Metal Electronics

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Stretchable electronics are central to the future of soft and wearable technologies. Among the most promising materials are gallium-based liquid metal alloys (LM), which offer great conductivity and deform without breaking. When embedded into soft elastomers, these LM enable circuits that stretch, bend, and move with the surface they're mounted on—something traditional rigid electronics cannot do<sup>1</sup>. But despite their appeal, making reliable and scalable liquid metal devices remains a major challenge. Fabricating fine, consistent features from an LM that wants to bead up or flow uncontrollably is not straightforward. Unlike solid conductors, LM is hard to pattern using conventional manufacturing methods, and it poses risks like leakage or smearing. Developing processing techniques that can achieve narrow lines, strong adhesion, and stable interfaces is still an open problem<sup>2</sup>. Material interactions add further complexity. Gallium alloys can corrode or embrittle solid metals like copper or aluminium at contact points, leading to early failure<sup>3</sup>. At the same time, the soft encapsulants used to contain and protect the LM (and the LM itself) can degrade over time due to oxygen, moisture, or mechanical fatigue. These issues can significantly impact device reliability and lifetime<sup>4</sup>. SUBLIME focuses on tackling these core challenges in fabrication, materials interactions, and reliability. The project studies how LM interacts with solid contacts, aiming to develop barrier layers or surface treatments to prevent unwanted reactions. It also explores new stretchable encapsulants that improve protection and durability, including materials with self-healing properties. A strong emphasis is placed on scalable and rapid processing techniques, such as spray coating and direct writing, respectively. In parallel, the project investigates long-term reliability through dedicated testing, including mechanical cycling and environmental stress tests. These tests help identify failure mechanisms and guide improvements in materials and processing. To validate the outcomes, functional demonstrators are being developed that combine stretchable circuits with embedded components, serving as proof of concept for future applications<sup>5</sup>. The overall goal is to bring liquid metal-based stretchable electronics closer to practical use by solving the key scientific and engineering challenges that currently limit their performance, stability, and manufacturability.

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## [P14] Surfactant-free synthesis and characterization of highly dispersible antimony-doped tin oxide nanoparticles

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Antimony-doped tin oxide (ATO) nanoparticles (NPs) are widely utilized in transparent conductive films, solar cells, sensors, and smart coatings due to their excellent electronic conductivity, optical transparency, and chemical stability.<sup>1,2</sup> Although various colloidal synthesis methods for ATO NPs exist, achieving narrow size distribution and good dispersibility remains challenging. Most reported strategies rely on steric stabilization using bulky ligands or surfactants; however, this approach often compromises the electronic conductivity of ATO NPs. 1-5 In the present study, we demonstrate a surfactant-free approach for the hydrothermal synthesis of monodisperse ATO NPs with antimony doping levels ranging from 1% to 13% under alkaline conditions at 150°C in the presence of tetramethylammonium hydroxide (TMAH). Capped by N(CH<sub>3</sub>)<sub>4</sub>+ cations, the ATO NPs are highly stabilized via electrostatic repulsion, which significantly improves dispersibility and prevents agglomeration of the as-synthesized ATO NPs in water. X-ray diffraction (XRD) analysis on ATO NPs demonstrated that the samples contained SnO<sub>2</sub> with a tetragonal (rutile-like) symmetry, without any antimony-containing side phases. Further, gradual peak broadening was observed with increasing antimony content, indicating incorporation of antimony into the SnO<sub>2</sub> lattice. ATO NPs dispersed in water exhibited high transparency that increased with higher doping levels. The hydrodynamic diameter measured with dynamic light scattering (DLS) decreases from 25 nm for undoped SnO<sub>2</sub> to 5 nm for 13% Sb-doped ATO, accompanied by a narrow size distribution for all ATO NPs. Transmission electron microscopy (TEM) analysis revealed that undoped SnO<sub>2</sub> NPs possessed a cubic morphology, which progressively becomes less defined as antimony content increased. Crystallite sizes obtained from XRD, particle size distributions from DLS, and particle sizes measured by TEM were in close agreement, indicating that the nanoparticles consist of primary crystallites without significant aggregation. This work has received financial support from the Energy Transition Fund of the Belgian federal government through the ETF project BE-HyFE.

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# [P15] Synthesis and characterisation of high energy density polyanion compounds as cathode active materials for miniature, formable Li-ion batteries

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The rapid evolution of modern technology has been strongly driven by improvements in energy storage systems, such as lithium-ion batteries (LIBs). Since their commercial introduction in 1991, LIBs can be found everywhere, powering devices ranging from mobile phones and laptops to electric vehicles and grid storage systems. Their high energy density, long cycle life, and relatively low weight have made them the default choice for various applications. However, as emerging technologies such as medical implants, wearable electronics, and compact IoT devices become more prevalent, conventional battery designs face critical limitations.<sup>2</sup>

While the microelectronic components controlling these devices have undergone significant miniaturisation at rapid pace, the development of equally compact, flexible, and reliable power sources has lagged behind. Conventional rechargeable batteries are bulky and have a fixedform, causing severe limitations in device design. In practice, medical device developers are forced to design their products around the limited form factors of commercially available batteries. Ideally, batteries should be conformable, able to adapt to the available space within the device.<sup>3,4</sup>

To address these challenges, this research investigates the integration of high-energy-density polyanion cathode materials into lightweight, high-surface-area metal nanomeshes. In this study, lithium vanadium oxyphosphate (LiVOPO<sub>4</sub>) is studied as a promising high-voltage cathode material capable of multiple lithium-ion (de)intercalation reactions. Phase-pure LiVOPO<sub>4</sub> was synthesized using a hydrothermal approach, followed by a controlled thermal conversion of a hydrated precursor (LiVOPO<sub>4</sub>·2H<sub>2</sub>O) under oxygen-rich conditions. To ensure compatibility with nanostructured current collectors, synthesis parameters are being optimised to reduce the processing temperatures below 350 °C. The study further examines how synthesis strategy influences crystal structure, morphology, and electrochemical behaviour, with particular attention to particle size reduction to improve conductivity and reaction kinetics.

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## [P16] An In-Depth Study of the Thermodynamics and Kinetics of the Structural Phase Transition of Hydrothermally Synthesized W/VO<sub>2</sub> Microparticles

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Thermochromic vanadium dioxide (VO<sub>2</sub>) is widely recognized for its reversible structural phase transition (SPT) from a semiconducting monoclinic VO<sub>2</sub>(M) phase to a metallic rutile VO<sub>2</sub>(R) phase near 68 °C, accompanied by a sharp modulation in infrared (IR) transmittance. <sup>1,2</sup> This unique feature has positioned VO<sub>2</sub> as a strong candidate for smart window coatings in energy-efficient buildings.3 However, the high intrinsic transition temperature and optical limitations of bulk VO<sub>2</sub> have motivated intensive research into lowering the transition temperature and improving phase transition behaviour through metal doping and particle engineering.<sup>4,5</sup> In this study, we present a comprehensive investigation of both the thermodynamic and kinetic properties of the SPT in hydrothermally synthesized, tungstendoped W:VO<sub>2</sub> microparticles. A benign, oxalic acid-based hydrothermal method was employed to produce phase-pure VO<sub>2</sub>(M) particles with W concentrations ranging from 0.5 to 2.5 at.%. Differential scanning calorimetry (DSC) was used to extract key transition parameters, including transition temperature ( $T_{spt}$ ), enthalpy ( $\Delta H_{spt}$ ), and hysteresis width, while isoconversional kinetic analysis provided activation energy estimates for both heating and cooling transitions. Our analysis shows that W-doping successfully lowers the transition temperature (T<sub>spt</sub>) across the full doping range. A reduction of approximately 22 °C per atomic percent of W was expected, and while a decrease was observed for all samples, inhomogeneous W incorporation into the VO<sub>2</sub> lattice resulted in higher transition temperatures than theoretically predicted for the respective doping levels. High transition enthalpies ( $\Delta H_{spt}$ ) were achieved across all compositions, indicative of a highly crystalline material. However, inhomogeneous W distribution and broad particle size distributions contributed to relatively wide hysteresis widths. Calorimetric and kinetic data indicate measurable differences in activation energy barriers, suggesting that dopant level and microstructure influence switching behaviour. Results are compared to the kinetic characteristics of VO<sub>2</sub> materials prepared via classic bead milling, as reported in the literature by Calvi et al., to contextualize these findings. This work addresses a critical knowledge gap in VO<sub>2</sub> synthesis and transformation kinetics, supporting future design strategies for VO<sub>2</sub>-based smart coatings that are optically viable, thermally responsive, and kinetically stable under repeated environmental exposure. Financial support: Interreg VlaanderenNederland project U-SAVE, VLAIO network "Flanders Innovation & Entrepreneurship.

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#### [P17] Ultrasonic spray coating of PHA encapsulated silver particles for the development of safe Ag/PHA coated packaging films

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Incorporating silver nanoparticles (Ag NPs) in biobased and biodegradable polymers such as polyhydroxyalkanoates (PHA) can introduce functionality, such as antimicrobial properties <sup>1</sup>. However, the method must ensure effective interactions between Ag and microorganisms, while minimizing Ag migration under safe limits <sup>2,3</sup>. Therefore, this study aims to develop stable dispersions of Ag NPs encapsulated in PHA, which are applied as thin layers of Ag/PHA particles at the surface of extruded PHA films and analysed for potential migration of Ag/Ag<sup>+</sup>.

Ag NPs (50 nm) were encapsulated in PHA via mini emulsion encapsulation (ME) at varying loadings (0-1-5-10-40 wt.%). The resulting aqueous dispersions (<300 nm) were diluted (0.25 wt.% solid content) and ultrasonically spray coated (50 layers) onto film-extruded PHA substrates (250  $\mu$ m). Finally, the films were washed (10 or 20 times) for surfactant removal, and annealed at the PHA melting temperature (145 °C) for particle embedment. Migration was measured after 10 days submerging in food simulant A and B at 40°C ((EU) No 10/2011) using SP-ICP-MS technology (Figure 1).

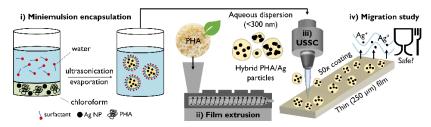


Figure 1 – Fabrication and analysis of Ag/PHA coated PHA films

Optical and SEM images show uniform coating coverage with homogeneous particle distribution. Ag migration from coated films with the highest loadings (10-40 wt.%) (absolute Ag content film <0,0056 wt.%), remained below the specific migration limit (SML) (<50  $\mu g/kg$ ) in food simulant A (<1.3  $\mu g/kg$ ), but exceeded in acidic food simulant B. By lowering the silver content in the ME process to 1-5 wt.% (absolute Ag content film <0.00034 wt.%), silver migration remained under the SML in food simulant A and B. These findings highlight the potential of the ME process to encapsulate Ag NPs in PHA as aqueous inks for USSC. Further optimization in post-treatment and NP loading can enhance scalability, processing flexibility, active performance and silver migration safety.

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## [P18] Toward reliable molar mass determination of glycolated polymer channel materials for organic electrochemical transistors

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The molar mass of polymer channel materials plays a crucial role in the performance of organic electrochemical transistors (OECTs), significantly impacting their charge transport properties. While high-molar-mass polymers typically show an enhanced mobility ( $\mu$ ) and overall performance ( $\mu C^*$ ), accurate molar mass determination remains very challenging, especially for glycolated polymers as used most often in OECTs. As a result, reported molar masses often lack validation, and literature comparisons become unreliable.

To address these challenges, dedicated batches of the benchmark p-type OECT material, pgBTTT, were synthesized using droplet flow chemistry, allowing control over molar mass via the residence time in the flow reactor. Preliminary OECT measurements suggest an optimal performance window at intermediate residence times. To accurately determine the molar mass, we are developing a new diffusion NMR calibration curve based on structurally matched gBTTT monomer, dimer, trimer, and two STM (scanning tunneling microscopy) characterized pgBTTT polymers. This approach aims to establish a reproducible link between synthesis conditions and device performance for glycolated materials.

#### Acknowledgement

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### [P19] Centrifugally spun hybrid polyhydroxyalkanoate/dextran nanocapsule fiber matrix for the delivery of hydrophilic payloads

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Biopolymeric micro- and nanofibers with active ingredients have gained significant attention for biological applications. However, the incorporation of hydrophilic compounds into hydrophobic matrices via spinning techniques remains rather unexplored. Here we report the incorporation of dextran nanocapsules (Dex-NCs) in centrifugally poly(3hydroxybutyrate-co-3-hydroxyhexanoate) (PHBHHx) fibers for the release of hydrophilic payloads. Inverse miniemulsion polymerization was employed to synthesize hydrophilic DexNCs with an average size of 0.25 µm. The Dex-NCs were embedded into PHBHHx via dual solvent centrifugal spinning at 0–7 wt% loading, resulting in beaded fibers with average fiber diameters of 4-6 µm. The effect of Dex-NC loading on the melting and crystallization behavior of PHBHHx was limited, while the strength and stiffness of the hybrid fibers was retained. The elongation of the hybrid fiber mats is reduced with increasing Dex-NC loading, but remains suitable for biological applications. Further, the in vitro release measurements showed a time dependent release of embedded Dex-NCs and the payload from the hybrid fibers. We anticipate this hybrid fiber matrix to be a starting point for the development of non-woven mats for slow release of hydrophilic payloads for biological applications, especially for medical wound dressings.

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## [P20] Multiscale modelling of reactively sputtered meso-porous titanate-based thin films

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Glancing Angle Deposition (GLAD) combined with reactive magnetron sputtering can be a method of choice where film structure must be controlled at the nanoscale for improved material performance. One promising application is the fabrication of nanostructured Titanate-based thin film anodes in the domain of Lithium-ion batteries.

In this work, we are investigating mesoporous thin films deposited by reactive magnetron sputtering process in GLAD mode, using Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> target. The aim is to show how the process can be optimized to maximize (1) the air-connected surfaces of the coating while keeping the pores size in a range of 2-50 nm, and (2) the amount of lithium in the coating after deposition.

The deposition process is modelled by using the kinetic Monte-Carlo software Virtual Coater<sup>1</sup>, allowing to simulate the complete sputtering process, from the design of the coater to the atomic-scale film growth simulation and film characterization (see Fig.1). A special attention is paid to the influence of the surface reaction constants, like sticking coefficients of deposited species, on the final composition of the coating. Such constants are provided by DFT simulations.

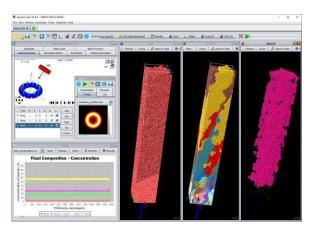


Figure 1 - PVD process modelling to atomic scale Monte-Carlo simulation of LTO film growth and porosity prediction.

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#### [P21] Multiscale modelling of LTO PVD growth

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In an ever-increasingly electrified society, investigation, characterisation and improvement of the production methods of battery-related material are becoming central to pave the way for the development of new technologies. Within the framework of the BatFactory consortium, our group focuses on lithium-titanate oxide (LTO) materials, which are generally regarded as an alternative to carbon-based anodes in batteries: LTO has been shown to significantly improve the charging time and lifespan of the batteries, yet at a cost of a lower energy density [1]. We aim at delivering the most complete description of the plasma vapor deposition (PVD) growth of LTO crystals, from first-principles calculations to kinetic Monte-Carlo (kMC) simulations.

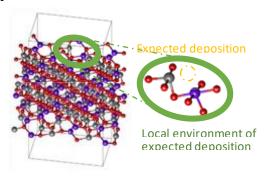


Figure 1 - LTO slab in the (100)-crystallographic orientation. A specific reactive surface site is highlighted, along with the expected position of the deposition site.

To bridge the gap between the microscopic and macroscopic realms, we first model surfaces as slabs, on which several reactive sites will be characterised through the absorption energy of different species (Li, Ti, O). Calculations are carried out using the Vienna ab-initio simulation package (VASP) implementation of the density functional theory (DFT).

Upon completion of the first-principles investigation, absorption energies are translated into sticking coefficients providing relative probabilities for each species to stick on a LTO substrate. Using Virtual Coater [2], we perform kMC simulation of the growth according to several macroscopic parameters such as temperature, pressure, plasma compositions. Our results will provide our partners with indications on how to optimize production methods depending on their specific needs. We propose this workflow as a versatile approach to describe PVD growth in various crystalline materials.

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## [P22] Correlation between structural and optical properties of 2D hybrid perovskites

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Over the past decade, hybrid organic-inorganic perovskites (HOIPs) have received significant research consideration mainly because of their use as active layers in perovskite solar cells (PSC) <sup>1</sup>. Lower-dimensional 2D HOIPs are currently receiving increased attention because of their generally enhanced material stability compared to their 3D counterparts and their much higher degree of compositional flexibility <sup>2,3</sup>. One of the points of strength of the 2D HOIPs is that - whereas the A cation in 3D HOIPs (ABX3, B = Pb2+ and X = I-, Br-, Cl-) can only be selected from a very limited range of small organic cations - the bulkier A\* cation in 2D HOIPs (A\*2BX4) can be selected from a huge potential cation pool. While most 2D HOIPs synthesized so far primarily utilize relatively simple A\* cations, the unique 2D structure offers exciting opportunities to develop more sophisticated A\* cations with enhanced functionalities, such as specific optical and/or (semi-)conducting properties.

In this work, we explore the use of a benzotriazole derivative with a three-carbon alkyl spacer (BtaC3) to form a 2D HOIP. Single-crystal X-ray diffraction (SCXRD) analysis revealed that the benzotriazole-based organic layers in the 2D HOIP structure show interdigitation, reducing the thickness of the organic layer and leading to an unusually dense packing layer. We monitored the material's behavior by temperature using in situ PXRD; the stability is preserved for high temperatures until a phase transition occurs at  $\pm 170$  °C, however the sample changes the from single crystal to polycrystalline. Therefore, structure determination of the 2nd phase could only be effectively achieved using 3D Electron Diffraction (3DED). According to the obtained structure, the 2D packing is still maintained, but the interdigitation between the organic layers is lost. The 2D HOIPs could be regarded as natural multiple-quantum-well structures in which the semiconducting inorganic layers act as "wells" and the insulating organic layers act as "barriers", giving to the organic spacer a key role in the optical properties of those materials  $^4$ .

In the current case, considering the phase transition above 170 °C, we measured the photoluminescence (PL) spectra of the BtaC3 HOIP in situ with increasing temperature. We observed a blue shift of the maximum peak of the 2nd phase compared to the 1st one, followed by an enhanced intensity. This confirms the loss of interdigitation of the organic spacer and the increasing of the distance between the inorganic layers, changing the electronic nature of the material.

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## [P23] Less is More: A Direct (Arylation) Approach to Near-Infrared TADF Emitters for Solution-Processed Organic Light-Emitting Diodes

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Developing efficient deep red to near-infrared (NIR) emitting materials is crucial for applications in optical data transmission, medical phototherapies, biosensing, cryptography. The challenge to achieve efficient NIR emission from all-organic  $\pi$ -conjugated systems can be tackled by the design of donor-acceptor type chromophores affording high quantum yields by leveraging triplets in materials optimized for thermally activated delayed fluorescence (TADF). While internal quantum efficiencies of up to 100% can be realized through TADF, harmonizing this mechanism with the design of NIR emitters remains particularly complex. Despite steady advancements, many reported NIR-TADF materials still rely on large, planar acceptor cores such as dibenzo[a,c]phenazine, which often suffer from poor solubility and strong  $\pi$ - $\pi$  stacking, possibly leading to processing issues and aggregationcaused fluorescence quenching.<sup>[2]</sup> To address these limitations, there is growing interest in the development of solution-processable NIR-TADF emitters featuring condensed but highly electron-deficient acceptor moieties. However, functionalizing these acceptors with the necessary donor groups remains synthetically challenging. In this work, we explore the direct arylation reaction as a promising alternative to conventional cross-coupling strategies such as Suzuki coupling. This approach eliminates the need for prefunctionalized acceptors, streamlining synthetic pathways while enabling the discovery of novel materials previously inaccessible through established methods. In this work, we report the design, synthesis, and full characterization of new NIR-TADF materials incorporating (novel) low-LUMO acceptors like benzo[c][1,2,5]thiadiazole-4,7-dicarbonitrile (CNBT) and benzene-1,2,4,5-tetracarbonitrile (TCNB). Density functional theory (DFT) calculations were employed to investigate and compare the relative differences in the molecular geometry, torsion angle, and excited state energy distribution, and to correlate these with specific changes in the structure and electron density. Afterwards, time-resolved emission spectroscopy was used to probe the TADF characteristics in (doped) films, providing insight into the excited state dynamics. Finally, these materials were integrated into basic solution-processed organic light-emitting diodes (OLEDs), demonstrating their practical application potential. Through this direct arylation strategy, we systematically examine the impact of molecular geometry, donor orientation, and donor group quantity on the emission properties of novel (and existing) NIR-TADF compounds. In that regard, our findings may offer a potential step forward in the development of more efficient, solution-processable NIR-OLEDs.

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## [P24] Engineering Advanced BiVO<sub>4</sub> Photoanodes for Efficient Photoelectrochemical Water and Ethylene Glycol Oxidation

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Bismuth vanadate (BiVO<sub>4</sub>) is a leading photoanode material for solar-driven water splitting due to its visible-light absorption and stability in alkaline media, though its performance is limited by poor charge transport and slow oxygen evolution kinetics. In this study, we developed advanced BiVO<sub>4</sub> photoanodes by integrating a NiO hole transport layer and a FeOOH co-catalyst to enhance charge separation and catalytic efficiency. BiVO<sub>4</sub> thin films were synthesized via spin-coating with optimized parameters for nanoporous morphology, high crystallinity, and strong light absorption. NiO layer was deposited by reactive sputtering to improve interfacial charge extraction and provide a stable scaffold for FeOOH, which was electrodeposited to accelerate oxygen evolution. We fabricated four configurations: pristine BiVO<sub>4</sub> (BVO), NiO/BVO, FeOOH/BVO, and FeOOH/NiO/BVO and evaluated them by XRD, FESEM, and photoelectrochemical testing under AM 1.5G illumination (100 mW cm<sup>-2</sup>). PEC measurements were conducted in 1 M KBi buffer for water oxidation and in a mixed electrolyte with 10 vol% ethylene glycols (EG) for organic oxidation. FeOOH/BVO and FeOOH/NiO/BVO achieved photocurrent densities of ~2.3 and ~1.8 mA cm<sup>-2</sup> at 1.23 V<sub>RHE</sub> for water oxidation, around eightfold and sixfold higher than pristine BVO, confirming improved interfacial charge transport and catalytic performance. For EG oxidation, pristine BVO yielded the highest photocurrent (~3.5 mA cm<sup>-2</sup>), suggesting possible competing catalytically active sites on unmodified sample. All photoanodes exhibited higher photocurrents for EG oxidation than for water, highlighting the kinetic favorability of organic oxidation. These results emphasize the importance of interfacial engineering and requirement of further detailed surface analysis to attain optimized PEC performance. Building on this platform, the high-performing BVO photoanode was be integrated with a halide perovskite photovoltaic absorber to construct an artificial leaf device for unassisted solar fuel production. This monolithic tandem system is also designed to couple solar energy harvesting with selective oxidation reactions, aiming for high solar-to-fuel conversion efficiency.

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