

Biobased Chemistry and Technology Annual report 2024



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Catalysis/Conversion

Team Leaders: Dr. Elinor Scott/Dr. Tomas van Haasterecht/Prof.dr. Harry Bitter

PhD students/Post doc: Roel Bisselink, Yangming Ding, Martijn Ekhart, Maurice Essers, Torin de Groot, Matthijs van der Ham, Freek Karaçoban, Ellis van Keulen, Frits van der Klis, Ivo van Luijk, Pedro Mazaira Couce, Imogen Morris, Ida Ngongkum, Dmitry Pirgach, Xiaojie Qin, Edwin Schreuder, Nena Zwart



Contact: elinor.scott@wur.nl or harry.bitter@wur.nl

Background and goal

The aim in this theme is to develop sustainable conversions routes and processes utilising renewable feedstocks. To achieve this aim a multi-disciplinary approach is used i.e. catalyst development, synthesis and process development that goes hand in hand with computational methods and multi-scale modelling to underpin scientific understanding at every level.

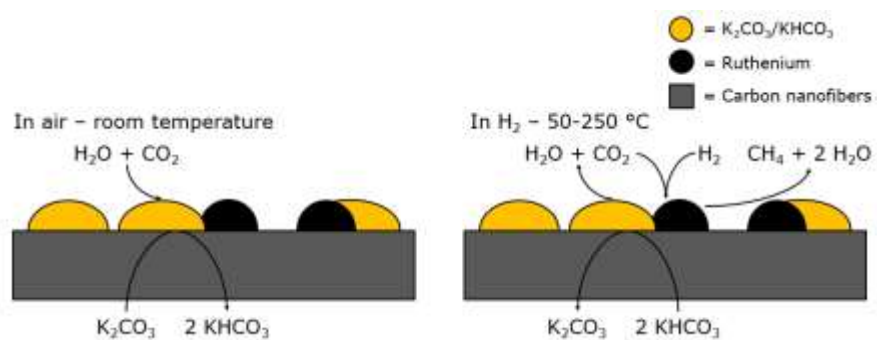
Important and emerging chemistry and technology in the area of CO₂ capture and conversion, as well as the use of electricity as an input to drive reactions using biobased molecules or to produce chemicals is also a major theme.

Main topics:

- Catalyst development for biobased feedstock conversion (heterogeneous, homogenous, bio)
- Conversion of biobased feedstocks and synthesis of biobased chemicals
- Use of non-noble metal catalyst to replace scarce noble metals in synthesis
- Electrochemical/electrocatalytic conversion of (larger) biobased molecules
- Integration of thermal catalysis with electro catalysis/chemistry
- CO₂ capture and conversion

Highlights from last year

The figure below illustrates research into a dual material for direct CO₂ capture and conversion of CO₂ to methane. This research was recognised with the poster of Freek Karaçoban winning an award at the ExxonMobil EU R&D Days.



Students project envisioned

Thesis subjects are related to the research of the Ph.D. projects described on the next pages. Projects are mainly lab based but modelling can also be performed. Contact Elinor Scott (Elinor.scott@wur.nl) for further information.

Electrochemical cell design for the production of valeric acid and hydrogen peroxide

Name PhD: Roel Bisselink

Involved staff members: Prof. Dr. J.H. Bitter; Dr. J. van Haveren

Project sponsor: NWO program, TKI BBEG-program, EU H2020 program

Start/(expected) end date of project: August 2020 – July 2026



Background and goal of project

The availability of cheap electricity presents an opportunity to drive chemical transformations and thus enables electrification / decarbonization of the chemical industry. Possibilities to decarbonize current processes can be found in the electrochemical conversion of 1. bio-based levulinic acid to valeric acid and 2. oxygen (O_2) to hydrogen peroxide (H_2O_2). But to come to an efficient electrochemical process design for these routes it is vital to increase understanding of various fundamental aspects of each conversion.

Highlight of the past year

In the past year the electrochemical reduction of O_2 to H_2O_2 progressed from electrolysis under flow conditions using a dual membrane electrolyser and 0.5 M K_2SO_4 electrolyte towards integration of porous solid polymer electrolyte. To enable cost-effective production of H_2O_2 a dual membrane electrolyser is proposed having porous solid polymer electrolyte sandwiched in between both membranes. This reactor configuration enables production of 'electrolyte-free' and concentrated H_2O_2 . First the influence anion exchange membranes (AEMs) and catalyst presence were evaluated by stepwise increasing the electrical current of the electrolyser and determining the influence on FE and cell voltage. Significant differences in cell voltages are obtained using different membranes (Fig. 1 left). The faradaic efficiency for H_2O_2 formation was initially $>80\%$ for all AEMs, however at increasing current density the FE depends on the nature of the AEM (Fig. 1 right). These findings shows the impact of the nature of the AEM on the electrolytic process, moreover, the differences in cell voltage cannot be explained by solely the electric resistance differences between the AEMs. We therefore tentatively explain the obtained differences in cell voltage by differences in contact resistance, i.e. between the gas diffusion layer and the AEM, within the membrane electrode assembly.

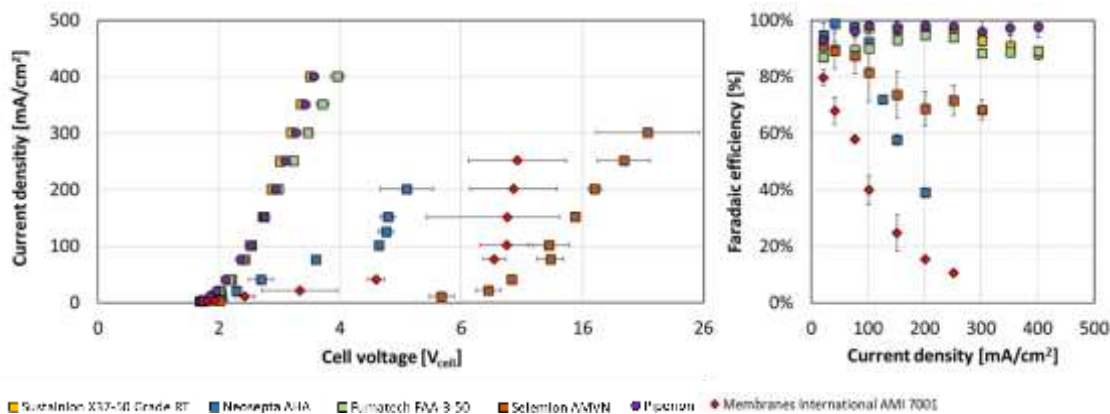


Figure 1. Performance of a dual membrane electrolyser, having 0.5 M K_2SO_4 in the centre compartment, for the electrocatalytic reduction of O_2 to H_2O_2 using different AEMs.

Next step involves the integration of ion exchange resin as proton conductive material in the electrolyser. By tuning the flow and current density a concentration of 20% H_2O_2 was achieved. This system will be optimized in order to understand the influence of operating parameters on the process.

Type of student projects envisioned

Experimentally oriented projects are available such as for example: Diversification of the electrochemical reduction of the ketone functionality to other keto-compounds, related to levulinic acid to improve understanding of the involved electrochemical reaction or 2. Improve understanding of the electrochemical cell design via characterisation of the individual cell components and/or its effect on the performance on the electrochemical reactor.

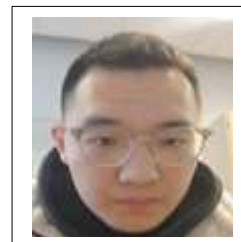
Atomically dispersed Pt₁/S-C for selective reductive amination of furfural

Name PhD/PD: Yangming Ding

Involved staff members: Prof. dr. Harry Bitter, Dr. Guanna Li, Dr. ir. Tomas van Haasterecht

Project sponsor: China Scholarship Council (CSC)

Start/(expected) end date of project: 12-04-2023/12-04-2027



Background and goal

Primary amines are key intermediates in the chemical industry with extensive applications in the manufacture of polymers, pharmaceuticals, dyes and detergents etc. but produced from fossil resources. Utilizing renewable biomass platform molecules such as furfural to produce primary amines via reductive amination is a sustainable strategy. Pt has been widely used for catalyzing this reaction. However, to achieve high selectivity for desired primary amines is a challenge because Pt favors the hydrogenation of intermediate Schiff base to secondary amines and even hydrogenation of ketone/aldehydes due to its strong hydrogenation capability.

In this project, I aim to develop Pt₁/S-C single atom catalyst for selective production of furfurylamine and investigate the electronic effect on its catalytic performance by preparation of different Pt nano species and isolated Pt₁ single atoms with fine-tuned electronic states.

Highlight of the past year

2 wt%, 5 wt%, 10 wt% Pt_{nano}/S-C with a similar average Pt particle size were prepared (Fig. 1A-C). In addition, Atomically dispersed Pt₁/S-C was confirmed by the k₃-weighted Fourier transform of EXAFS (Fig. 1D). The Pt₁/S-C presented a prominent peak around 1.8 Å, which could be ascribed to the Pt-S coordination without Pt-Pt contribution around 2.65 Å. The order of oxidation state was confirmed and speculated according to XANES (Fig. 1E) and the literature: PtO₂ > 2wt%Pt₁/S-C > 2wt%Pt_{nano}/S-C > 5 wt%Pt_{nano}/S-C > 10wt%Pt_{nano}/S-C > Pt foil.

Pt₁/S-C exhibited the highest yield of furfurylamine up to 89 %. However, for Pt nanocatalysts, with the Pt loading increased, the yield of furfurylamine dropped from 60% to 33%, along with the production of furfural alcohol increasing from 21% to 62%, meanwhile the electronic density of Pt species increased. Since the particle sizes of Pt nanocatalysts are similar according to TEM, it is speculated that the electronic state has a significant influence on the performance of Pt/S-C catalysts.

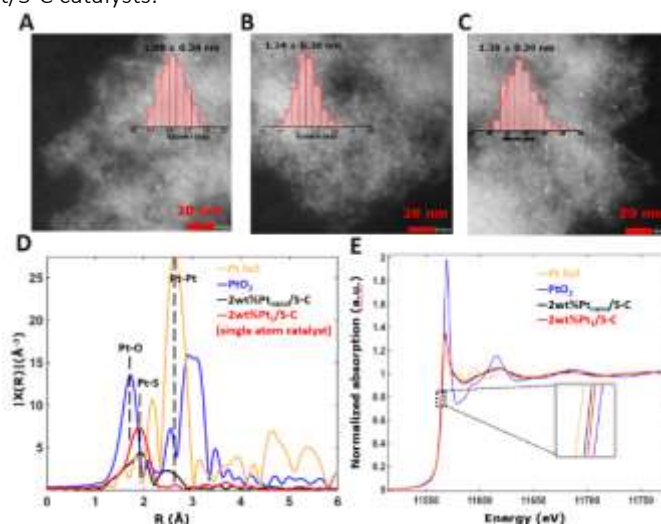


Figure 1. (A-C): TEM images of Pt_{nano}/S-C catalysts: 2wt%, 5wt%, 10wt%. D) EXAFS. E) Normalized XANES spectra of 2wt% Pt₁/S-C, 2wt% Pt_{nano}/S-C, Pt foil, and PtO₂.

Type of student projects envisioned

I offer projects including catalyst synthesis (single atom catalysts, Carbon support etc), characterization (physisorption, chemisorption, XRD, TEM, etc), and reaction tests.

If interested, please feel free to contact me (yangming.ding@wur.nl).

Investigating the Enzymatic Remodeling of Starch for Enhanced Functional and Physiological Properties

Name PhD/PD: Maurice Essers

Involved staff members: Harry Bitter

Project sponsor: AVEBE

Start/(expected) end date of project: 1-10-2020 - 1-10-2025



Background and goal of project

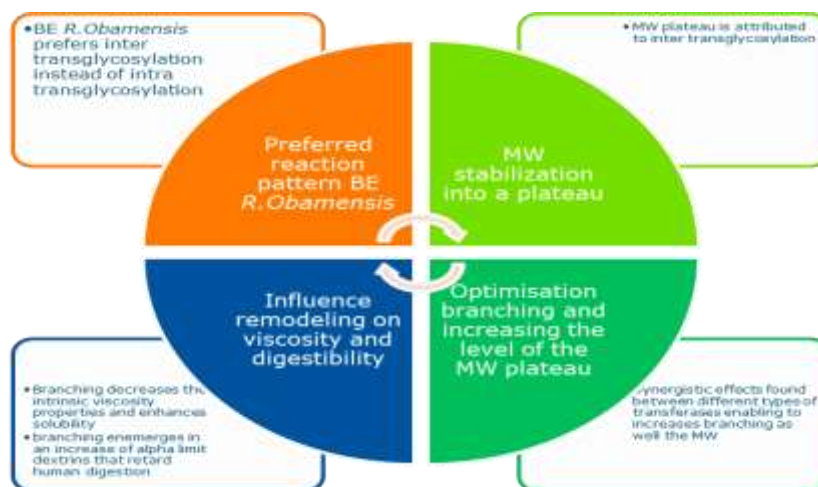
Carbohydrates like starch are fully converted into glucose by human digestive enzymes in the small intestine. However, excessive consumption of highly digestible carbohydrates is linked to health issues such as obesity and diabetes. This highlights the need for carbohydrates that are less prone to digestion, which can be achieved through the remodeling or restructuring of starches. Starch remodeling can be accomplished using starch-modifying enzymes, such as 1,6- α -glucotransferases (branching enzymes). These enzymes increase the number of α -1,6 glycosidic bonds, but this modification alone is insufficient to make starch fully resistant to digestion in the small intestine. A key observation during the branching process is a reduction in molecular weight (Mw), which occurs at the start of the reaction and then stabilizes into a plateau during subsequent branching. However, the underlying mechanisms remain unclear. This research aims to address the following key questions:

- Is the reduction in Mw primarily caused by the branching reaction itself, or is it due to a side reaction involving hydrolysis?
- What mechanisms drive the stabilization of Mw into a plateau during the later stages of the reaction?
- Can the molecular weight plateau be adjusted at different levels while optimizing the degree of branching?
- How does the degree of branching influence starch digestibility, viscosity, and functional properties?

The overarching goal of this study is to deepen our understanding of the enzymatic remodeling mechanisms of starch. By uncovering these insights, we aim to design novel starch structures that offer both enhanced physiological benefits and desirable functional characteristics.

Highlight of the past year

- 1) Scientific article submitted in Carbohydrate polymers regarding the activity of the branching enzyme in modified starches
- 2) Polymerization effect found between different types of transferases, included the branching enzyme, this enables to increase the level of the molecular weight plateau as well optimized the degree of branching



Enabling Direct Air Capture of CO₂ through efficient and stable sorbent materials

Name PhD: Torin de Groot

Involved staff members: Prof. dr. Harry Bitter, Dr.ir. Tomas van Haasterecht, Dr. Akbar Asadi Tashvigh

Project sponsor: NWO, Shell LIFT

Start/(expected) end date of project: September 2021-September 2025



Background and goal of project

Direct air capture (DAC) of carbon dioxide is a method that can help reduce emissions, including emissions from mobile sources and historical emissions already present in the atmosphere. This technique requires a sorbent material capable of capturing CO₂ at atmospheric concentrations and functioning across varying humidity levels. For this project, potassium carbonate supported on carbon is used as the sorbent material. Potassium carbonate reacts with CO₂ and water vapor to form potassium bicarbonate, which can then be heated to regenerate the sorbent and release the captured CO₂, allowing it to be stored or utilized. However, the precise reaction mechanism remains unclear.

The goal of the research is to establish property-performance relationships for these materials in CO₂ capture. Key research questions include:

1. Understanding the role of water in the reaction mechanism.
2. Investigating how the polarity of the support affects sorption capacity.
3. Examining the stability of sorbent materials during both storage and use.

Highlights of the past year

In-Situ XRD was used to track intermediate phases during CO₂ capture under different levels of relative humidity. Intermediates could clearly be observed (Fig 1a) and a reaction mechanism could be proposed (Fig 1b). The same sequence of phases was observed at all humidity levels (figure 1B), increasing the humidity caused new phases to appear faster. However, the total capture capacity decreased at high humidity. Further quantification of phases is still ongoing

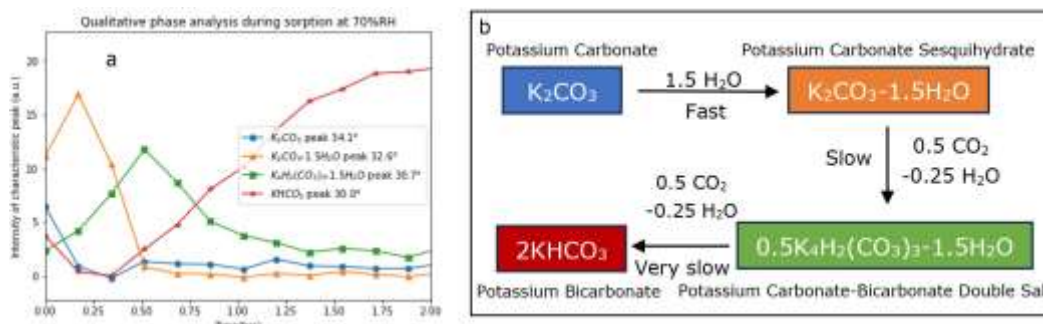


Figure 1: a) Intensity of characteristic diffraction peaks of different phases during sorption. This qualitatively illustrates the formation and disappearance of intermediate phases. b) Suggested mechanism of carbonation

Increasing the level of surface polarity of the carbon nanofibers used to support K₂CO₃ particles was found to shift the deliquescence point of the K₂CO₃ to lower humidity. Once humidity surpasses the deliquescence point K₂CO₃ dissolves in adsorbed water forming a solution instead of a solid which drastically changes CO₂ capture capacity. Isobaric water adsorption measurements were used to quantify this shift in deliquescence point

Type of student projects envisioned

Potential projects consist of either lab work or modelling. However, the project is ending this year so it is unlikely I will have any new student projects available

Dual Functional Materials for the Direct Air Capture and Conversion of CO₂

Name PhD/PD: Freek Karaçoban

Involved staff members: Prof. dr. Harry Bitter, dr.ir. Tomas van Haasterecht

Project sponsor: VLAG Graduate School

Start/(expected) end date of project: December 2021-December 2025



Background and goal of project

To reach the goal of the Paris agreement, and limit the increase in global average temperature to 1.5 °C above pre-industrial levels, negative carbon technologies are needed. One of these technologies is direct air capture (DAC). In DAC, CO₂ is captured directly from air. The CO₂ can then be stored or used to make renewable fuels and chemicals.

In this project, we aim to combine the DAC and conversion processes in a single reactor. To do so, we develop a dual functional material (DFM) that is capable of both capturing and converting CO₂. This DFM consist of a CO₂ sorbent and metal nanoparticles that catalyzes the conversion of CO₂. To deepen our understanding of the DFM, we focus on elucidating the interaction between the sorbent and the catalyst. We have shown that there is a synergy between the two components that improves conversion, but the underlying mechanism is not yet fully understood.

Highlight of the past year

In the past year we gained insights into the interaction between the carbonate and the metal catalysts. By making DFMs with different carbonates (Na, K, Rb, Cs) we have shown that the methanation temperature of the catalyst depends directly on the alkali metals. By tuning the loading of carbonate and catalyst, a stable material was made that could be used in >25 cycles of CO₂ capture and conversion with 100% conversion of captured CO₂.

We have also performed in-situ X-ray adsorption studies to investigate the electronic structure of the metal catalyst throughout a cycle of capture and conversion. This allowed us to further understand the transitions the catalyst goes through while exposed to air and H₂, and how this is affected by the presence of K₂CO₃. An example of the XAS spectra during reduction of the catalyst is shown in Figure 1. Here, the catalyst transitioned from the oxidic to the metallic state.

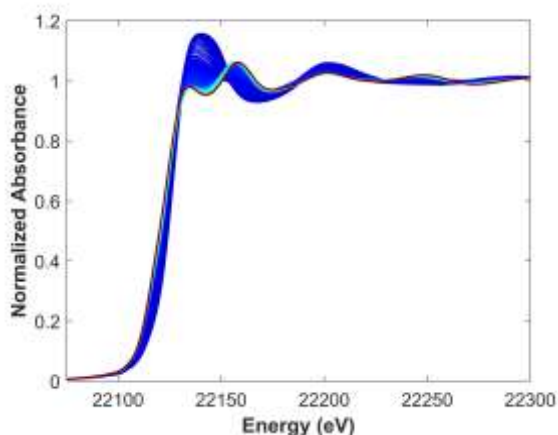


Figure 1: XAS spectra measured during the in-situ reduction of the catalyst in the DFM.

Type of student projects envisioned

Students are welcome for various projects in the lab. These projects will further explore the DFM we have presented. Lab work will include making the DFMs, testing these for capture and conversion, and characterizing them using various methods. These methods include X-ray diffraction, N₂ physisorption, electron microscopy and more.

Non-noble transition metal nanoparticles for the electrochemical production of hydrogen peroxide

Name PhD/PD: Ivo van Luijk

Involved staff members: Harry Bitter, Tomas van Haasterecht, Akbar Asadi Tashvigh

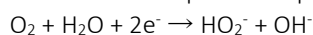
Project sponsor: NWO, Solvay

Start/(expected) end date of project: 1-11-2021/1-11-2025



Background and goal of project

Electrocatalytic hydrogen peroxide (H_2O_2) production offers a sustainable alternative to the traditional anthraquinone process, which is energy-intensive and produces CO_2 . Electrocatalytic H_2O_2 production via the oxygen reduction reaction (Eq. 1) is a less energy intensive method, potentially without CO_2 emissions when renewable energy is used. The reaction product HO_2^- is the alkaline form of H_2O_2 , which can either be protonated or used in this form. To perform this reaction, a catalyst is needed. The properties of the catalyst determine the efficiency of the reaction, thus studying the property performance relationships of the catalyst is vital towards improving the overall process. With sufficient understanding, catalysts can be developed that will help the electrochemical process replace the current anthraquinone process.



Eq. 1

Highlight of the past year

This year we investigated the effect of the oxygen functional groups of carbon nanofiber supported nickel nanoparticle based electrodes on the electrochemical production of hydrogen peroxide. The oxygen groups on a support have been shown in previous studies to have a strong effect on a variety of reactions. The oxygen groups. For the production of hydrogen peroxide some studies suggest that phenolic oxygen groups can improve the performance of carbon for this reaction. In this study oxygen groups, such as phenols and carboxylic acids, were added to the catalyst in order to determine the influence of the oxygen groups on nickel nanoparticles. Figure 1 shows the relationship between catalytic performance and oxygen content of the catalyst support. Clearly, there is a positive correlation between the oxygen groups and the performance. It is hypothesized that there is a synergistic effect between the support and the nickel nanoparticles in this case, oxygen can coordinate to the phenol, react, and the intermediate can then transfer to the nickel in order to complete the reaction. This means that oxidizing the support, in particular with phenols, is an effective strategy to improve the performance of electrochemical hydrogen peroxide production with nickel nanoparticles.

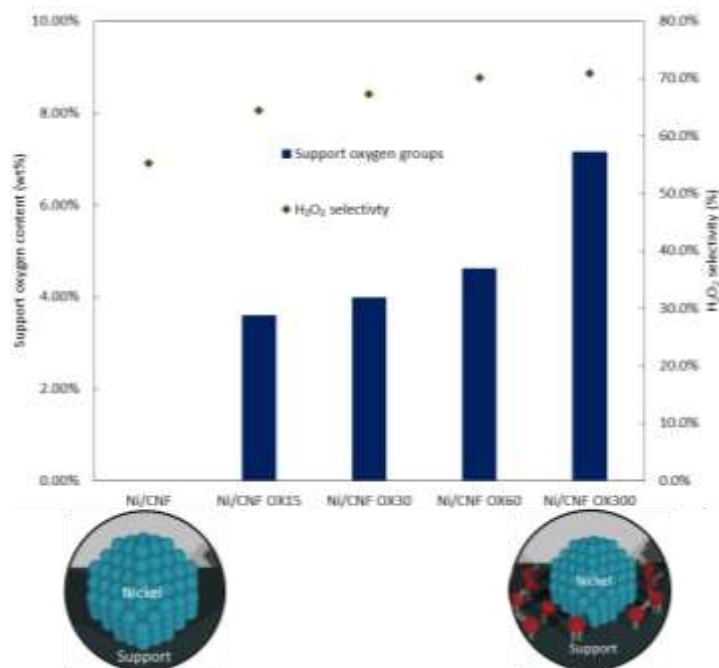


Figure 1: Relation between oxygen group content and performance

Clearly, there is a positive correlation between the oxygen groups and the performance. It is hypothesized that there is a synergistic effect between the support and the nickel nanoparticles in this case, oxygen can coordinate to the phenol, react, and the intermediate can then transfer to the nickel in order to complete the reaction. This means that oxidizing the support, in particular with phenols, is an effective strategy to improve the performance of electrochemical hydrogen peroxide production with nickel nanoparticles.

Type of student projects envisioned

This project will end in November 2024 therefore there are no more possibilities for student projects.

On the effect of the oxygen groups over carbon catalyst for the electrocatalytic reduction of O₂

Name PhD/PD: Pedro Mazaira Couce

Involved staff members: Harry Bitter, Tomas van Haasterecht

Project sponsor: EU

Start/(expected) end date of project: 1-2-2023/1-2-2027



Background and goal of project

Industrial manufacture of hydrogen peroxide (H₂O₂) produces 3 times more CO₂ than H₂O₂. The electrocatalytic oxygen reduction reaction (ORR), powered by renewable energy, represents a viable eco-friendly pathway to produce H₂O₂. Carbon-based catalysts are active towards ORR, however, it is necessary to oxidize its surface to increase its polarity and facilitate the access of dissolved O₂ to the catalyst's active sites. Surface oxidation improves catalytic performance by introducing oxygen functional groups (OGs), like hydroxyls (C–OH) or carboxylic acids (COOH) or ketones (C=O). Nevertheless, the impact of the specific OGs over the catalyst performance is not yet understood. In this project we aim to understand the effect of this OGs on the performance of different carbon materials like carbon nanofibers (CNF), graphene nanoplatelets (GNP) or active carbon.

Highlight of the past year

During this year we were able to chemically modified the OGs over CNF and GNP to selectively increase the concentration of carboxylic acid, phenols or ketones. GNP with a higher concentration of phenol groups show the highest activity and selectivity (97%) towards H₂O₂. (Figure 1 a) Using thermal oxidation, phenol groups were selectively introduced in GNP, after electrochemical testing thermally oxidized GNP showed similar currents to chemically modified GNP but a perfect selectivity toward H₂O₂.

Moreover, by using a flow cell set up which the mass flow oxygen towards the catalyst, it was possible to increase the performance of the system from ≈ -1 mA/cm² to ≈ -400 mA/cm² showing that by using thermally oxidized metal free carbon catalyst it is possible to reach industrially relevant conditions. (figure 1 b))

Type of student projects envisioned

There are many avenues to explore in this project. From the use of different carbon materials, research the influence of pH in the reaction or coping with heteroatoms. Nevertheless, any project will consist on the development of a novel catalyst. Its characterization using a wide range of techniques as electron microscopy, boehm titration, TGA or TPD and finally, analyze the electrocatalytic performance using H-Cell, flow cell or ring disk electrode.

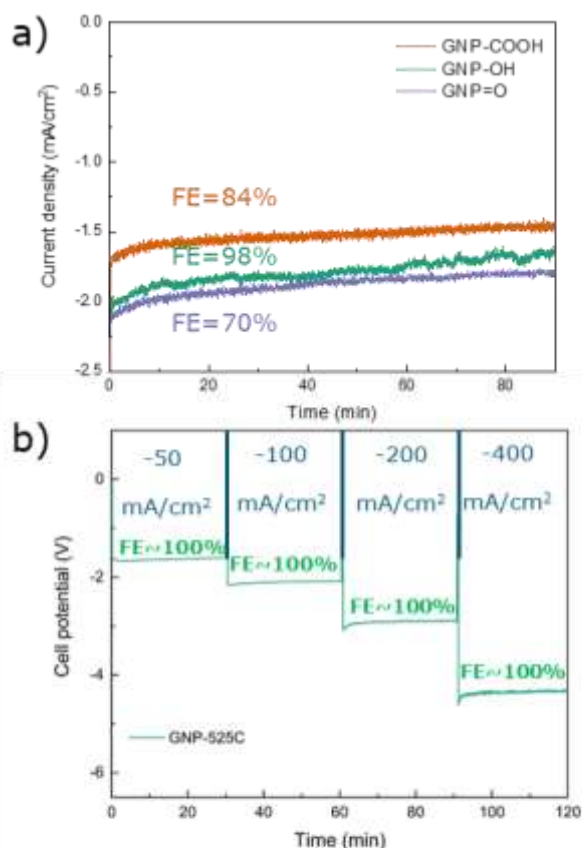


Figure 1: a) electrochemical performance in an H-cell set up of the different GNP at -0.25 V vs HgO. **b)** Electrochemical performance of thermally oxidized GNP using a flow cell at different current densities

Biobased Soft Matter

Team Leader: Dr. Costas Nikiforidis

PhD candidates: Gijs Konings, Sybren Zondervan

Researcher/technician: Imogen Morris

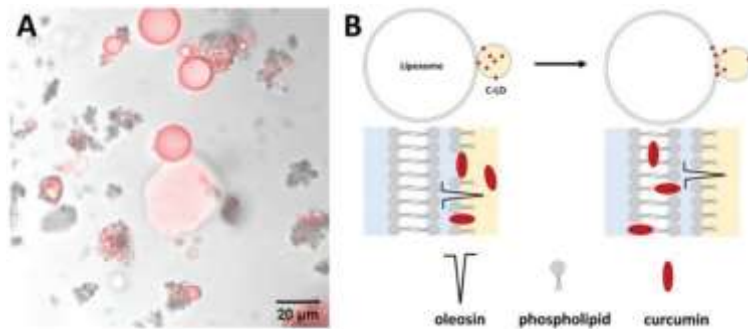
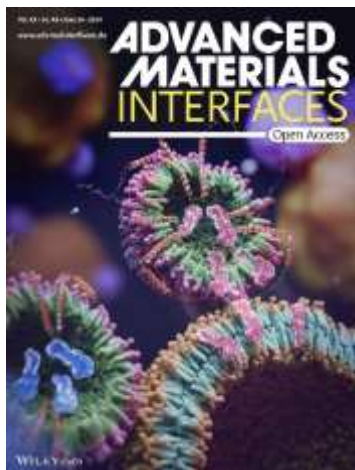
Contact: costas.nikiforidis@wur.nl



Background and goal

The Biobased Soft Matter team develops bioinspired functional materials using molecules derived from natural sources. We focus on designing efficient extraction processes and studying how the properties of these molecules relate to their functions in the soft materials we create. Our research spans multiple scales, from the molecular level to the macroscopic, using approaches from soft matter physics, chemistry, and biology.

Our work relies on advanced analytical tools like fluorescence and confocal microscopy, combined with interfacial and bulk rheology, to understand and optimize these materials.



Main topics

- Interplay between LDs and lipid bilayers
- Trafficking lipophilic molecules with natural lipid droplets (LDs)
- Behaviour of proteins and polar lipids on interfaces
- Plant protein/phenol interactions and their use in functional materials
- Jammed emulsions to mimic animal fat
- Investigating protein adhesive properties
- Design super stable bio-inspired oil droplets

Highlights from last year

- The team published 18 peer-reviewed articles in highly-ranked journals
- Understood the role of oleosins and phospholipids on lipid droplet (oleosome) stability
- Understood the effect of cargo's polarity on transporting molecules from lipid carriers to membrane bilayers
- 5 invited keynote lectures at international meetings and conferences

Student project envisioned

The available thesis subjects relate to the research of the team's projects, which are predominantly experimental.

Electrophoretic Fractionation of Rapeseed Components

Name PhD/PD: Kübra Ayan

Involved staff members: Dr. Costas Nikiforidis

Project sponsor: National Education Ministry of Türkiye

Start/(expected) end date of project: September 2020 / September 2024



Background and goal of the project

Fractionating plant materials is crucial for creating functional ingredients and supporting sustainable food production. Oilseed proteins have valuable emulsifying, foaming, and gelling properties for the food industry. However, phenolic compounds in oilseeds can bind to proteins, making them insoluble and indigestible. Current separation methods are resource-intensive, so this project explores an electric field-assisted process as a more efficient alternative.

This process separates rapeseed components by charge or size. Phenolics (sinapic acid) and proteins are separated using an electric field and solvent flow since phenolics are negatively charged and have higher electrokinetic mobility. In Figure 1, besides the effect of flow and charge, a membrane allows phenolics to migrate while retaining larger protein molecules.

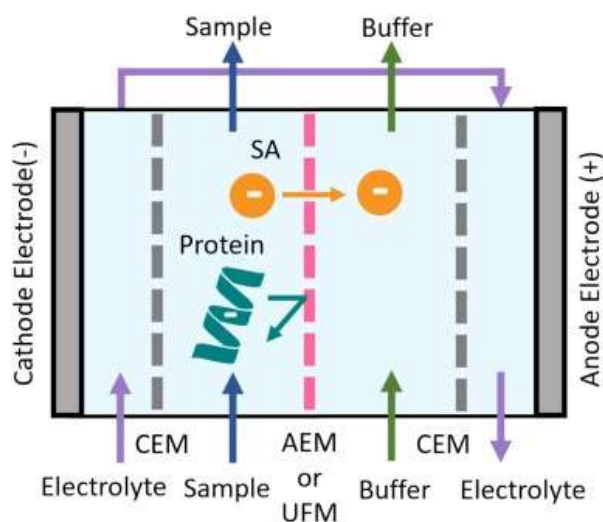


Figure 1. Charge and size-based electrophoretic separation principle. Arrows indicate the migration direction of the compounds.

Highlights of the past year

- It has been shown that introduction of an electric field increases separation selectivity of rapeseed oleosomes and proteins.
- Electrodialysis based separation method was developed.
- Electrophoretic removal of sinapic acid from rapeseed protein extract was accomplished.

Type of student projects envisioned:

This project has been finalised

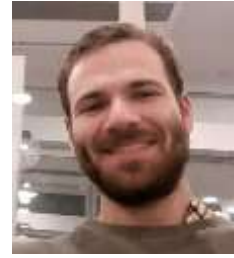
Bridging the gap between supramolecular interactions and mesoscale structure using pea proteins

Name PhD/PD: Gijss Konings

Involved staff members: Dr. Costas Nikiforidis

Project sponsor: Graduate School Green Top Sectors TKI, Planted Foods AG (Zürich, Switzerland)

Start/(expected) end date of project: May 2023 / April 2027



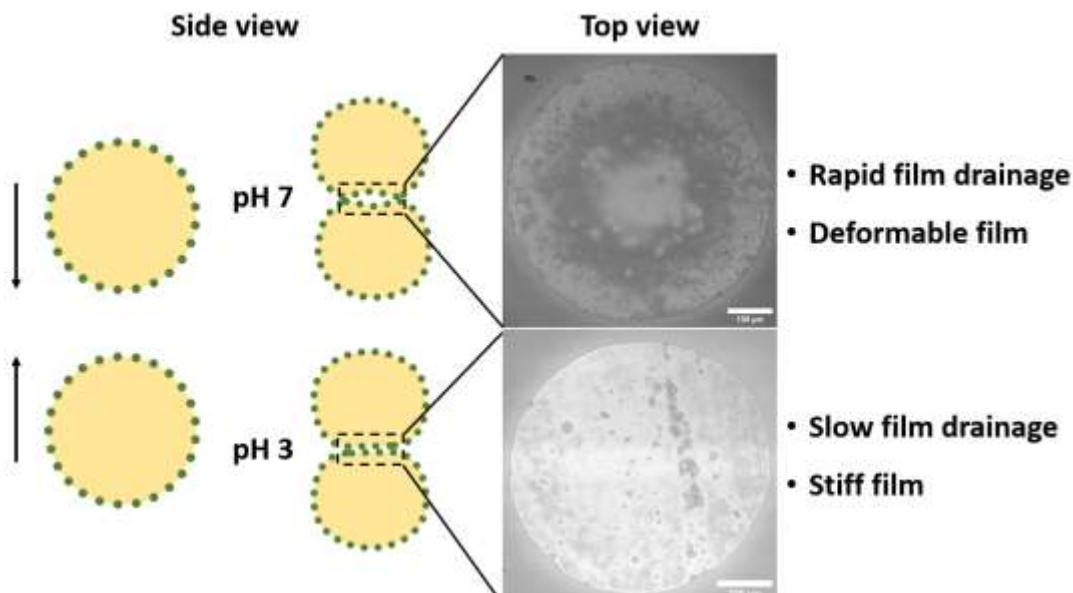
Background and goal of project

The adipose tissue is a densely packed system of fat cells around and in between muscle tissue. In meat products this adipose tissue is responsible for the flavour and the perceived juiciness of meat. Mimicking these properties is essential to create meat analogues with good sensory quality. We could mimic the structure and mechanical properties of adipose tissue at elevated temperatures by binding oil droplets with pea proteins. However, the remaining challenges are to mimic the system hardness at ambient temperatures and melting behaviour during heating. To design a material with the required characteristics it is key to also better understand the contribution of individual components of the material.

Highlight of the past year

Using laser diffraction and confocal microscopy, we found that after a heating-cooling-heating circle, fat crystals protrude from the oil droplet interface and bridge neighbouring droplets which led to droplet coalescence and consequently a decrease of viscoelasticity (melting). By changing the crystalline fat content we could control the extent of coalescence either by reducing the crystal protrusion into the continuous phase or by modulating the cluster size of aggregated crystal droplets.

In parallel, we collaborated with TU/e where they have a system capable of measuring the attractive/repulsive forces between oil droplets. With this model system we could quantify the adhesive effect of self-assembled protein particles between two oil/water interfaces. Together with data obtained by a student we could uncover the mechanism with which these protein particles provide our system with its rigidity.



Type of student projects envisioned

Student projects would consist of mostly labwork revolving around protein extraction, rheological characterization of materials, and protein-protein interactions.

Nature knows best – Lessons from plants on how to design stable emulsions resistant to lipid oxidation

Name PhD/PD: Lorenz Plankensteiner

Involved staff members: Dr. Costas Nikiforidis

Project sponsor: Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), Botaneco INC. (Calgary, AB, Canada)

Start/(expected) end date of project: 01.07.2020 / 01.07.2024



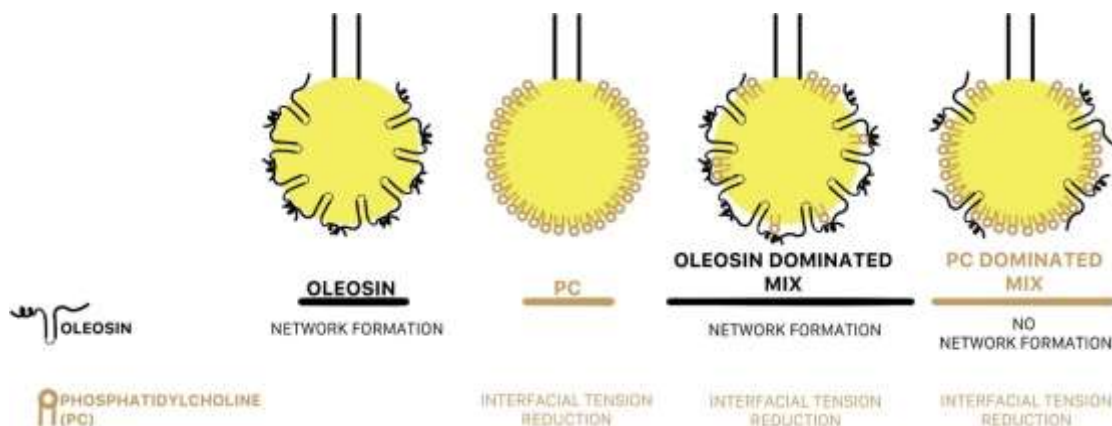
Background and goal of project

Preventing lipid oxidation is crucial for the food and personal care industries, as it limits product shelf life. Many products, like oil-in-water emulsions, contain unsaturated lipids (triacylglycerides or TAGs) that easily oxidize, causing off-flavors and the loss of bioactive compounds, which harms product quality. Interestingly, inspiration to prevent oxidation can come from oilseeds, the primary source of TAGs.

In seeds, TAGs are energy reserves for germination and are protected from oxidation by being stored in oleosomes—natural droplets stabilized by a phospholipid monolayer with embedded proteins. Oleosomes also contain antioxidants like tocopherols and carotenoids that may help prevent oxidation. Traditional oilseed processing destroys oleosomes to extract TAGs, but intact oleosomes could be used directly as oil droplets in emulsions. Our research explores whether using oleosomes this way reduces lipid oxidation and aims to uncover the mechanisms behind their stability.

Highlight of the past year

We understood the role of oleosins and phospholipids on the oleosomes' stability. Oleosins formed viscoelastic solid interfacial films due to network formation via in-plane interactions. Weak interactions were observed between adsorbed phosphatidylcholines, suggesting the surface stress response upon dilatational deformations was dominated by density changes. In mixtures with 3:1 and 1:1 oleosin-to-phosphatidylcholine ratios, oleosins dominated the interfacial mechanics and formed a network, while phosphatidylcholines contributed to interfacial tension reduction. At higher phosphatidylcholine concentrations (1:3 oleosin-to-phosphatidylcholine), phosphatidylcholine dominated the interface, and no network formation occurred. Our findings improve the understanding of both components' role for oleosomes.



Type of student projects envisioned

The project has been finalized

On the functional properties of rapeseed protein extracts

Name PhD/PD: Sybren Zondervan

Involved staff members: Harry Bitter, Costas Nikiforidis, Atze Jan van der Goot (FPE), Julia Keppler (FPE)

Project sponsor: NWO-TKI "INTRINSIC"

Start/(expected) end date of project: October 2022 / September 2026

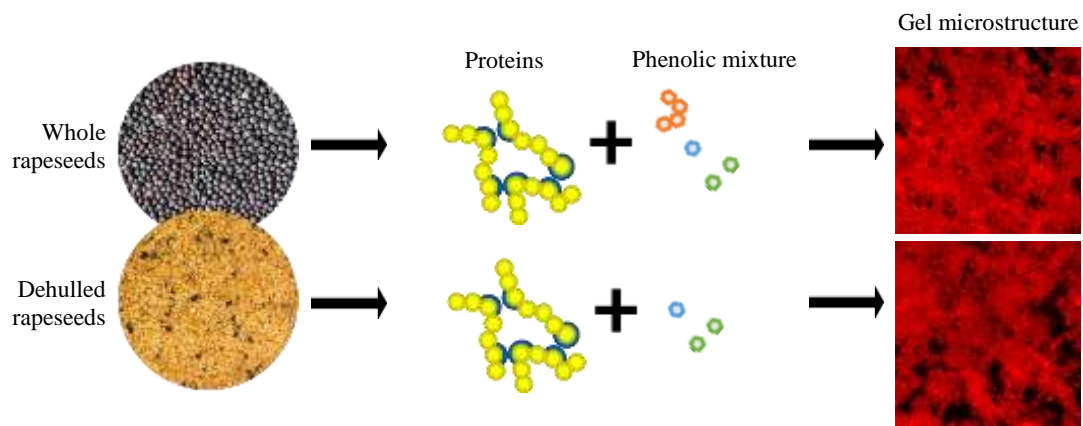


Background and goal of project

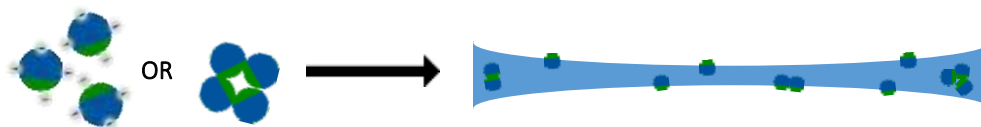
Rapeseed proteins are a promising plant-based protein source due to their balanced amino acid profile and global large production. For foods, proteins can also be used to make structures in the form of gels or to stabilise bubbles and droplets in foams and emulsions respectively. The formation of gel networks and stabilisation of oil/water and air/water interfaces by rapeseed proteins has been demonstrated before. However, the functional properties can be affected by a few factors which need to be well-understood for the proteins to be used in food materials.

Highlight of the past year

One factor affecting the protein functional properties is the co-extraction of phenolic compounds during the rapeseed protein extraction. Phenolic compounds may affect the protein gelation. We unveiled the past year to what extent the primary phenolic compounds in rapeseeds and in rapeseed protein extracts affect the protein gelation. The results of these studies are currently drafted into a publication.



Another factor changing the protein functional properties is the pH of the dispersion – proteins can be charged at specific pH-values which causes electrostatic repulsion between them. This affects their aggregation behaviour. It was hypothesized that the surface charge may change how rapeseed proteins stabilize the air-water interface. This was studied for the rapeseed albumins, napins.



Type of student projects envisioned

In 2025, we envision student projects related to the functional properties of napins. This can be in relation to their potential to stabilize emulsions or air-water interfaces, or related to the way napins behave in dense solid-like dispersions. A thesis would primarily involve lab-work with a focus on protein chemistry and physics.

Utilizing conserved lipid structures as nanocarriers

Name PhD/PD: Imogen Morris

Involved staff members: Harry Bitter and Costas Nikiforidis

Start/(expected) end date of project: 2023 – Ongoing



Background and goal of project

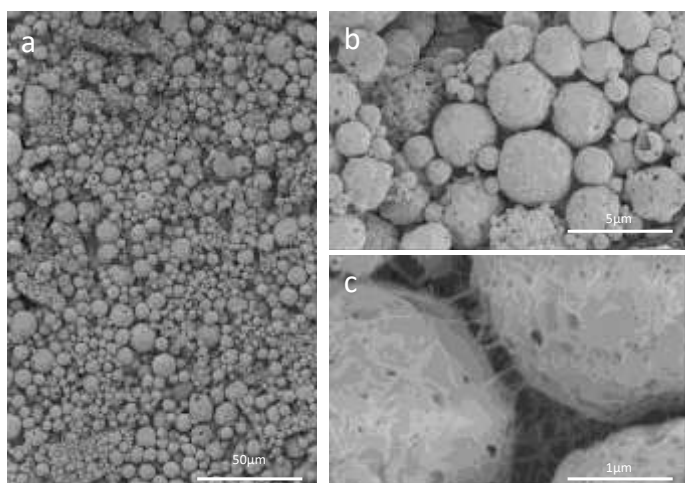
Repurposing lipid droplets, oleosomes, extracted from seeds into nanocarriers for direct therapeutic delivery

Various cellular mechanisms restrict the bioavailability and, therefore, the efficacy of many therapeutics; most notably, the cell membrane acts as a highly selective barrier. By utilizing the natural membrane fusing properties of plant-based lipid droplets, and oleosomes, we can enhance delivery and bio-availability of therapeutics. This project combines cell culture techniques with advanced imaging to study oleosome-cell membrane fusion, aiming to optimize oleosomes as nanocarriers with high encapsulation efficiency and selective therapeutic delivery.

Highlight of the past year

Optimizing colloidosome nanocarrier production and loading capacity.

Using Scanning Electron Microscopy at high magnification, we observed how various solvents affect the structure of colloidosomes. Using this knowledge, we were able to modulate their production and, therefore, boost their ability to load, transport, and deliver their payload.



Scanning Electron Microscopy of colloidosomes.

Illustrating the fine detail of structural changes caused by different solvents during production.

a. 1000 X, b. 10000 X and c. 50000 X

Type of student projects envisioned

Optimizing nanocarrier-encapsulated therapeutic delivery to the gut. This project focuses on using advanced confocal microscopy to elucidate and optimize the delivery of therapeutics to gut cell model systems. By adapting established cloning assays and tools, we aim to integrate expertise in genetics and microscopy to enhance and modulate our nanocarriers for gut-specific therapies.

Developing co-culture cell models and transitioning to Organoids for high throughput screening. Exploring oleosome-cell interactions will involve co-culturing diverse cell lines to establish organoid models long-term. Here, cell lines will be used as functional tools, allowing us to study the metabolic impact of oleosome-delivered therapeutics in a high throughput manner.

Modeling & Technology



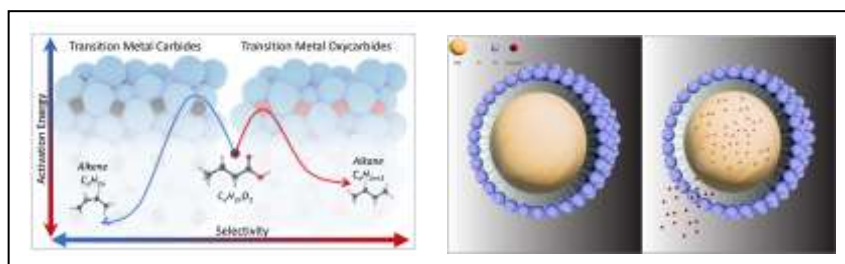
Theme leader: Guanna Li & Akbar Asadi Tashvigh

Background and goal of this theme

Computational modeling geared with large data and AI/ML has become an indispensable tool in catalysis research domain. By simulation of the system at different time and space scales, computational modeling can *in silico* screen a broad spectrum of potential catalysts, provide valuable insights into the catalytic reaction processes, and deliver recipes for rational design of catalytic materials and reactions. With close collaboration with experimentalists in BCT group and external collaborators, in this theme we carry out cross-disciplinary researches and maximize modeling-experiment knowledge exchange and utilization.

In the past year, we continued to apply multiscale quantum chemical modeling methodologies combined with ML models to rationalize catalyst design principles based on molecular level understandings of the reaction mechanisms of catalytic biomass conversion, CO₂ hydrogenation, waste plastic recycling. Meanwhile, we carried out numerical simulations at reactor level to study the mass and heat transfer in porous materials for electrocatalytic conversion of biomass, encapsulation and separation processes of biological membranes, and mechanisms of CO₂ adsorption and capture processes. All research topics have direct collaborations with the ongoing experimental projects of physical chemistry and catalysis/conversion themes.

For the coming period, the objectives are to further develop operando and ML modeling approaches to narrow the gap between models and real systems and to strengthen the reaction mechanism investigations of electrocatalytic systems.



Main topics running in the theme

- **Solid (electro)catalysts for biomass conversion (Akbar)**
Development of kinetic models
Investigation of diffusion in porous materials
- **Capture of CO₂ from air (Direct Air Capture, DAC) (Akbar)**
Development of kinetic models
Modeling condensation in micro- and mesopores
Reactor/process design and heat integration
- **Reaction mechanism and catalyst design for CO₂ conversion (Guanna)**
Rationalization of the CO₂ conversion reaction network and data-driven new catalyst discovery
- **Multiscale modeling of carbide catalyst for biomass conversion (Guanna)**
Investigation of the structure-reactivity relationships of metal carbide catalysts
- **Reaction mechanism of catalytic waste plastic upcycling (Guanna)**
Investigation of PP/PE chemical upcycling by hydrogenolysis and oxidation

Student projects envisioned

Thesis subjects are related to the research work of Ph.D. students and Postdocs in the Modeling & Technology theme or cooperation with the other BCT themes. If you are interested in a thesis, please contact guanna.li@wur.nl or akbar.asaditashvigh@wur.nl to discuss specific details and possibilities.

Biocompatible and sensitive MRI sensors - Elucidating the complex contrast mechanisms of nanoparticles by synergy of experiment and modelling

Name PhD/PD: Merlin Cotessat, MSc

Involved staff members: dr. Guanna Li (dr. Julia Krug and prof. Aldrik Velders (BNT))

Project sponsor: VLAG

Start/(expected) end date of project: 1-Oct-2021 to 19-Mar-2026



Background and goal of project

The goal of the project is to develop new Magnetic Resonance Imaging (MRI) contrast agents, in order to increase the sensitivity of clinical MRI. In order to do so, an interdisciplinary approach combining magnetic resonance imaging, computational chemistry, and organic synthesis will be employed. Systems other than the traditional gadolinium chelates employing new ways to generate contrast (like CEST, Chemical Exchange Saturation Transfer) and supramolecular systems potentially capable of multimodal imaging are the current focus of the project.

Highlight of the past year

In 2024, we managed to achieve the successful multi-step synthesis of a novel water-soluble artificial porphyrin. Once sufficiently pure, in-depth characterization of its spectrophotocemical properties was undertaken. When in solution with metallic elements such as europium, the evolution of its different absorbance bands and their associated fluorescence is asymmetrical (see figure 1 below) which is normally not expected from such systems. Furthering understanding of these phenomena in order to eventually make use of them in more complex systems is now the main focus of the project.

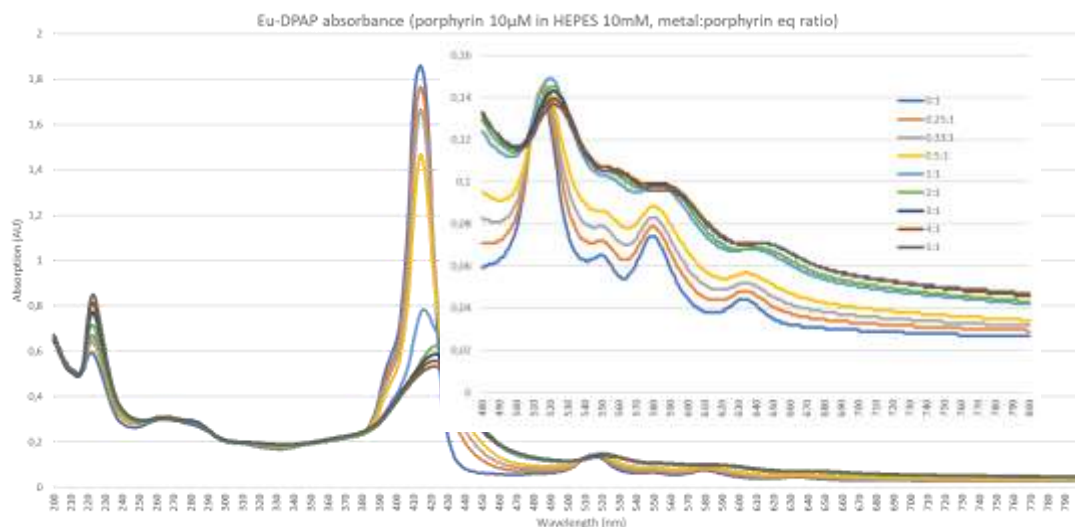


Figure 1. A graph showing the evolution of the absorbance in the UV and visible range of a novel porphyrin as an increasing quantity of europium is added to the solution ; the multiple absorption bands of the porphyrin evolve in different and separate ways.

Type of student projects envisioned

Since 2025 is the last full year of the project, no opportunity for student supervision is foreseen.

Urea Removing Membranes for Artificial Kidney

Name PhD/PD: Martijn Ekhart

Involved staff members: Akbar Asadi

Project sponsor: UKID (Nierstichting)

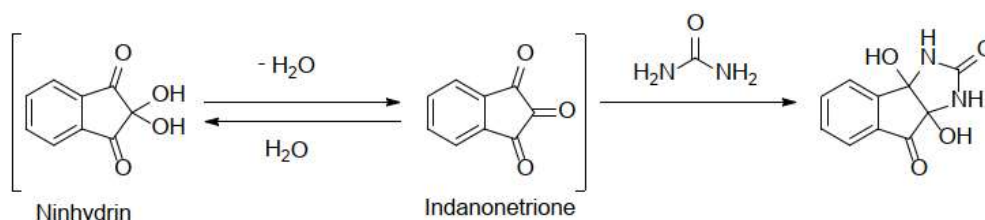
Start/(expected) end date of project: 01-04-2024 / 31-03-2028



Background and goal of project

Patients with end-stage kidney disease undergo hospitalized dialysis for 3-4 times per week to replace kidney function. Although lifesaving, it drastically impacts patients' lives, severely burdens health care costs and produces large amounts of waste. A lot of water could be saved when the dialysate is purified during dialysis in a closed-loop system, which enables dialysis at home and could potentially lead to a so-called wearable artificial kidney.

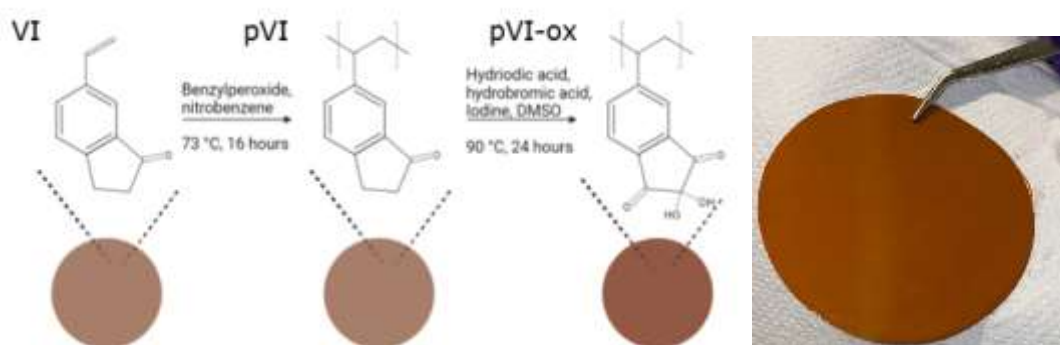
For this, we use ninhydrin based sorbents. These ninhydrin groups are in an equilibrium with their indanonetrione which can covalently bind to urea to remove it from the dialysate.



Previous research already showed that 'polymer beads' (small balls of polymer) could be made with these ninhydrin groups incorporated in them. These beads already showed a quite good binding capacity but their reactivity was still too low for application. In this project, sorbent membranes are being developed to increase the reactivity of the sorbent.

Highlight of the past year

The first sorbent membranes have been developed! Their binding capacity, reactivity and stability are all still unclear but this is a major step towards making functional sorbent membranes.



Type of student projects envisioned

- A background in (organic/polymer) chemistry, and wanting to apply it to membranes
- Curious to use different techniques relating to chemistry, flow-testing and data analysis.
- Looking to contribute to help people suffering from kidney disease and reduce the climate impact of dialysis.
- Wanting to work in a collaborative project with BCT at WUR but also with Utrecht University and UMC Utrecht (stationed at WUR).

Exploring the potential of non-fluorinated proton exchange membranes for hydrogen fuel cells

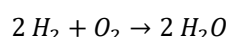
Name PhD/PD: Ellis van Keulen
Involved staff members: dr. Akbar Asadi Tashvigh
Prof. dr. Harry Bitter

Start/(expected) end date of project:
November 2022-November 2029



Background and goal of project

Balancing the grid is challenging due to a mismatch between renewable energy production (e.g., solar or wind) and energy consumption [1]. Hydrogen is expected to have a key role in the future electrical grid. Hydrogen can be used as a chemical storage component, produced via water electrolysis. When there is an electricity demand, hydrogen can be utilised using a proton exchange membrane fuel cell (PEM-FC). The overall reaction within the hydrogen fuel cell is:



In a PEM-FC, the proton exchange membrane (PEM) is the heart of the cell and its function is to conduct protons while forming a barrier between hydrogen and oxygen gasses. Currently, perfluorosulfonic acid polyelectrolyte-based membranes are mainly used because of its high conductivity and stability. However, with the growing awareness of polyfluoroalkyl compounds (PFAS), it is key to develop an alternative proton exchange membrane which is more sustainable.

Highlight of the past year

This year we have focused on the development of characterisation methods for our PEMs, as can be seen in Figure 1. Here several impedance setups (to evaluate to proton conductivity) have been tested, such as a through-plane and in-plane configuration. In addition, we have established a lab setup for hydrogen fuel cell testing of our membrane electrode assembly. Currently, we are focusing on the development of polymer blend membranes using sulfonated polymers.

Type of student projects envisioned

In this project, generally the membrane development workflow shown in Figure 1 is followed. Here membranes are synthesized, characterized and tested for hydrogen PEM-FC. Student's projects will follow this workflow too and consist working in the lab. Some projects will focus on the modification of polymers (such as side chain modifications). All project consist of membrane characterization using techniques such as electrochemical analysis (e.g., impedance, polarization curves), thermal gravimetric analysis and chemical analysis such as Fourier transform infrared (FTIR). Affinity with (polymer) chemistry is an advantage.



Figure 1. Membrane development workflow consisting of membrane synthesis, characterization and testing.

[1] T. Capurso, M. Stefanizzi, M. Torresi, and S. M. Camporeale, "Perspective of the role of hydrogen in the 21st century energy transition," *Energy Convers Manag*, vol. 251, p. 114898, Jan. 2022, doi: 10.1016/j.enconman.2021.114898.

Advanced Polymer Synthesis for Proton Exchange Membrane Fabrication

Name PhD: Sam Pikavet

Involved staff members: Prof. Dr. Harry Bitter, dr. Akbar Asadi Tashvigh, dr. Tomas van Haasterecht

Project sponsor: NWO groenvermogen

Start/(expected) end date of project: December 2024 - December 2028



Background and goal of project

As part of the global energy transition aiming to limit the effect of global warming, one key area is energy storage. The use of hydrogen based storage is attracting attention due to its advantages of excellent capacity and low emissions. Currently, a great deal of research is focused on improving the viability of hydrogen in the individual steps of circular production, storage, and consumption.

Proton exchange membrane fuel cells (PEMFCs) are a clean and efficient way to convert hydrogen and oxygen into electricity, producing water as a side product. Compared to other fuel cells, PEM type fuel cells are highly efficient and operate at lower temperatures. Their compact and portable size makes them especially suitable for automotive applications. The proton exchange membrane is responsible for selectively conducting protons between the anode and cathode, while blocking gas and electron crossover. However, improving the durability remains the key area of improvement.

Currently, Nafion-type membranes are predominantly used in PEMFCs because of their high conductivity and excellent mechanical and physical properties. However, as a fluorinated compound, Nafion raises significant environmental concerns, especially regarding its long-term impact. This highlights the need for alternative, high-performance, PFAS-free membranes. In this project, comb-like polymers with sulfonated side chains will be developed to replace Nafion-type membranes. These functionalized side chains are expected to facilitate microphase separation and formation of hydrophilic pathways, which should result in improved performance. Additionally, the project aims to better understand the underlying mechanisms and properties of these new materials.

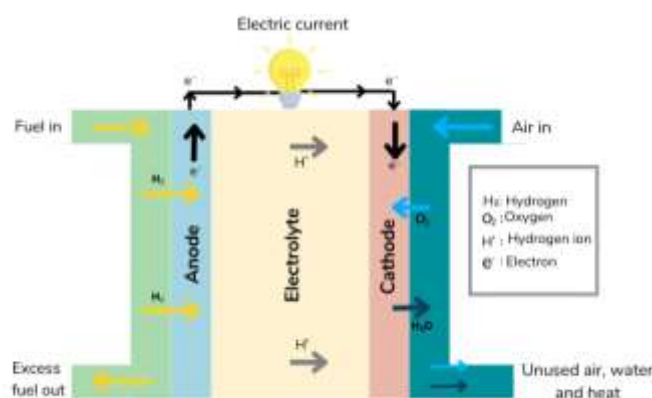


Figure 2 Schematic representation of a proton exchange membrane fuel cell (PEMFC)

Highlight of the past year

-Start of the project.

Type of student projects envisioned

Projects will be focused on synthesis of monomers, including their characterization and purification, followed by polymerization processes to develop PFAS-free polymers. These polymers will then be used for membrane fabrication to be used in a fuel cell with performance characterized in terms of conductivity, mechanical strength, and durability.

Enhancing micropollutant biodegradation in municipal wastewater through synergy with “fit for purpose” nanofiltration membranes

Name PhD/PD: Nena Zwart

Involved staff members: Akbar Asasi Tashvigh, Harry Bitter, Dainis Sudmalis (ETE), Nora Sutton (ET)

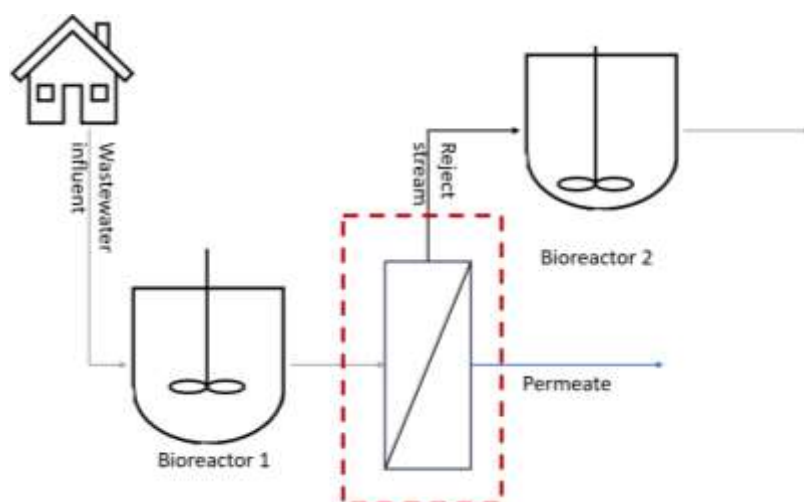
Project sponsor: WUR

Start/(expected) end date of the project: 01-10-2024 til 30-09-2028



Background and goal of the project

Increasing amounts of organic micropollutants (OMPs) for instance, medicines, pesticides, PFAS, etc., end up in our wastewater. The OMPs pose a risk to public health and the environment when they are not removed. Current OMP removal methods are often energy-intensive, chemically intensive, or both. Another removal option would be the biodegradation of OMPs since this would lower the energy and chemical demand. However, to improve the biodegradation the OMPs need to be concentrated with nanofiltration (NF) membranes. Developing Covalent Organic Framework (COF)-NF membranes could be a suitable option, since the crystalline nature of such membranes gives high control over the characteristics, such as pore size and active groups. However, the challenge is to make them suitable for membrane use without losing their highly crystalline nature. In this project new NF membranes, using COFs will be developed and integrated into a bench-scale wastewater treatment, to look into the potential of COF-NF membranes and their effect on biodegradation, such as the effects of the OMP concentration and salinity on the biodegradation. The figure below shows an overview of the envisioned system, where the municipal wastewater is treated in the first bioreactor, followed by an NF membrane to concentrate the OMPs, which are in turn treated in the second bioreactor.



Highlight of the past year: This project started in October and the first two batches of COF polymers have been made.

Type of student projects envisioned: As a thesis student in 2025, you could be involved in developing and improving new COF-NF membranes for OMP removal! Examples of projects could be the optimization of COF synthesis (polymer chemistry), the development of COF-NF membranes, and the characterization of the COFs and COF membranes. Once the synthesis of COF-NF membranes is developed, the performance of the COF-NF membranes can be tested. These projects could be interesting for students with lab experience, an affinity for organic chemistry and preferably experience in chemical synthesis.

Education

Bachelor and Master courses BCT and contribution to other courses

Code	Course title
BCT-10302	Organic Chemistry BAT
BCT-10805	Process Engineering Basics
BCT-20306	Modelling Dynamic Systems
BCT-22803	Physical Transport Phenomena
BCT-23306	Biorefinery
BCT-23806	Principles of Biobased Economy
BCT-24306	Renewable Resources and the (Bio)Chemical Production of Industrial Chemicals
BCT-30806	Physical Modelling
BCT-32306	Advanced Biorefinery
BCT-33806	Conversions in Biobased Sciences
BCT-34818	Micromaster Biobased Chemistry
BCT-35306	Catalysis and bio-organic synthesis
BCT-40306	Biobased Materials Science

Code	Course title
BPE-20806	Separation Process Design
BPE-60312	Bioprocess Design
FTE-12803	Introduction Biosystems Engineering part 2
PCC-33808	From Molecule to Designer Material
PPH-31804	Frontiers in Molecular Life Sciences
YWU-60312	Research Master Cluster: Proposal Writing

BCT: Biobased Chemistry and Technology

FTE: Farm Technology

PPH: Plant Physiology

BPE: Bioprocess Engineering

PCC: Physical Chemistry and Soft Matter

YWU: Wageningen University

BSc Theses

- Kluijtmans, Wouter - Optimisation of hydrodeoxygenation reaction on different surfaces of the hexagonal-Mo₂C
- Jonker, Wes - Effect of Solid Fat Content and Interfacial Protein Density on Partial-Coalescence in Packed Emulsions (YFS, BCT 45%)
- Osté, Iris – The effect of fat, in combination with temperature, on the foaming properties of faba bean protein (YFS, BCT 20%)

MSc Theses

- Sanchez Bedoya, Maria - Extraction of rapeseed proteins and the impact of phenolic compounds on their gelling properties
- Bassil, Michelle – Investigation of Transfer of Bioactives from Oleosome into Cells (FPH, BCT 50%)
- Weelden, Ilias van - Investigating the Extent of Binding of Sinapic Acid and Rapeseed Proteins, and its Consequences for Protein Gelling Properties
- Rajwade, Sreya – The effect of oil extraction from rapeseeds on the characteristics of the proteins (FPE, BCT 30%)
- Giusepponi, Giona - Understanding the influence of the extraction methods on the stabilisation and material properties of pea proteins stabilized emulsions
- Hocevar, Manca – Encapsulation of bioactive component in oleosome-membrane loading (FPH, BCT 50%)
- Kuang, Daisy – Pea Protein Assembly Mediated Stabilization of High Internal Phase Emulsions for Plant-Based Adipose Tissue Mimics (FPH, BCT 50%)
- Krauss, Raphael - Does the addition of oleosomes make biobased food packaging more flexible and hydrophobic? (PCC, BCT 50%)
- Ozobodo, Kingdavid - Dual enzymatic remodeling approach to enhance digestibility properties of starch
- Fellermaier, Julia – In Vitro Lipid Digestion: Impact of Co-Extracted Storage Proteins on Rapeseed Oil Body Emulsions (FQD, BCT 50%)
- Sim, Wai-Yin - Electrochemical Br[O]mination of Furfural
- Sawant, Ajinkya - Electrocatalytic synthesis of H₂O₂ over carbon nanofiber supported Ninanoparticles: Elucidating the role of surface oxygen groups
- Purcell, Michael - Structure-Performance Relationship of Molybdenum Carbide Catalysts for Hydrodeoxygenation Reaction
- Rebollo Campo, Claudia - Effect of pH during rapeseed protein concentration by membrane filtration
- Ferryka Sekar, Bernadetha Efata - Evaluating Conductivity: Characterization of Hydrocarbon-based Proton Exchange Membrane
- Kovacs, Stan - Phospholipids affect the functionality of mildly extracted rapeseed proteins by covering their surface
- Becerril Gama, Ximena - Process Design to Obtain Calcium Carbonate and Proteins from Chicken Eggshell