## Biobased Chemistry and Technology Annual report 2022





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## Contents

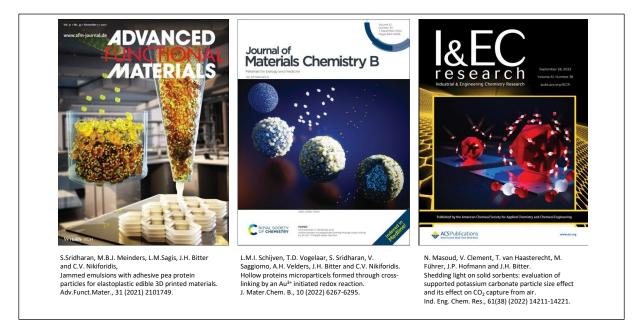
INTRODUCTION
CATALYSIS/CONVERSION
Electrochemical cell design for the production of valeric acid and hydrogen peroxide
Novel enzymatic routes for making starch derivatives with retarded digestibility and enhanced functional properties
Mixed metal carbides for biomass upgrading9
Enabling Direct Air Capture of CO2 through efficient and stable sorbent materials
Electrocatalytic conversion of (poly)saccharides over 3D electrodes11
Integrating CO2 capture and utilization: towards a more efficient use of CO2 from the air
Specific dietary fiber combinations for decreasing antibiotics use and faster recovery of gut microbiota 13
Carbon supported nickel nanoparticles for the electrochemical production of hydrogen peroxide
Electrochemically induced conversion of biobased compounds15
Recycling and valorising residual keratin materials from chicken feathers into biobased nanocarriers16
Strategies for hydrogen evolution catalyst integration in Microbial Electrosynthesis
BIOBASED SOFT MATTER18
Electrophoretic Separation of Oleosomes and Proteins from Oilseeds
Exploring sustainable transformation of plant extract industry
Oleosomes as carriers of cannabidiols21
Nature knows best – Lessons from plants on how to design stable emulsions resistant to lipid oxidation 22
Oleosoemes (Lipid Droplets) as Carriers of Therapeutics23
Continuous extraction of oleosome from rapeseed24
How does oleosin influence mechanical properties of oil body surface?
Application of oleosome as biodegradable/edible films and coatings in food packaging
Self-assembled oleosin micelles for resveratrol delivery
Finetuning oilseed protein-phenol interactions towards novel functional materials
MODELING & TECHNOLOGY

Biocompatible and sensitive MRI sensors - Elucidating the complex contrast mechanisms of nanoparticles synergy of experiment and modelling	-
Reomval of Perfluorinated Acids Contaminant from Water by Pillararenes	31
Multiscale modeling of transition metal carbides for biomass conversion	32
Membranes Separation Processes	33
Smart membranes for high temperature proton exchange membrane fuel cells (HT-PEMFC)	34
EDUCATION	.35
SCIENTIFIC PUBLICATIONS 2022	.38
OTHER OUTPUT	.41

#### Introduction

It is my pleasure to present to you the annual report 2022 of the Biobased Chemistry and Technology (BCT) group.

Luckily this year we were able to work again without too many Covid restrictions. Working in the lab and working with each other does increase the quality of our research. That resulted in nice papers with 3 front covers showing the span of our research.



We are happy that we can contribute to a sustainable future. With our research we contribute to new sustainable materials and processes. By striving for a fundamental understanding of catalysts, extraction procedures and materials properties we develop new materials and processes. We do not only do this in the lab but also at the computer. I am very excited that we have both laboratory skill and computational skills in one group.

The outcome of our research is summarized in this annual report. I hope you will enjoy reading it.

With kind regards

Prof. J.H. (Harry) Bitter Chair holder Biobased Chemistry and Technology

#### Catalysis/Conversion

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

**PhD students/Post doc:** Roel Bisselink, Roxani Chatzipanagiotou, Maurice Essers, Marlene Fuhrer, Xinhua Windt, Torin de Groot, Matthijs van der Ham, Tim Hoogstad, Freek Karaçoban, Frits van der Klis, Cynthia



Klostermann, Ivo van Luijk, Dmitry Pirgach, Edwin Schreuder, Xiaojie Qin, Sanne de Smit. Contact: <u>elinor.scott@wur.nl</u> or <u>harry.bitter@wur.nl</u>

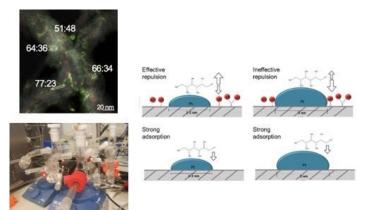
## **Background and goal**

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 CO<sub>2</sub> 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:

- o Catalyst development for biobased feedstock conversion (heterogeneous, homogenous, bio)
- $\circ$   $\quad$  Conversion of biobased feedstocks and synthesis of biobased chemicals
- o Use of non-noble metal catalyst to replace scarce noble metals in synthesis
- o Electrochemical/electrocatalytic conversion of larger (biobased) molecules
- o Integration of thermal catalysis with electro catalysis/chemistry
- CO<sub>2</sub> capture and conversion



Some examples: STEM/EDX (in collaboration with Prof. P.E. de Jongh (UU) of Mixed Mo-W carbides/CNF for deoxygenation (top left). Electrochemical cell for testing of foam based electro catalysts (bottom left). Representation of surface oxygen groups in Pt/CNF for glucose oxidation

#### Highlights from last year

- New project started on electrocatalytic production of H2O2 together with Utwente, WUR-FBR, Solvay
- Front cover of Industrial and Engineering Chemistry Research of Nazila Masoud on direct air capture of CO<sub>2</sub> using K<sub>2</sub>CO<sub>3</sub>/CNF
- Guanna Li (Modeling & Technology) and Harry Bitter started a collaboration with Nanjing University of Science and Technology (prof. Jing Zhang) on CO<sub>2</sub> capture and photocatalytic conversion.

## 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, TKI programs 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 (LA) to valeric acid (VA) and 2. oxygen to hydrogen peroxide. 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 LA to VA progressed from conversions in a glass H-cell to flow cell operation. Therefore focus was directed to 'scale-up' aspects, such as corrosion, reactivity of the reactants and products at the other electrode and reactor configuration. As the reaction mechanism involves formation of an organo-metallic specie, cathodic corrosion could take place. Therefore, corrosion of selected cathodes were determined by using intermittent electrolysis as shown in the figure below with Pb as example. A steep increase in Pb concentration is noticed after switching the current on and off, which is the result of the dissolution or formation of a PbSO<sub>4</sub>-film. But most importantly, the results indicate that with Pb, and the other materials, dissolution of the cathode does either not occur or is minimal compared to corrosion under zero current conditions. Next, we investigated the influence of the type of anode, based on lead dioxide (PbO<sub>2</sub>) or iridium oxide (IrO<sub>x</sub>) on the cathodic process. No reactivity of reactants and products were observed at IrO<sub>x</sub> in contrast to PbO<sub>2</sub>. This reactivity is attributed to the formation of reactive hydroxyl radicals at PbO<sub>2</sub>. In addition, the determined stability of IrOx anodes is >3 orders of magnitude higher compared to PbO2. However, low amounts of dissolved iridium negatively influence the cathodic reduction reaction of LA to VA. This negative influence is tentatively explained by the formation of iridium particles, which catalyse the cathodic formation of hydrogen. Therefore four different flow cell configurations, divided and undivided and with a PbO2 or IrOx anode, were evaluated based on selectivity and energy usage. As a result the energy consumption can be as low as 3.2 kWh/kgvA at 100 mA/cm<sup>2</sup>.

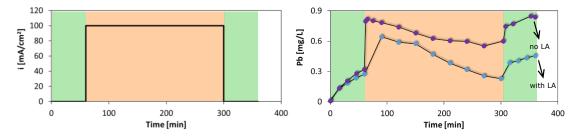


Figure 1. Effect of intermittent electrolysis (left) on the corrosion of Pb cathode in 1 M  $H_2SO_4$  with and without 0.5 M LA (right).

#### Type of student projects envisioned

Experimentally oriented projects are available to improve understanding of the involved reactions, e.g. assessing the influence of reactant on the conversion, other reactants include different keto-acids, diketo-acids and alike. Work involving oxygen reduction to hydrogen peroxide has started in September 2022, here synthesis and characterisation of electrocatalysts are foreseen.

#### References

Bisselink et al., *ChemElectroChem* **2019**, 6, 3285. Bisselink (**2017**). Electrochemical process and reactor. (Patent No. WO2017222382)

# Novel enzymatic routes for making starch derivatives with retarded digestibility and enhanced functional properties

Name PhD: Maurice Essers Involved staff members: Harry Bitter Project sponsor: AVEBE Start/(expected) end date of project: 1-10-2020-1-10-2024



## Background and goal of project

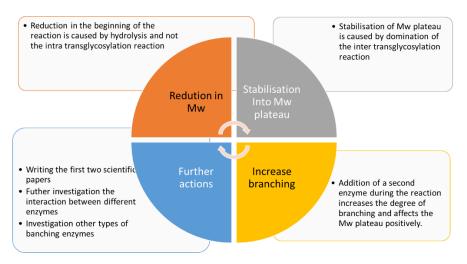
Carbohydrates, such as starch, will be completely converted into glucose by the human digestive enzymes in the small intestine. Consumption of high levels of digestible carbohydrates can lead to diseases such as obesities, diabetes etc. Hence there is a need of carbohydrates that are less prone to human digestion. This can be achieved via remodeling or re-structuring of starches. Remodeling can be achieved via starch modifying enzymes e.g., 1,6- $\alpha$ -glucotransferases such as branching enzymes. Still, the increase of the  $\alpha$ -1,6 glycosidic bonds are still insufficient to induce complete resistance towards digestion in the small intestine. Another aspect is the reduction in molecular weight, which already occurs in the beginning of the reaction and stabilizes into a plateau during the further branching reaction. Hence in this research we aim to investigate

- 1. Is the Mw reduction due to the branching reaction or hydrolysis (side reaction)?
- 2. The cause of the stabilization into Mw plateau during the further reaction.
- 3. How the process conditions affect the degree of branching and Mw plateau and if this can be further enhanced.
- 4. What the influence is of the degree of branching on the digestibility properties and the corresponding viscosity/functional properties.

The goal is to gain insight in the enzymatic remodeling mechanism in order to make a novel starch structure with both physiological as well functional properties.

## Highlight of the past year

- 1) Mw reduction is beginning of the reaction is due to hydrolysis and not the intra transglycosylation as reported in literature; branching reaction seems to be Mw depended.
- 2) Mw stabilization is caused by inter transglycosilation which is proven via Malditof Ms analyses after enzymatic branching with two different types of modified starches.
- 3) Further progress realized via addition of a second enzyme, amylomaltase, resulting in an Increase of the degree of branching is observed.



## Type of student projects envisioned

We envision a student project which is focused on the execution (lab work) of which we would like to investigate different types of starch branching enzymes form different bacterial hosts.

#### Mixed metal carbides for biomass upgrading

Name PhD: Marlene Führer Involved staff members: Prof. dr. Harry Bitter, dr. ir. Tomas van Haasterecht Project sponsor: NWO & FAPESP Start/(expected) end date of project: September 2018- December 2022



#### Background and goal of the project

Transition metal carbides like molybdenum and tungsten are viable replacements for scarce noble metal catalysts. We have shown that carbon-supported Mo (8.5 wt%) and W (15 wt%) carbides are active for decarboxylation/decarbonylation and hydrodeoxygenation of renewable triglyceride-based feedstock to chemicals such as oxygenates, alkenes and alkanes. Interestingly, when comparing the supported W-carbides to the supported Mo-carbides catalysts the former ones were more selective (>50%) towards the high-valued alkenes, while the latter were more selective towards the also valuable oxygenates.

In our research, we want to understand how the catalysts behave when using mixed W/Mo-carbides. The first challenge in this research was to make a MoW carbide of one mixed phase. For this several characterization measurements during and after synthesis (e.g. TGA, TPD/MS, TEM, XRD) have been used to indicate the preparation of bimetallic MoW carbides.

#### Highlight of the past year

We were able to show that both methods the carbothermal reduction (CR) method and the temperatureprogrammed reduction (TPR) method result in well-mixed bimetallic carbide phases. The TEM-EDX images in Figure 1 display the TPR (left) and CR (right) synthesised mixed MoW-carbide with a molar ratio of 1:1 (Mo:W). The composition of the nanoparticles itself varies; some particles contain >85 wt% Mo, and others are fully mixed (50:50 wt%).

Although both methods lead to well-mixed MoW-carbide nanoparticles, the available carbon source during the synthesis influences the crystalline phases and the particle size of the nanoparticles. A cubic carbide ( $MeC_{1-x}$ ) phase with 3-4 nm nanoparticles was obtained when using TPR method while a hexagonal phase ( $Me_2C$ ) with 4-5 nm nanoparticles was found when using the CR method.

In addition, the carbide catalysts were tested for the deoxygenation of stearic acid. The TPR-synthesized carbides showed higher activity in comparison to the CR-prepared catalysts after 1 h. This higher activity of the TPR samples was tentatively related to the cubic crystal structure, particle size or a combination of those two effects. These results highlight that the crystal structure and/or the particle size have more impact the catalytic on performance than the composition of the mixed metal carbides.

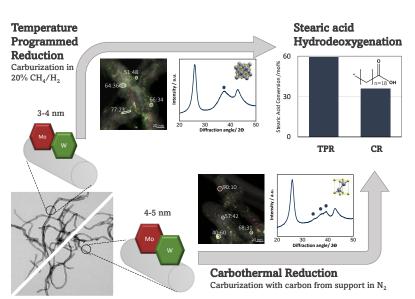


Figure 1. The characteristics and deoxygenation performance of mixed carbides prepared via the CR and the TPR synthesis

#### Type of student projects envisioned

This project has ended by the end of 2022.

## 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

Anthropogenic carbon dioxide is a major contributor to climate change. Direct air capture of carbon dioxide is one way to reduce emissions. In my project, potassium carbonate on a carbon support is used to capture  $CO_2$  from air, known as direct air capture (DAC). Potassium carbonate reacts with  $CO_2$  and water vapour to form potassium bicarbonate. This can then be heated to regenerate the sorbent and release the  $CO_2$  which can then be stored or utilised.

The aim of the research is to establish property-performance relationships of these materials for  $CO_2$  capture; key sub questions are:

- 1. Identifying the role of water in the reaction mechanism.
- 2. Investigating effects of support polarity and porosity on sorption capacity
- 3. Explore stability of sorbent materials during both storage and use

#### Highlight of the past year

Sorbent materials were prepared using carbon nanofiber supports with different surface polarities. These supports were characterised and tested in terms of CO<sub>2</sub> capture performance at high water vapour concentrations. Polar sorbent materials showed lower sorption capacities (Figure 1), however increasing polarity further had no clear effect.

Experiments were also done at different water vapour concentrations using an apolar sorbent (Figure 2). These showed an inhibitory effect of water vapour concentration on CO<sub>2</sub> sorption capacity as greater quantities of potassium carbonate hydrate were formed. CO<sub>2</sub> breakthrough curves for different sorbents

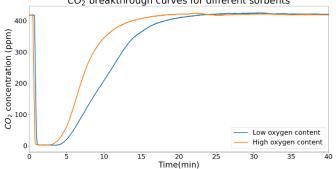


Figure 1: Breakthrough curves of sorbents with different surface polarity. 4.4% oxygen groups returns to the inlet concentration sooner and has less area above the curve, indicating a lower sorption capacity.

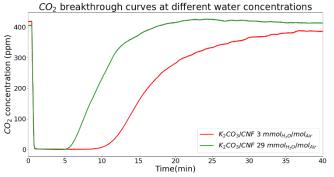


Figure 2: Breakthrough curve at different water concentrations. Lower water vapour concentrations causes sorption to continue for longer and gives a higher sorption capacity.

#### Types of student projects envisioned

Student projects could include characterising and testing supports with different polarity using TGA, XPS and TPD; investigating K2CO3 particle size using physisorption, chemisorption and TEM; exploring sorbent stability under different conditions with XRD. There is also room for some modelling of breakthrough curves .

#### Electrocatalytic conversion of (poly)saccharides over 3D electrodes

Name PhD: Matthijs van der Ham Involved staff members: Prof. Dr. Harry Bitter, Dr. Akbar Asadi Project sponsor: NWO, Avebe, TNO, Brightlands Start/(expected) end date of project: 08-2019/08-2023



#### Background and goal of project

The electrocatalytic conversion of biomass-based feedstocks can be used for the sustainable production of platform molecules and specialty chemicals, such glucose and starch to glucaric acid and anionic starch. Electrocatalytic conversions can be performed at mild reaction conditions and can use water as the oxidizing and reducing agent, thereby enabling the sustainable production of chemicals. Moreover, in electrocatalysis the driving force to surpass the activation energy barrier of the reaction is the applied potential, which can easily be tuned, giving good control over the electrocatalyst selectivity. In this project, platinum (Pt) is used as the electrocatalyst, which is decorated as nano-sized Pt particles on two different supports (carbon nanofibers (CNF) and nickel (Ni) foam) to increase the Pt surface to volume ratio, thereby reducing the amount of scarcely available Pt. The aim of this project is to synthesize Pt on CNF and Pt on Ni foam electrocatalysts, and to evaluate their activity, stability and selectivity for the oxidation of glucose and starch.

#### Highlight of the past year

Last year we had shown that an increase in content of support oxygen groups on a CNF support decorated with Pt particles (Fig. 1A) increases the catalytic activity of Pt for the electrocatalytic oxidation of glucose. The increase in catalytic activity was related to an enhanced adsorption of glucose in the perimeter of the Pt particle (Fig. 1B), facilitating an increase in available glucose to be catalyzed by Pt. In parallel, we have studied the effect of Pt oxidation state on the catalyst selectivity for the electrocatalytic oxidation of glucose. For this study a novel analytical approach was developed where a combination of chromatographic techniques (HPLC and HPAEC) allowed us to quantify the 10 different glucose oxidation products. For electrocatalytic glucose oxidation, Pt favors the dehydrogenation of the primary alcohol groups ( $C_6$ ), whereas PtO<sub>x</sub> favors the oxidation of the anomeric carbon ( $C_1$ ) (Fig. 1C).

Current research focusses on the use of Pt functionalized foam reactors for the catalytic oxidation of starch (Fig. 1D), preferably achieving the oxidation of the primary alcohol groups (C<sub>6</sub>). The foam is macroporous (> 0.4 mm), facilitating the diffusion of starch molecules and therefore reducing mass transport limitations. Here we aim to synthesize and characterize the Pt functionalized foams, and study whether it can electrocatalytically oxidize starch and characterize the anionic starch.

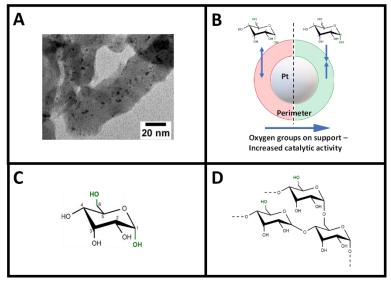


Figure 2. A) Self-synthesized Pt nanoparticles supported on carbon nanofibers. B) The effect of support oxygen groups on Pt/CNF on the electrocatalytic activity of Pt/CNF for glucose oxidation. C) For glucose it was found that Pt favors the dehydrogenation of the  $C_1$  group and PtO<sub>x</sub> favors the oxidation of the  $C_1$  group. D) shows the aim for next year, where we intent to oxidize starch at the  $C_6$  group Pt functionalized foam reactors.

#### Type of student projects envisioned

This project is close to its end and therefore there are no new student projects.

## Integrating CO2 capture and utilization: towards a more efficient use of CO2 from the air

Name PhD: 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 decrease  $CO_2$  levels in the atmosphere and simultaneously produce useful chemicals,  $CO_2$  Capture & Utilization (CCU) technologies are necessary. Currently, it is technologically possible to capture  $CO_2$ , release it, and then convert it into interesting product. However, this remains unfeasible due to high energy demands.

In this project, we develop a dual functional material (DFM) that is capable of both capturing CO2 and converting it to interesting products. This DFM consist of a CO2 sorbent and a metal that catalyzes the conversion of CO2. Figure 1 shows an envisioned process using a DFM.

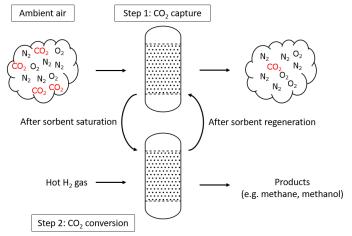


Figure 1: Envisioned integrated  $CO_2$  capture & conversion process which we aim to explore during this PhD project.

We thus attempt to integrate  $CO_2$  capture and conversion. This hopefully results in a more energy efficient process. To do so, there are two main challenges that we will tackle:

- 1) The material must capture  $CO_2$  ambient air, as this allows it to capture all  $CO_2$  that is emitted.
- 2) The CO<sub>2</sub> must be converted at a low temperature.

## Highlight of the past year

In the past year we aimed to develop our first dual functional materials. We successfully combined the  $CO_2$  sorbent  $K_2CO_3$  with a noble, and a non-noble metal. These metals were capable of partly reducing  $CO_2$  into interesting products. We found that the selectivity and yield of the conversion is tunable by modifying the  $K_2CO_3$ /catalyst interactions. We now aim to elucidate what kinds of interactions are present.

## Type of student projects envisioned

Students are welcome for various projects in the lab. Now we have produced multiple functional DFMs, we can further characterize these. We will attempt to identify the most important aspects that influence the performance of the materials. Additionally, we aim to understand how exactly these materials capture & convert CO<sub>2</sub>. Modelling projects may also be available, as we will eventually compare the developed DFM to separate CO<sub>2</sub> capture & conversion.

## Specific dietary fiber combinations for decreasing antibiotics use and faster recovery of gut microbiota

Name PhD: Cynthia Klostermann Involved staff members: prof. dr. Harry Bitter Involved members: prof. dr. Henk Schols (FCH), prof. Dr. Paul de Vos (UMCG) Project sponsor: NWO, CCC (Carbobiotics) Start/(expected) end date of project: 15-11-2018 / 15-02-2023



## Background and goal of project

Resistant starch type 3 (RS-3) is known to have great potential as a prebiotic by supporting beneficial gut microbiota after intestinal digestion. In contrast, antibiotics have a negative effect on beneficial microbiota and barrier function. This research investigates the opportunity of RS-3 to be used as a prebiotic after antibiotics use. RS-3 is considered a dietary fibre since it escapes digestion in the small intestine and arrives in the colon. Previously, the factors influencing resistance to digestion of specific RS-3 have been studied [1]. It has been concluded that especially a specific crystal type and chain length are of interest, since such RS-3 preparations are fully resistant to digestion in the small intestine and thus arrive in the colon. *In vitro* fermentation of such substrates revealed that depending on the physico-chemical characteristics, the ratio between expected primary degraders *Ruminococcus*, *Bifidobacterium* and *Lachnospiraceae* differed.

#### Highlight of the past year

RS-3 preparations with different physico-chemical characteristics were *in vitro* fermented with known primary RS degrading strains of *Ruminococcus bromii* and *Bifidobacterium adolescentis*. Results revealed that *R. bromii* degraded all substrates tested approximately equally well, whereas *B. adolescentis* only degraded some specific substrates. This thus highlights that certain RS-3 preparations are highly specific dietary fibers, that require advanced enzymatic machineries to be degradable by gut microbes.

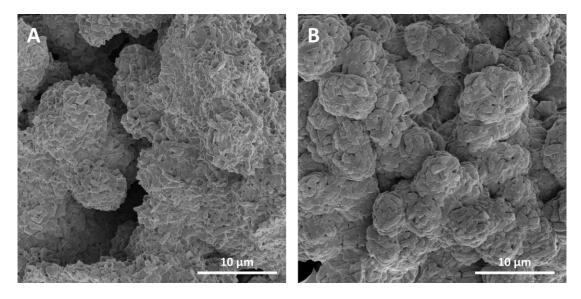


Figure A represents an RS-3 preparation incubated with *R. bromii*, whereas figure B represents the same RS-3 preparation, incubated with *B. adolescentis*.

#### Type of student projects envisioned

This project is close to its end and therefore there are no new student projects.

[1] Klostermann et al. 2021. Carbohydrate Polymers

#### Carbon supported nickel nanoparticles for the electrochemical production of hydrogen peroxide

Name PhD: Ivo van Luijk Involved staff members: Harry Bitter, Akbar Asadi Tashvigh Project sponsor: NWO, Solvay Start/(expected) end date of project: 1-11-2021/1-11-2025



(1)

#### Background and goal of project

Hydrogen peroxide is a very versatile and important oxidant, that has found many applications. However, current production of the chemical via the anthraquinone process, relies on non-renewable hydrogen and fossil derived organic compounds. These factors give rise to the 1.1 million tons of  $CO_2$  to be emitted in the EU alone. To mitigate these emissions, this project aims to improve the alternative  $CO_2$  neutral electrochemical method via the development of better cathode materials. The electrochemical method works by a reduction reaction of oxygen, as is shown in Equation 1.

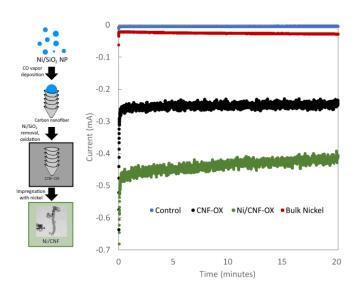
$$O_2 + 2H_2O + 2e^- \rightarrow H_2O_2 + 2OH^-$$

To improve the efficiency of this reaction, better and abundant electrode materials are needed. In this project cathode materials consisting of abundant transition metal nanoparticles supported by carbon are developed for this method. The properties of the materials, dictating the efficiency (kinetics) of the oxygen reduction reaction, can be altered by changing the nanoparticle morphology or the composition of the carbon support.

#### Highlight of the past year

This year we showed the potential of using nickel based nanoparticles in the electrochemical oxygen reduction reaction. The addition of nickel nanoparticles to the carbon nanofiber support increases the current compared to the bare carbon support. Additionally the nanoparticles demonstrate far greater activity than bulk nickel.

Furthermore, it was also demonstrated that the size of nickel nanoparticles has a significant impact on its reactivity. We saw a clear trend towards higher activity at lower particle sizes. It is hypothesized that the smaller particles have better kinetics due to their different electronic structure.



the smaller particles have better Figure 3: Synthesis of catalysts with performance comparison

#### Type of student projects envisioned

There are many possibilities to develop better materials and understanding of this process. Different projects are possible with the improvement of the nanoparticles, carbon support or the system in general. Projects will start with the synthesis of various novel materials, than analysis of the material properties with various characterization techniques and finally performance testing with various electrochemical methods.

#### Electrochemically induced conversion of biobased compounds

Name PhD: Dmitry Pirgach Involved staff members: Prof. Dr. Harry Bitter, Prof. Dr. Pieter Bruijnincx (UU), Dr. Daan van Es (WFBR) Project sponsor: WUR 1<sup>st</sup> stream Start/(expected) end date of project: 01.12.2020 – 01.12.2024



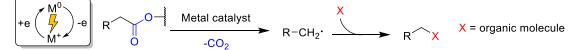
#### Background and goal of project

Lately, developing green and sustainable synthetic and catalytic methods for the production of chemical buildingblocks is gaining more and more attention from the chemists. In addition to electrosynthesis which is nowadays becoming an alternative to the traditional chemical synthesis , it also concerns homogenous transition metal catalysis. Despite being currently widely used, this process is usually burdened with soluble metal species or byproducts. Traditionally, isolation methods like precipitation, distillation, chromatography and recrystallization are employed, however they still suffer from increased waste production and high energy demand.

The goal of the project is to develop sustainable electrochemical approach to conduct the catalytic reactions. This method would allow to conduct homogenous catalytic catalysis, but at the same time would make the catalyst easy-to-separate from the reaction mixture. Developing this method would provide a competitive sustainable alternative to traditional way of conducting the catalytic reactions and separating the catalyst, without high energy demand and waste production.

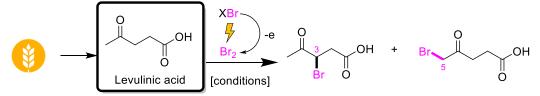
#### Highlight of the past year

During the past year, new approaches for (electro)catalytic valorization of biobased molecules were discovered and studied. First project being developed is electrocatalytic decarboxylative coupling. Carboxylic acids are stable, inexpensive, and widely available in nature compounds. Transformations of carboxylic acids can give access to various valuable product classes, given the variety of readily available acids, they find wide application in organic synthesis as ready or half-ready building blocks.



During the past year the method was being developed to conduct the transition metal catalyzed transformations by means of electrocatalysis, which would offer convenient way to recollect the metallic catalyst from the solution and yield more pure product. Using this electrocatalytic technique allows to reach low levels of transition metal ions in the final product without high energy consumption and waste generation.

Another project developed is electrochemical bromination of renewable levulinic acid. Products of this reaction lead to valuable 3- or 5-bromolevulinic acid - precursors of anti-cancer agents, herbicides, insecticides or precursors of biologically active compounds. Electrochemical approach could be more beneficial solution by using bromide salts as bromine source, avoiding utilization of molecular bromine or other brominating agents. In this case bromine is formed in-situ during the anode process in that way the concentration will remain low and bromine will be consumed immediately. It has been found that depending on the reaction conditions, it is possible to steer the regio selectivity towards the certain brominated product.



## Type of student projects envisioned

Student projects include lab work such as planning and performing the electrochemical experiments, isolating and purifying the desired product and analyzing the samples by means of TLC, NMR and ICP.

## Recycling and valorising residual keratin materials from chicken feathers into biobased nanocarriers

Name PhD: Xiaojie Qin Involved staff members: Dr. Elinor Scott (BCT), Prof. Dr. Harry Bitter (BCT) and Prof. Dr. Chunhui Zhang (CAAS) Project sponsor: China Scholarship Council (CSC) Start/(expected) end date of project: 01-01-2020/01-01-2024



## Background and goal of project

Feather keratin is a promising natural biopolymer with excellent structural stability resulting from abundant disulfide bonds, possessing good stability, biocompatibility, biodegradability, and non-toxicity. It has been developed into various products, including gels, films, micro/nanoparticles. The tripeptides "Arg-Gly-Asp" and "Leu-Asp-Val" in keratin have been reported to own the ability to bind with cell surface ligands and promote cell adhesion. Therefore, feather keratin could be a potential material for preparing drug nanocarriers with high stability and penetrability. However, there are still challenges in nanoparticle stability and drug encapsulation capacity due to the low solubility and dispersity of keratin in aqueous solution.

The project aims to develop a novel nanocarrier system based on keratin materials using insulin as the targeted drug. In this study, keratin nanoparticles (KNPs) will be obtained by controlled hydrolysis, the stability of which will be first explored under various conditions, e.g., heating and enzymolysis. Then, insulin will be encapsulated into keratin nanoparticles in different ways, including self-assembly and covalent bonding. After investigating the insulin loading capacity, *in vitro* stability, and release, a high-performance keratin-based oral route for drug delivery will finally be established.

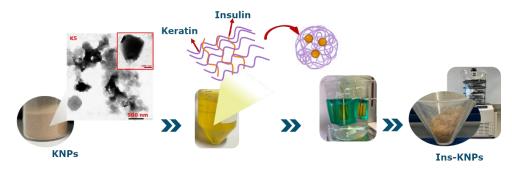


Fig.1 Scheme of keratin nanoparticle preparation for insulin delivery

## Highlights of the past year

- Keratin nanoparticles (KNPs) have been successfully prepared with an average particle size of 123 nm via partial hydrolysis.
- The KNPs presented good stability under heating at 37  $^{\circ}$ C and enzymatical digestion in vitro, demonstrating potential in oral-delivering drugs.
- The KNPs exhibited a reversible "open and closed" structure as a function of pH, which could be used as an encapsulation method.

## Type of student projects envisioned

Preparation and characterization of drug-loaded KNPs in different forms will be carried on. The lab work of this project will mainly include physical and chemical characterization of nanoparticles involving such means as FT-IR, XRD, TEM, DLS, UV, and HPLC. Additionally, the work regarding in-vitro drug release will be explored at later stage.

## Strategies for hydrogen evolution catalyst integration in Microbial Electrosynthesis

Name PhD: ir. Sanne de Smit
Involved staff members: prof. dr. Harry Bitter (BCT), prof. dr. ir. Cees Buisman (ETE), dr. ir. David Strik (ETE)
Project sponsor: WIMEK, ChainCraft
Start/end date of project: Sep 2018 – Nov 2022 (finished)



## Background and goal of project

A sustainable way of reutilisation CO<sub>2</sub> is conversion to higher value compounds. For this process, energy is required, which can be supplied as electricity during Electrosynthesis. To catalyse the CO<sub>2</sub> conversion to volatile fatty acids, microorganisms are used as a catalyst. A biofilm of bacteria grows on the electrode. The fatty acids from the conversion can be used as animal feed additive or platform chemical for e.g. fuel production.

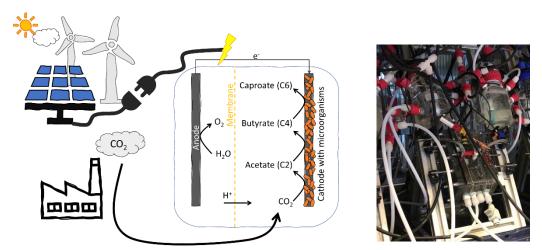
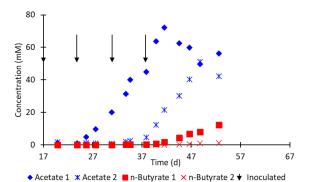


Figure 1. Schematic overview of the process (left) and picture from the set-up in the lab (right).

The goal of the PhD project is gain a better understanding of the working mechanisms at the cathode to obtain steering tools to optimize the system in the lab and work towards practical application.

#### Highlight of the past year

The microbial activity can be boosted by improvement of the hydrogen supply to the biofilm. Hydrogen is an important energy carrier between the electrode and the microbial community. Hydrogen production at the cathode was stimulated by integration of a mixed metal-catalyst. With the integrated catalyst, microbial production of volatile fatty acids acetate and *n*-butyrate was observed within one week after inoculation. This is a substantial improvement compared to the state of art processes which take at least 20 days for start-up.



*Figure 2.* Fast start-up of microbial activity shown as acetate and n-butyrate production 7 days after first inoculation.

## Type of student projects envisioned

No student projects available because the project is finished.

## **Biobased Soft Matter**

Team Leader: Dr. Costas Nikiforidis

**PhD candidates:** Kübra Ayan, Mingzhao Han, Zhaoxiang Ma, Lorenz Plankensteiner, Umay Sevgi Vardar, Chenqiang Qin, Yufan Sun, Mingming Zhong, Sybren Zondervan **Visiting researcher:** Dr. Feng Xue

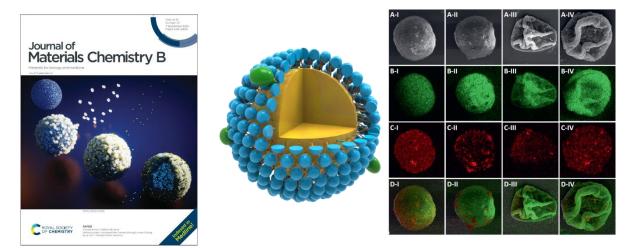
Contact: costas.nikiforidis@wur.nl

#### Background and goal

The Biobased Soft Matter team aims to create bioinspired functional materials using

biosourced molecules and complexes. The property-function relationship of the biosourced molecules and the created soft materials are investigated from a soft matter physics, chemistry, and biology perspective at multiple length scales, from molecular to macroscopic.

The typical analytical tools we are using in our research are fluorescent, confocal, atomic force, scanning and transmission electron microscopy, dynamic light scattering, interfacial and bulk rheology.



#### **Main topics**

- Trafficking molecules with natural lipid droplets (Oleosomes)
- Behavior of lipid droplets (oleosomes) on interfaces
- Plant protein/phenol interactions and their use in functional materials
- Jammed emulsions to mimic animal fat
- Design bio-inspired oil droplets resistant to lipid oxidation
- Efficient extraction of proteins and oleosomes

## Highlights from last year

-The team published 7 peer reviewed articles in highly ranked journal

-Cover at Journal of Materials Chemistry B (https://doi.org/10.1039/D2TB00823H)

-1 Article amongst the Most Downloaded of Journal of Materials Chemistry B

-2 articles in the Most Downloaded of Food Hydrocolloids

-Research on jammed emulsions to mimic animal fat featured in multiple media and the Italian science show Superquark

-5 invited keynote lectures in international meetings and conferences

## Student project envisioned

Thesis subjects are related to the research of the Ph.D. projects of the team including mainly experimental and in some cases computational work.



## Electrophoretic Separation of Oleosomes and Proteins from Oilseeds

Name PhD: Kübra Ayan Involved staff members: Dr. Costas Nikiforidis (BCT) & Prof. Remko Boom (FPE) Project sponsor: National Education Ministry of Turkey Start/(expected) end date of project: September 2020 / September 2024

## Background and goal of the project

Lipids and proteins are major components of food production. In the case of plant-based foods, they can be extracted from oilseeds, like rapeseeds<sup>[1]</sup>.

Aqueous extraction is used to extract oil in the form of oleosomes and proteins simultaneously, and the final separation between the two is accomplished by centrifugation<sup>[2]</sup>. It is, however, not an efficient path due to the large amount of water consumption. To provide a more resource-efficient step for the separation, we are developing a continuous electrophoretic separation process.

Oleosomes and proteins can be separated by a combination of electrophoresis and a counter-acting solvent flow when the magnitude of the latter is set between the electrophoresis rate of oleosomes and proteins. Oleosomes exhibit higher electrophoretic mobility than rapeseed proteins at pH > 5.0, meaning that oleosomes are retained by electrophoresis and proteins are dragged by the flow.



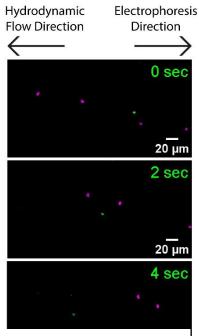


Figure 1: Time – lapse images of the electrophoretic separation of rapeseed oleosomes and proteins under 50 V/cm electric field and 120 mBar pressure difference (~100  $\mu$ m/s solvent flow velocity)

#### Highlight of the past year

- The separation of rapeseed oleosomes and proteins has been approved in a microscale application

- The microscale separation system was upgraded to a lab–scale process

- It is revealed that the retention and permeation mechanism of rapeseed oleosomes and proteins are governed by the balance between electrophoresis and pressure-driven flow

#### Type of student projects envisioned:

Lab-based MSc projects can be offered.

Tan, S. H., Mailer, R. J., Blanchard, C. L., & Agboola, S. O. (2011). Canola Proteins for Human Consumption: Extraction, Profile, and Functional Properties. Journal of Food Science, 76(1). https://doi.org/10.1111/j.1750-3841.2010.01930.x
 Nikiforidis, C. V. (2019). Structure and functions of oleosomes (oil bodies). Advances in Colloid and Interface Science, 274, 102039. https://doi.org/10.1016/j.cis.2019.102039

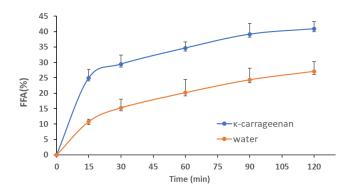
## Exploring sustainable transformation of plant extract industry

Name PhD: Mingzhao Han Involved staff members: dr. Costas Nikiforidis (BCT), Prof.dr. Remko Boom (FPE) Project sponsor: WUR-CAU (CSC) Start/(expected) end date of project: September 2019- December 2023



#### Background and goal of project

Oleosomes are promising natural oil-in-water emulsions due to their high physical and chemical stability. When oleosome dispersions are mixed with polysaccharides the viscosity of the system can altered and also the physicochemically stability of oleosomes can be enhanced. Additionally, in the case of food product, the gastric digestion rate of oleosomes might be altered when polysaccharides like k-carrageenan are present.



## Figure 1. Progression of lipolysis during the intestinal phase for oleosomes dispersions and oleosome/k-carrageenan mixtures samples.

## Highlight of the past year

- During digestion, oleosome dispersions with k-Carrageenan exhibited higher particle size in comparison to when only oleosomes where used.
- The gastric digestion significantly changed the interfacial protein composition, regardless of the presence of k-Carrageenan.
- The addition of k-Carrageenan lead to an increase of the free fatty acid release during intestinal digestion, enhancing the lipolysis of oleosomes.

## Type of student projects envisioned

No student projects available due to finalization of the project in 2023.

Nikiforidis, C. V., & Kiosseoglou, V. (2010). Physicochemical Stability of Maize Germ Oil Body Emulsions As Influenced by Oil Body Surface-Xanthan Gum Interactions. Journal of Agricultural and Food Chemistry, 527-532. Kaukonen, A. M., Boyd, B. J., Charman, W. N., & Porter, C. J. (2004). Drug solubilization behavior during in vitro digestion of suspension formulations of poorly water-soluble drugs in triglyceride lipids. Pharmaceutical Research, 254-260.

## Oleosomes as carriers of cannabidiols

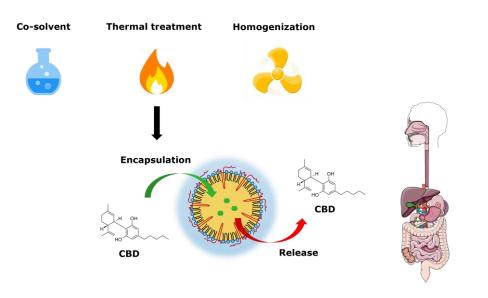
Name PhD: Zhaoxiang Ma Involved staff members: Prof. dr. Costas Nikiforidis (BCT), Prof. dr. Harry Bitter (BCT), Prof. dr. Remko boom (FPE) Project sponsor: Botaneco Inc. (Canada) Start/(expected) end date of project: March 2020-February 2024



#### Background and goal of project

Oleosomes, the natural lipid droplet in oil seeds, have a unique structure that could act as carriers of hydrophobic therapeutics, like cannabidiols (CBD). CBD is an active compound extracted from hemp, which has exhibited beneficial pharmacological effects, including antioxidant and anti-inflammatory activities. However, the application of CBD is hindered due to poor water solubility, low bioaccessibility, and low chemical instability. The use of carriers has therefore been a preferred strategy for delivering CBD.

This project focuses on understanding the mechanisms of encapsulation and release of CBD from oleosomes and enhancing the potential utilizations of oleosomes in food, pharmaceuticals, and cosmetics. We are following different strategies to encapsulate the CBD and also investigating the release during gastric digestion, as it is shown in the figure.



#### Oral administration

#### Highlight of the past year

- The morphology and dispersion method of CBD affect its encapsulation efficiency.
- Different encapsulation methods were developed using various mechanisms.
- Oleosome presents good properties as a carrier with a high encapsulation efficiency of CBD.
- The bioaccessibility of CBD encapsulated in oleosomes was improved through the in vitro digestion model.

#### Type of student projects envisioned

Student projects include lab work, focusing on investigating the bioactivity of CBD released from oleosomes through the human skin model and the potential application of oleosomes (like 3D printing).

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

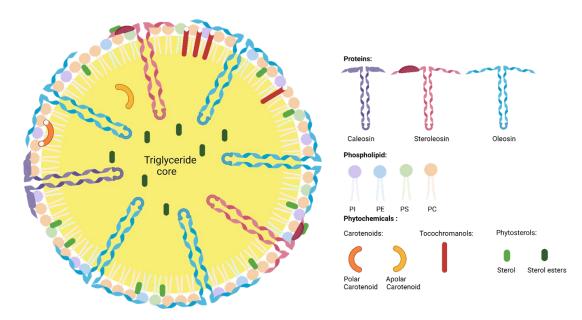
Name PhD: Lorenz Plankensteiner Involved staff members: Dr. Costas Nikiforidis Project sponsor: Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), Botaneco INC. (Calgary, AB, Canada) Start/(expected) end date of project: 01.07.2020 / 01.07.2024



#### Background and goal of project

Lipid oxidation is a big challenge for the food industry, as it is one of the main causes of degradation of many lipid based products like oil-in-water emulsions. New strategies for preventing oxidation, could be inspired by plants. Plants are storing energy as triacylglycerols in the core of oil droplets within the cells. These oil droplets are called oleosomes and besides their core of triglycerols (TAG) they have a membrane of phospholipids (PL) and proteins and packed with phytochemicals (Figure).

First studies showed that oleosomes have a higher oxidative stability than classical emulsions, which makes them very attractive for the food industry. In our research we want to further investigate and understand the oxidative stability of oleosomes to test if they could be a new strategy for preventing lipid oxidation.



#### Highlight of the past year

In the last year we focused on testing the stability of oleosomes emulsions. The oxidative and physical stability of oleosomes were compared against emulsions stabilized with commonly used food emulsifiers (lecithin (rapesed) and whey protein) in a shelf life test. The physical stability of oleosomes was comparable to the benchmark emulsions, no droplet coalescence was observed during the storage.

Oxidatively oleosomes were more stable than the benchmark emulsions, forming  $\sim$ 40 % less primary oxidation products. Our finding suggest that, using oleosomes could be a promising strategy for making stable oil-in-water emulsions.

#### Type of student projects envisioned

We offer a broad spectrum of thesis topics in the fields of food/analytical chemistry and soft material science. Various topics are possible with a focus on experimental lab work.

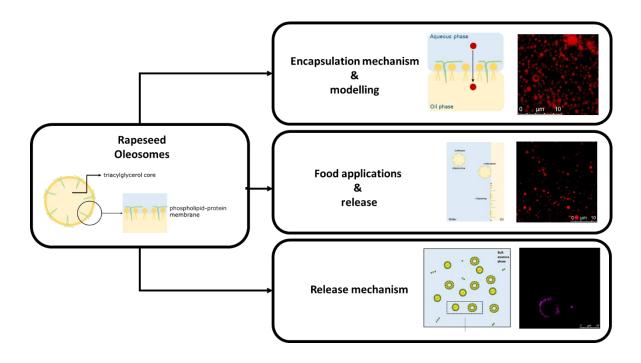
## Oleosoemes (Lipid Droplets) as Carriers of Therapeutics

Name PhD: Umay Sevgi Vardar Involved staff members: Costas Nikiforidis, Harry Bitter Project sponsor: Republic of Turkey Ministry of Education Start/(expected) end date of project: 09.2019/09.2023



## Background and goal of project

Oleosomes are specialized organelles to store hydrophobic molecules in oilseeds. They can be extracted from oilseed, and used as a carrier for hydrophobic therapeutics, to enhance therapeutics stability and bioaccessibility <sup>[1,2]</sup>. In the project, we aim to develop a carrier that could be used an alternative to synthetic carriers in food/medical applications and to understand encapsulation/release mechanism.



## Highlight of the past year

- Curcumin encapsulation into oleosome was modelled
- Effect of curcumin encapsulation on oleosome stability was determined and
- Release mechanism of curcumin was investigated using artificial cell bilayer

## Type of student projects envisioned

The project will be finalized in 2023

- 1. Nikiforidis, C. V. (2019). Structure and functions of oleosomes (oil bodies). Advances in Colloid and Interface Science, 274, 102039.
- 2. Kharat, M., & McClements, D. J. (2019). Recent advances in colloidal delivery systems for nutraceuticals: A case study–Delivery by Design of curcumin. Journal of colloid and interface science, 557, 506-518.

#### Continuous extraction of oleosome from rapeseed

Name PhD: Chenqiang Qin Involved staff members: Prof. dr. Costas Nikiforidis, Prof. dr. Remko Boom (FPE) Project sponsor: China scholarship council Start/(expected) end date of project: 2023.12



#### Background and goal of project

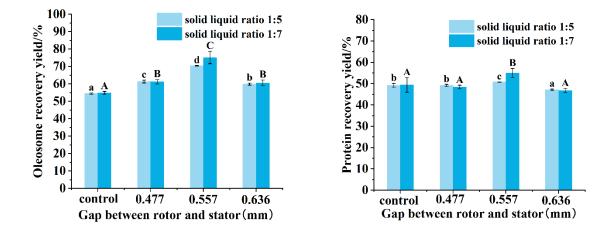
Oleosomes from oilseeds could be used in food and pharmaceutical application, however their extraction yield is currently around 60 wt% and needs to be optimised. The combination of different extraction process steps like the twin-screw press and the colloid mill might improve the disruption of the seed cells and the subsequent oleosome and protein extraction.

In this project we aim to track the extraction yield of oleosomes and proteins from seeds using equipment that could also be applied in large scale and continuous extraction.

#### Highlight of the past year

1. By combining the colloid mill and twin-screw press the recovery yield of oleosome was improved.

- 2. Seed-water ratio at 1:5 had a similar extraction yield of oleosomes and proteins comparing to 1:7
- 3. The oleosome recovery yield that was achieved at 86 wt %.



## Type of student projects envisioned

My project is focused on lab work. MSc and BSc students can perform experiments on the extraction of oleosomes and proteins and also on using them to design model food products

## How does oleosin influence mechanical properties of oil body surface?

Name PhD/PD: Yufan Sun Involved staff members: Costas Nikiforidis, Renko de Vries (PCC) Project sponsor: China Scholarship Council (CSC) Start/(expected) end date of project: February 2022-February 2023



## Background and goal of project

Oleosomes have been suggested as potential sustainable route to produce emulsions for applications in food and pharmaceuticals. Besides extracting them and using them as such, we could also be inspired by their structure to form oleosome-inspired oil droplets that could even outperform the natural ones. However, exploiting the full potential of oleosomes requires a deep understanding of the relationship between their structural motifs and functions. Therefore, further understanding of the interactions between the molecules in their interface is needed. In this work we aim to provide theoretical guidance for the preparation of artificial oleosome emulsions, by investigating their structure using Atomic Force Microscopy.

## Highlight of the past year

- Artificial oleosomes were successfully prepared
- At pH 3 and 10 oleosin emulsions are stable against aggregation
- Phospholipids and oleosin are needed to make artificial oleosomes with a droplet size distribution similar to the natural ones
- AFM is a promising method to study the mechanical properties of oleosomes, but further developments are needed

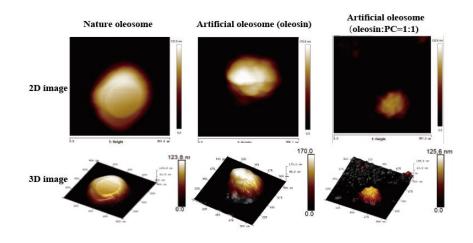


Figure. Oleosomes under the Atomic Force Microscope

## Type of student projects envisioned

The project is finalised in January 2023

## Application of oleosome as biodegradable/edible films and coatings in food packaging

Name visiting researcher: Feng Xue Involved staff members: Dr. Costas Nikiforidis, Dr. Mehdi Habibi (FPH) Project sponsor: Jiangsu Overseas Visiting Scholar Program for University Prominent Young & Middle-aged Teachers and Presidents Start/(expected) end date of project: 01/06/2022-01/07/2023



## Background and goal of project

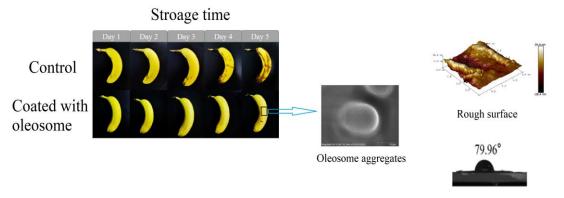
In order to limit the excessive use of non-degradable plastics as materials for food packaging, studies about the development of more sustainable and environmentally friendly packaging materials has grown rapidly over the past few decades. The incorporation of oleosomes to develop composite films or coating materials is an emerging trend to produce sustainable films with improved physical and functional properties, such as higher flexibility, lower water vapor permeability, and encapsulation of functional compounds (antioxidants and antimicrobials).

## Highlight of the past year

-Oleosome was extracted from plan seed and used to prepare coating solution.

-Oleosome-based coating solution was sprayed on the surface of bananas to expand their shelf life.

-Oleosomes can form a thin layer films on the surface of bananas and prevent weight loss and browning during the storage time.



Hydrophobic surface

## Type of student projects envisioned

This project welcomes the students with material science and food preservation background. The lab work mainly includes the characterization of material functional properties and evaluation of food freshness.

## Self-assembled oleosin micelles for resveratrol delivery

Name PhD: Mingming Zhong Involved staff members: Costas Nikiforidis, Renko de Vries (PCC) Project sponsor: China Scholarship Council (CSC) Start/(expected) end date of project: 2/4/2022-2/3/2023



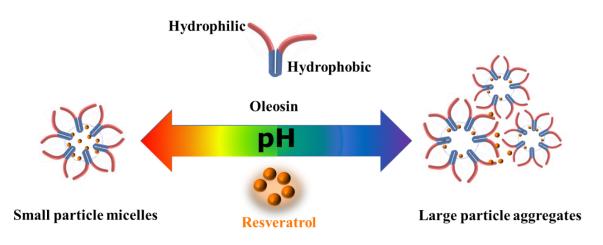
## Background and goal of project

Rapeseed oleosins are unique proteins consisting of a long hydrophobic hairpin bordered by hydrophilic arms. Oleosin has become very attractive in the development of formulations in functional food and pharmaceutical fields due to its unique hydrophobic long-chain structure and non-toxic properties in biological systems. Especially for the encapsulation of hydrophobic nutrients and drugs.

#### Highlight of the past year

-Oleosins self-assembled into small-particle core-shell micelles of  $\sim$ 30 nm at pH 3 and large-particle irregular aggregates of  $\sim$ 100 nm at pH 8 after stirring overnight.

-Oleosin nanoparticles can encapsulate resveratrol in the hydrophobic nanocore at pH 3 .



#### Type of student projects envisioned

The project is finalised in January 2023

## Finetuning oilseed protein-phenol interactions towards novel functional materials

Name PhD: Sybren Zondervan Involved staff members: Harry Bitter, Costas Nikiforidis Project sponsor: NWO-TKI "INTRINSIC" Start/(expected) end date of project: October 2022 / September 2026



## Background and goal of project

Oilseed oil is one of the most predominantly used edible oils in the food industry. After the oil extraction, a seed meal remains, which is high in protein, making them a promising protein resource supporting global food security. Oilseed proteins can form gels and stabilise emulsions and foams making them valuable for creating functional materials, such as plant-based foods or biodegradable packaging materials.

However, besides proteins, there are phenols present in seed meals, which are reacting with proteins and significantly affect their physicochemical properties. It is difficult to avoid the protein-phenol reactions, therefore, we are aiming to gain insights into the specific binding spots and also their effect when using the proteins to create materials. Thereby, the 'wasted' meal of vegetable oil production can be valorised. The project setup is visualised in Figure 4.

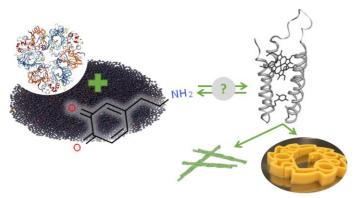


Figure 4. Project schematic depicting the initial molecular studies on oilseed protein-phenol interactions, and the subsequent relationship with functional properties of materials made up of protein-phenol complexes, such as fibres or 3D-printed materials.

#### Highlight of the past year

In the first three months of this project, we completed the first explorational protein extraction which will be continued in 2023.

#### Type of student projects envisioned

A few projects are envisioned for 2023 for which students are very welcome to apply:

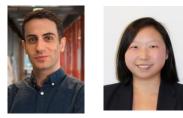
- Show how extraction parameters can be employed to produce oilseed protein isolates depleted from phenols (refinery, processing, lab work)
- Unveil the impact of processing parameters on oxidation states of phenolic compounds (chemistry, lab work)

## Modeling & Technology

Theme leader: Guanna Li & Akbar Asadi Tashvigh

## Background and goal of this theme

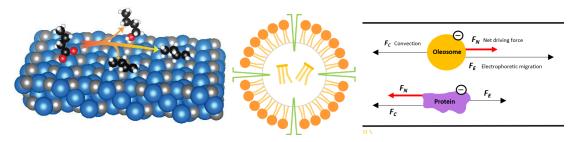
Computational modeling has become an indispensable approach to investigate scientific questions in chemistry and related research areas. By simulation of the system at different time and space scales, It helps to get insights into the reaction processes and provide recipes for optimization or rational design of catalytic materials and reactions.



With close collaboration with experimentalists, it is feasible to carry out cross-disciplinary research and realize knowledge exchange and utilization.

In the past year, we continued to apply quantum chemical modeling methodologies to investigate the reaction mechanism of heterogeneous catalytic biomass conversion and numerical simulations to study the mass and heat transfer in porous materials for electrocatalytic conversion of biomass. Meanwhile, simulation of encapsulation and separation processes of biological membranes, and mechanisms of CO<sub>2</sub> adsorption and capture processes have been carried out. 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 multiscale and operando 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, vacancy available)
 Development of kinetic models

Investigation of diffusion in porous materials

- Capture of CO<sub>2</sub> from air (Direct Air Capture, DAC) (Akbar, vacancy available) Development of kinetic models
   Diffusion of CO<sub>2</sub> in K<sub>2</sub>CO<sub>3</sub>
   Modeling condensation in micro- and mesopores
  - Reactor/process design and heat integration
- Mass transfer in biological membranes (Akbar) Modeling of encapsulation process of bioactive compounds in lipid droplets Modeling of protein separations
- Electro-conversion of biomass to valuable platform chemicals (Guanna, vacancy available) Development of model electrocatalyst for biomass conversion
- Multiscale modeling of carbide catalyst for biomass conversion (Guanna, vacancies available) Investigation of the structure-reactivity relationships of metal carbide catalysts Development of operando modeling approaches

## 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 <u>guanna.li@wur.nl</u> or <u>akbar.asaditashvigh@wur.nl</u> 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: Merlin Cotessat, MSc Involved staff members: dr. Guanna Li, prof.dr. Harry Bitter Project sponsor: VLAG Start/(expected) end date of project: 1-Oct-2021 to 1-Oct-2025



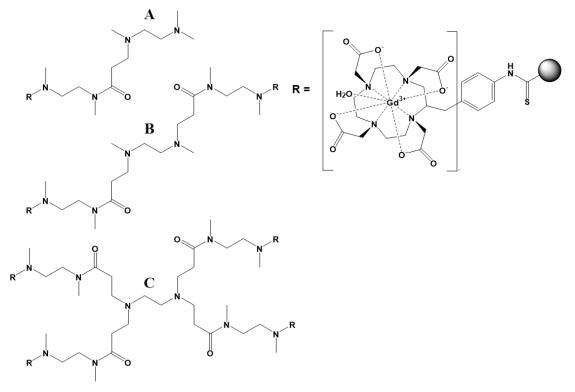
## Background and goal of project

This fundamental and interdisciplinary research project aims to link three fields of science: magnetic resonance, computational chemistry, and chemical synthesis. The project is shared between the BCT, BNT and ORC research groups.

As the commercial pool of clinical MRI contrast agents keeps shrinking due to safety concerns, a better fundamental understanding of their properties and effects is needed, in order to improve the design process of this essential class of pharmaceuticals. This project aims to explore specific questions related to relaxivity theory with computational chemistry methods, and to test new insights by synthetizing novel kinds of contrast agents like soft nanoparticles.

## Highlight of the past year

An MSc thesis focused on synthesis of new MRI contrast agent materials was supervised to successful completion, leading to intermediary results that will be built on further in the coming year. The contrast agents are a group of pseudo-PAMAM dendrimers linked to a varying number of gadolinium-DOTA chelates.



## Type of student projects envisioned

This year there could be room for one or two computational student projects. This would allow for the modelling of a greater variety of structures than previously considered to check the current working hypothesis.

## Reomval of Perfluorinated Acids Contaminant from Water by Pillararenes

Name PhD: Tunan Gao Involved staff members: Guanna Li, Fedor Miloserdov, Han Zuilhof, Harry Bitter Project sponsor: VLAG graduate school Start/(expected) end date of project: 12/2019-12/2023

## Background and goal of project



Per- and polyfluoroalkyl substances (PFAS) are broadly used chemicals for a wide range of consumer and industrial applications, such as in stain-repellent sprays, non-stick pans, firefighting foams and food paper coatings. However, the extremely high stability of these materials also turns out to be one of their drawbacks, e.g. leading to increasing water pollution. Dangerous contamination levels of soils and surface waters with PFAS have already reached many parts of the world, frequently exceeding the US Environmental Protection Agency-advisory limit for perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) (70 ng/L) by several orders of magnitude. Toxicity research has demonstrated that this will cause developmental toxicity, immune function disorder, immunotoxicity, and a range of chronic diseases. This motivates research that can lead to an improved understanding of how to remove PFOS and PFAS from water.

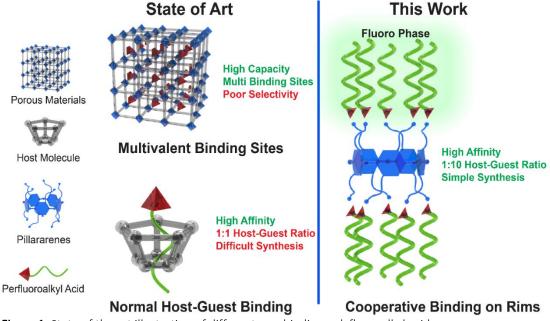


Figure 1. State of the art illustration of different way binding polyfluoroalkyl acids.

## Highlight of the past year

A new type of host-guest interaction between deca-ammonium-functionalized pillar-[5]-arenes (DAF-P5s) and perfluoroalkyl acids was reported. DAF-P5s show an unprecedented stoichiometry (1:10), as confirmed by isothermal calorimetry and X-ray crystallographic studies, and high binding constants (up to  $10^6 \text{ M}^{-1}$ ) to various polyfluoroalkyl acids. This novel host-guest chemistry also provides excellent removal of perfluorinated acids from water. A proof of concept experiment was done to remove PFOS from water, the residual concentration of PFOS decrease from 6 mg/L to 15 ng/L, which is lower than safety limit.

## Type of student projects envisioned

This project mainly involves lab work, specifically organic synthesis skills. Characterization like NMR, MS, UV-vis, ITC will be applied. Also some surface chemistry and supramolecular chemistry techniques like NMR titration, surface modification, will be needed in this project. Please contact <u>tunan.gao@wur.nl</u> or <u>guanna.li@wur.nl</u> if you are interested in doing a thesis related to these topics.

## Multiscale modeling of transition metal carbides for biomass conversion

Name PhD: Raghavendra Meena Involved staff members: Prof. Harry Bitter, Prof. Han Zuilhof, Dr Guanna Li Project sponsor: Sectorplan Chemistry and Physics Start/(expected) end date of project: 01.10.2020/30.09.2024

## Background and goal of project

With rapidly emerging potential applications of catalysis, design and discovery of



cheap-and-efficient catalysts must be addressed. On the other hand, efforts should be made to reduce our overreliance on fossil fuels which are limited in nature. Therefore, sustainable resources such as biomass for value-added chemicals is emerging. To convert biomass to valuable platform chemicals, heterogeneous catalysts belonging to platinum group metals (PGMs) have been used predominantly, but they are scarce and expensive. Hence, transition metal carbides (TMCs) have emerged as a potential alternative for PGMs.

The introduction of carbon (*C*) atoms in molybdenum (*Mo*) lattice shifts the M(*d*-band) close to the fermi level ( $E_F$ ), which resembles the electronic structure of PGMs. Therefore, as a result, it fetches  $Mo_2C$  PGM-like properties. Although, their catalytic activity is to some degree known, it is still not clear what the structure-activity relationships are for TMCs. These fundamental understandings are of great importance for the optimization and rational design of metal carbide catalysts. Therefore, I use the density functional theory (DFT) computational and other relevant mathematical modeling based approaches to get insights into the nature of active sites and the complicated reaction mechanisms involved. In such a way, I can address the originality of the activity and selectivity differences observed in the experiments.

## Highlight of the past year

In the past year, I studied the hydrodeoxygenation (HDO) reaction mechanism of butyric acid over orthorhombic phase of  $Mo_2C$  (101) catalytic surface. HDO is a fundamental reaction in biomass conversion, while butyric is an important model compound that mimics the functional group present in the biobased derived long-chain fatty acids (LCFAs). Using DFT and microkinetic modeling (MKM), we found the rate-controlling step in the HDO reaction mechanism. Later we used heteroatom doping to tune the activity of the catalytic surface. We then used the doping data to study the electronic structure of the doped surface,  $(Mo_{2-x})M_xC$ ; where M=(transition metals). The electronic structure analysis provided us with linear scaling relationships. Such linear scaling relationships were then used to establish descriptors for the activity of the doped  $(Mo_{2-x})M_xC$  catalytic surface. Such fundamental understandings at an atomic level provide us unique ideas in rational designing TMC catalysts for experimental validation.

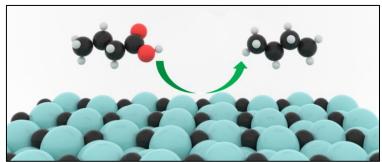


Figure 5: Conversion of butyric acid to butane on Mo2C (101) catalytic surface via HDO reaction mechanism.

## Type of student projects envisioned

The nature of the projects would reading/modeling. I offer short-term (3 months) projects in which a student can learn the basics of heterogeneous catalysis and DFT by reading and applying these techniques on simple systems. I also offer a couple of long-term (6 months) projects in which students can dive deep into the research involved in my PhD project.

If interested, please feel free to contact me (<u>raghavendra.meena@wur.nl</u>) or dr. Guanna Li (<u>guanna.li@wur.nl</u>) to schedule a talk.

#### Membranes Separation Processes

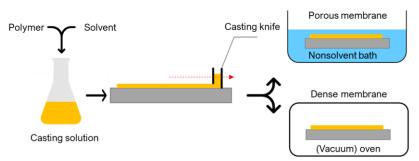
Team leader: Akbar Asadi Tashvigh (akbar.asaditashvigh@wur.nl) PhD students: Ellis van Keulen



## Background and goal of project

Separation and purification in chemical mixtures are responsible for up to 15% of the entire world's energy consumption. This energy is primarily used to power the evaporation/distillation towers as often a phase change is required to separate chemicals. Membrane separation technology removes the heating requirement from separation and requires substantially lower energy input.

The aim of this research is to synthesis highly selective and permeable polymer membranes for application is liquid separations, fuel cells and electrocatalysis.



Nonsolvent-induced phase separation and solvent evaporation processes for membrane fabrication.

#### Main topics

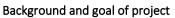
- Fabrication of highly ordered covalent organic polymer based membranes
- Synthesis of chemically resistant cation/anion exchange membranes
- Synthesis of thin film composite membranes
- Catalytic membranes for biobased valorization

#### Type of student projects envisioned

If you are interested in a thesis, please contact akbar.asaditashvigh@wur.nl to discuss specific details and possibilities.

## Smart membranes for high temperature proton exchange membrane fuel cells (HT-PEMFC)

Name PhD: Ellis van Keulen Involved staff members: Prof. dr. Harry Bitter, dr. Akbar Asadi Tashvigh Project sponsor: WUR Start/(expected) end date of project: November 2022-November 2029





An energy transition is required to limit global warming. Herein hydrogen has a key role for the energy storage of electricity obtained from wind-, hydro- or solar power. The advantages of hydrogen over e.g., lithium-ion batteries, are the storing efficiencies and the fast kinetics. However, for a smooth transition towards a cost-competitive hydrogen economy, the hydrogen technology (hydrogen production, storage, transport, and utilization) must be further developed.

In a fuel cell (FC) the hydrogen is oxidized (at the anode) and oxygen is reduced (at the cathode) with the generated hydrogen ions and electrons to form water, as the byproduct of hydrogen combustion. Several FC types have been developed in the past years, such as the proton exchange membrane FCs (PEMFCs) shown in Figure 1. PEMFC is ideally suitable for operation at low temperatures (below 100 °C). However, operation at high temperature (~120-250 °C) would be interesting due to improved reaction kinetics, higher tolerance for impurities and simplified heat and water management. However, the membranes currently used loose their conductivity over time due to hydration.

Nafion-like membranes are mostly used in PEMFC. However, during thermal degradation (mimicking high-temperature FC operation) of Nafion numerous perfluorinated compounds, such as the environmentally persistent perfluorocarboxylic acids are released in the environment. Alternatively, polybenzimidazoles (PBI) membranes could be used, which have excellent thermal stability and mechanical strength. Therefore, this study aims to develop a PBI membrane as Nafion replacement for high temperature proton exchange membrane fuel cells with high stability and conductivity. This project aims for better understanding on how to reduce PA-leaching from the membrane.

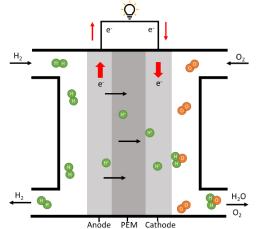


Figure 1: Schematic representation of a proton exchange membrane fuel cell (PEMFC).

## Highlight of the past year

-Start of the project

## Type of student projects envisioned

Students can work on membrane development. Here different PA-PBI membranes can be synthesized and characterized. Furthermore, students can study the use of a coating layer. Hereby the effect of a hydrophobic layer on a PA-PBI membrane can be evaluated. Characterization of membranes will include conductivity, thickness, PA-doping levels, PA leaching levels, mechanical strength (e.g., stress-strain curves), chemical composition (e.g., Fourier transform infrared spectroscopy), pore size and (thermal) durability (e.g., thermogravimetric analysis).

#### Education

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

## Bachelor and Master courses BCT and contribution to other courses

Code	Course title
BPE-12806	Bioprocess Engineering Basics BT
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**

- Ruijter, Martijn de The effect of reducing pectin in roadside grass on paper strength
- Frenk, Jordy Electronic features of sulfur(VI) fluoride exchange reactions (MLS, BCT 49.5%)
- Wirawan Hartanto, Arie Distribution and Characterization of Lipids Obtained from Side Fractions of Microfiltration of Lesser Mealworms (Alphitobus diaperinus) (FST, BCT 35%)
- Gros, Leane Electrochemical bromination of levulinic acid

## **MSc Theses**

- Hoogendoorn, Winnie Mathematical modelling of curcumin mass transfer into lipid droplets
- Triantafyllou, Thanasis Lipid droplets from Nannochloropsis oceanica for biotechnological applications: Process optimization and modeling (BPE, BCT 30%)
- Nikolau, Foivi Tribological properties of oleosome emulsions: the role of the membrane components (FPH, BCT 50%)
- Willems, Tomas Tribology of rapeseed oleosomes with added proteins (FPH, BCT 50%)
- Baldini Garcia, Carolina Stability of β-carotene encapsulated in rapeseed oil bodies during in vitro digestion and storage (FQD, BCT 50%)
- Leon Roldan, Maria Rapeseed Oleosomes as Curcumin Delivery Systems
- Kommer, Cynte In vitro fermentation of resistant starch type 3 and galacto-oligosaccharides by faecal microbiota of 6-month-old infants with and without amoxicillin (FCH, BCT 50%)
- Veen, Elske van der Evaluating the role of Pt precursor on the properties and performance of electroplated Pt on Cu and Ni wires for the electro-oxidation of glucose
- Keulen, Ellis van Electro-oxidation of glucose over bulk platinum: elucidating the reaction pathway and steering the selectivity
- Vergeer, Max Modelling the electrophoretic separation of oleosomes and proteins from oilseeds
- Chen, Mingzheng Exploring to produce dairy fat globules alternatives by using polysaccharides and oleosomes from capsicum seeds
- Fan, Kai-Ching Hydrogenation of cinnamaldehyde over carbon nanofiber supported Molybdenum carbide in a continuous flow reactor
- Koch, Joris Plant wide simulation of poly-3-hydroxyalkanoate extraction from wastewater and its conversion to value added biochemicals
- Pruim, Sebastian Catalyst-free production of crotonate esters and their deoxygenation towards biobased chemicals
- Bijman, Eline The tribological properties of rapeseed oleosome-protein mixtures (FPH, BCT 50%)
- Oorschot, Michel van Depolymerisation of Alginate
- Eissens, David RS3 crystal micro-attractiveness for keystone RS degraders *Ruminococcus bromii* and *Bifidobacterium adolescentis* (FCH, BCT 50%)
- Dam, Bastiaan van Mechanism of butyric acid hydrodeoxygenation reaction on the surface of Woxycarbide. A Density Functional Theory Study
- Voorde, Stefan ten Evaluating the potential of aqueous oleosome extraction to produce resourceefficient oil-in-water emulsions from capsicum seeds
- Desloover, Mariël Investigation of the continuous electrophoretic separation of polystyrene particles of different sizes (FPE, BCT 25%)

• Liu, Dongxuan – Exploring the in vitro digestion of capsicum seed oleosomes emulsion and the emulsion-filled gel (FPE, BCT 50%)

## **MSc Research Practices**

- Brink, Henk-Jan van den Unravelling the CO2 sorption kinetics of K2CO3/AC during direct air capture. Experiment based reactor modelling
- Fan, Kai-Ching Influence of surface-oxygen groups on molybdenum-carbide catalysts for the selective hydrogenation of cinnamaldehyde

## Scientific Publications 2022

## Refereed article in a journal

- <u>Covalent organic polymers for aqueous and organic solvent nanofiltration</u> Asadi Tashvigh, Akbar ; Benes, Nieck E. (2022) *Separation and Purification Technology 298*.
- <u>Recent Advances in Polybenzimidazole Membranes for Hydrogen Purification</u> Bitter, Johannes H. ; Asadi Tashvigh, Akbar (2022) Industrial & Engineering Chemistry Research 61 (18). - p. 6125 - 6134.
- <u>Sulfur–Phenolate Exchange : SuFEx-Derived Dynamic Covalent Reactions and Degradation of SuFEx Polymers</u> Chao, Yang ; Krishna, Akash ; Subramaniam, Muthusamy ; Liang, Dong Dong ; Pujari, Sidharam P. ; Sue, Andrew C.H. ; Li, Guanna ; Miloserdov, Fedor M. ; Zuilhof, Han (2022) *Angewandte Chemie-International Edition 61 (36)*.
- <u>Concentration-dependent effects of nickel doping on activated carbon biocathodes</u> Chatzipanagiotou, Konstantina Roxani ; Jourdin, Ludovic ; Bitter, Johannes H. ; Strik, David P.B.T.B. (2022) *Catalysis Science & Technology 12 (8). - p. 2500 - 2518.*
- <u>Tuning UV Absorption in Imine-Linked Covalent Organic Frameworks via Methylation</u> Dautzenberg, Ellen ; Lam, Milena ; Nikolaeva, Tatiana ; Franssen, Wouter M.J. ; Lagen, Barend van; Gerrits-Benneheij, Ilse P.A.M. ; Kosinov, Nikolay ; Li, Guanna ; Smet, Louis C.P.M. de (2022) The Journal of Physical Chemistry Part C: Nanomaterials and Interfaces 126 (50). - p. 21338 - 21347.
- <u>Cinnamaldehyde hydrogenation over carbon supported molybdenum and tungsten carbide catalysts</u> Führer, Marlene ; Haasterecht, Tomas van; Bitter, Johannes Hendrik (2022) *Chemical Communications 58 (98). - p. 13608 - 13611.*
- <u>The Synergetic Effect of Support-oxygen Groups and Pt Particle Size in the Oxidation of α-D-glucose: A</u> <u>Proximity Effect in Adsorption</u> Führer, Marlene ; Haasterecht, Tomas van; Masoud, Nazila ; Barrett, Dean H. ; Verhoeven, Tiny ; Hensen, Emiel;

Führer, Marlene ; Haasterecht, Tomas van; Masoud, Nazila ; Barrett, Dean H. ; Verhoeven, Tiny ; Hensen, Emiel; Tromp, Moniek ; Rodella, Cristiane B. ; Bitter, Harry (2022) *ChemCatChem 14 (19).* 

• The Use of Virtual Reality in A Chemistry Lab and Its Impact on Students' SelfEfficacy, Interest, Self-Concept and Laboratory Anxiety

Gungor, Almer ; Kool, Denise ; Lee, May ; Avraamidou, Lucy ; Eisink, Niek ; Albada, Bauke ; Kolk, Koos van der; Tromp, Moniek ; Bitter, Johannes Hendrik (2022)

Eurasia Journal of Mathematics, Science and Technology Education 18 (3).

- <u>Environmental Impact Evaluation for Heterogeneously Catalysed Starch Oxidation</u> Hoogstad, Tim M.; Timmer, Stijn M.; Boxtel, Anton J.B. van; Buwalda, Pieter L.; Bitter, Johannes H.; Kiewidt, Lars (2022) *ChemistryOpen 11 (10).*
- Enhancing the Formation and Stability of Oil-In-Water Emulsions Prepared by Microchannels Using Mixed <u>Protein Emulsifiers</u>
   Liao, Yan : Zhao, Yuntai : Chang, Ying : Ma, Zhaoxiang : Kohayashi, Isao : Nakajima, Mitsutoshi : Neves, Marc

Jiao, Yan ; Zhao, Yuntai ; Chang, Ying ; Ma, Zhaoxiang ; Kobayashi, Isao ; Nakajima, Mitsutoshi ; Neves, Marcos A. (2022)

Frontiers in Nutrition 9.

• Carbohydrate structure—activity relations of Au-catalysed base-free oxidations: gold displaying a platinum lustre

Klis, F. van der; Gootjes, L. ; Verstijnen, Noud ; Haveren, J. van; Es, D.S. van; Bitter, J.H. (2022) RSC Advances : An international journal to further the chemical sciences 12 . - p. 8918 - 8923.

• <u>A plant wide simulation of polyhydroxyalkanoate production from wastewater and its conversion to methyl</u> <u>crotonate</u>

Koch, Joris ; Scott, Elinor ; Bitter, Johannes ; Asadi Tashvigh, Akbar (2022) *Bioresource Technology 363*.

• Optimizing pea protein fractionation to yield protein fractions with a high foaming and emulsifying capacity Kornet, Remco; Yang, Jack; Venema, Paul; Linden, Erik van der; Sagis, Leonard M.C. (2022) Food Hydrocolloids 126.

- <u>Fractionation methods affect the gelling properties of pea proteins in emulsion-filled gels</u> Kornet, Remco; Sridharan, Simha; Venema, Paul; Sagis, Leonard M.C.; Nikiforidis, Constantinos V.; Goot, Atze Jan van der; Meinders, Marcel B.J.; Linden, Erik van der (2022) *Food Hydrocolloids 125*.
- <u>Solvent-Assisted Ketone Reduction by a Homogeneous Mn Catalyst</u> Krieger, Annika M. ; Sinha, Vivek ; Li, Guanna ; Pidko, Evgeny A. (2022) *Organometallics 41 (14). - p. 1829 - 1835.*
- <u>CO2 Hydrogenation to Methanol over Cd4/TiO2 Catalyst : Insight into Multifunctional Interface</u> Li, Guanna ; Meeprasert, Jittima ; Wang, Jijie ; Li, Can ; Pidko, Evgeny A. (2022) *ChemCatChem 14 (5).*
- <u>Shedding Light on Solid Sorbents : Evaluation of Supported Potassium Carbonate Particle Size and Its Effect on CO2Capture from Air</u> Masoud, Nazila ; Clement, Victorien ; Haasterecht, Tomas van; Führer, Marlene ; Hofmann, Jan P. ; Bitter, Johannes Hendrik (2022)
  - Industrial & Engineering Chemistry Research 61 (38). p. 14211 14221.
- <u>Ground-state properties of the narrowest zigzag graphene nanoribbon from quantum Monte Carlo and comparison with density functional theory</u> Meena, Raghavendra ; Li, Guanna ; Casula, Michele (2022) *Journal of Chemical Physics 156 (8).*
- <u>Sinapic acid impacts the emulsifying properties of rapeseed proteins at acidic pH</u> Ntone, Eleni ; Qu, Qiyang ; Gani, Kindi Pyta ; Meinders, Marcel B.J. ; Sagis, Leonard M.C. ; Bitter, Johannes H. ; Nikiforidis, Constantinos V. (2022) *Food Hydrocolloids 125*.
- <u>Napins and cruciferins in rapeseed protein extracts have complementary roles in structuring emulsion-filled</u>
   <u>gels</u>

Ntone, Eleni ; Kornet, Remco ; Venema, Paul ; Meinders, Marcel B.J. ; Linden, Erik van der; Bitter, Johannes H. ; Sagis, Leonard M.C. ; Nikiforidis, Constantinos V. (2022) *Food Hydrocolloids 125*.

- Antibiotic-Like Activity of Atomic Layer Boron Nitride for Combating Resistant Bacteria
   Pan, Yanxia ; Zheng, Huizhen ; Li, Guanna ; Li, Yanan ; Jiang, Jie ; Chen, Jie ; Xie, Qianqian ; Wu, Di ; Ma, Ronglin ; Liu, Xi ; Xu, Shujuan ; Jiang, Jun ; Cai, Xiaoming ; Gao, Meng ; Wang, Weili ; Zuilhof, Han ; Ye, Mingliang ; Li, Ruibin (2022)
   ACS Nano 16 (5). - p. 7674 - 7688.
- <u>A sustainable and efficient recycling strategy of feather waste into keratin peptides with antimicrobial activity</u> Qin, Xiaojie ; Xu, Xiong ; Guo, Yujie ; Shen, Qingshan ; Liu, Jiqian ; Yang, Chuan ; Scott, Elinor ; Bitter, Harry ; Zhang, Chunhui (2022)
   *Waste Management 144 . - p. 421 - 430.*

An advanced strategy for efficient recycling of bovine bone : Preparing high-valued bone powder via instant catapult steam-explosion
 Qin, Xiaojie ; Shen, Qingshan ; Guo, Yujie ; Liu, Jiqian ; Zhang, Hongru ; Jia, Wei ; Xu, Xiong ; Zhang, Chunhui (2022)
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- <u>Protein-stabilized interfaces in multiphase food : comparing structure-function relations of plant-based and animal-based proteins</u>
   Sagis, Leonard M.C.; Yang, Jack (2022)
   *Current Opinion in Food Science 43 . p. 53 60.*
- <u>Hollow protein microparticles formed through cross-linking by an Au3+ initiated redox reaction</u> Schijven, Laura M.I.; Vogelaar, Thomas D.; Sridharan, Simha; Saggiomo, Vittorio; Velders, Aldrik H.; Bitter, Johannes H.; Nikiforidis, Constantinos V. (2022) *Journal of materials chemistry. B, Materials for biology and medicine 10 (33). - p. 6287 - 6295.*
- <u>Starch controls brittleness in emulsion-gels stabilized by pea flour</u>
   Sridharan, Simha ; Meinders, Marcel B.J. ; Sagis, Leonard M.C. ; Bitter, Johannes H. ; Nikiforidis, Constantinos V. (2022)
   Food Hydrocolloids 131.

 <u>Phosphorus Tailors the d-Band Center of Copper Atomic Sites for Efficient CO2 Photoreduction under Visible-</u> <u>Light Irradiation</u>

Sun, Xiaohui ; Sun, Lian ; Li, Guanna ; Tuo, Yongxiao ; Ye, Chenliang ; Yang, Jiarui ; Low, Jingxiang ; Yu, Xiang ; Bitter, Johannes H. ; Lei, Yongpeng ; Wang, Dingsheng ; Li, Yadong (2022) Angewandte Chemie-International Edition 61 (38).

- <u>Highly dispersed Cd cluster supported on TiO2 as an efficient catalyst for CO2 hydrogenation to methanol</u> Wang, Jijie ; Meeprasert, Jittima ; Han, Zhe ; Wang, Huan ; Feng, Zhendong ; Tang, Chizhou ; Sha, Feng ; Tang, Shan ; Li, G. ; Pidko, Evgeny A. ; Li, Can (2022) *Chinese Journal of Catalysis*.
- <u>Fourier Transform Infrared Spectroscopy for Assessing Structural and Enzymatic Reactivity Changes Induced</u> <u>during Feather Hydrolysis</u>
   Windt, Xinhua ; Scott, Elinor L. ; Seeger, Thorsten ; Schneider, Oliver ; Asadi Tashvigh, Akbar ; Bitter, Johannes H. (2022)
  - ACS Omega 7 (44). p. 39924 39930.
- <u>Selective proteolysis of β-conglycinin as a tool to increase air-water interface and foam stabilising properties of soy proteins</u>

Xia, Wenjie ; Botma, Tjitske E. ; Sagis, Leonard M.C. ; Yang, Jack (2022) Food Hydrocolloids 130.

- <u>The impact of heating and freeze or spray drying on the interface and foam stabilising properties of pea protein extracts : Explained by aggregation and protein composition</u>
   Yang, Jack ; Mocking-Bode, Helene C.M. ; Hoek, Irene A.F. van den; Theunissen, Mira ; Voudouris, Panayiotis ; Meinders, Marcel B.J. ; Sagis, Leonard M.C. (2022)
   *Food Hydrocolloids 133*.
- <u>Rethinking plant protein extraction: Albumin From side stream to an excellent foaming ingredient</u> Yang, J. ; Kornet, C. ; Diedericks, C.F. ; Yang, Q. ; Berton-Carabin, C.C. ; Nikiforidis, K. ; Venema, P. ; Linden, E. van der; Sagis, L.M.C. (2022) *Food Structure 31*.
- Foaming and emulsifying properties of extensively and mildly extracted Bambara groundnut proteins : A comparison of legumin, vicilin and albumin protein
   Yang, Jack ; Wit, Annemiek de; Diedericks, Claudine F. ; Venema, Paul ; Linden, Erik van der; Sagis, Leonard M.C. (2022)

Food Hydrocolloids 123.

<u>Competition of rapeseed proteins and oleosomes for the air-water interface and its effect on the foaming properties of protein-oleosome mixtures</u>
 Yang, Jack ; Berton-Carabin, Claire C. ; Nikiforidis, Constantinos V. ; Linden, Erik van der; Sagis, Leonard M.C. (2022)
 *Food Hydrocolloids* 122

Food Hydrocolloids 122.

• Are micelles actually at the interface in micellar casein stabilized foam and emulsions?

Zhou, Xilong ; Yang, Jack ; Sala, Guido ; Sagis, Leonard M.C. (2022) *Food Hydrocolloids 129*.

## PhD Theses

 <u>Combining chemical and microbial electrocatalysis for CO2 utilisation</u> Chatzipanagiotou, Konstantina-Roxani (2022) Wageningen University. Promotor(en): J.H. Bitter; C.J.N. Buisman, co-promotor(en): D.P.B.T.B. Strik. -Wageningen : Wageningen University, - 189

 <u>Macrogels, microgels and microparticles : Au 3+-mediated cross-linking for constructing protein-based</u> <u>materials</u>

Schijven, Laura M.I. (2022)

Wageningen University. Promotor(en): J.H. Bitter; A.H. Velders, co-promotor(en): C.V. Nikiforidis; V. Saggiomo. -Wageningen : Wageningen University, - 124

## Other output

## **Orals contributed**

Structure and functions of oleosomes as lipid carriers Costas Nikiforidis, 22nd IUNS International Congress of Nutrition (ICN), Tokyo, Japan, 6/12/2022 - 11/12/2022

Sustainable conversions and sustainable projects Harry Bitter, FAPESP-NWO meeting, Sao Paulo, Brazil, 23/11/2022 - 25/11/2022

Designing elastoplastic edible 3D printable material using jammed emulsions stabilized with pea proteins Costas Nikiforidis, 2nd International Conference on Advanced Production and Processing (ICAPP) 2022, Novi Sad, Serbia, 20/10/2022 - 22/10/2022

The beauty of RS-3 degradation by gut microbiota Cynthia Klostermann, 8th Symposium on the Alpha-Amylase Family - ALAMY\_8 (2022), Smolenice, Slovakia, 9/10/2022 - 13/10/2022

Hydrodeoxygenation of butyric acid on Mo2C catalytic surface Raghavendra Meena, CHemistry As INnovating Science (CHAINS) 2022, Veldhoven, Netherlands, 21/09/2022 -22/09/2022

Unraveling the effect of support oxygen groups on the performance of Pt/CNF electrocatalysts Matthijs van der Ham, CHemistry As INnovating Science (CHAINS) 2022, Veldhoven, Netherlands, 21/09/2022 -22/09/2022

Carbon and its role in future catalysis Harry Bitter, CHemistry As INnovating Science (CHAINS) 2022, Veldhoven, Netherlands, 21/09/2022 -22/09/2022

Balancing Hydrogenation power and Oxophylicity in Carbon Supported Mixed Metal-Carbides for Deoxygenation of Stearic Acid Marlene Führer, 9th International Symposium on Carbon for Catalysis (CARBOCAT), Zaragoza, Spain, 28/06/2022 - 30/06/2022

On the role of support oxygen-groups in (electro)catalytic glucose oxidation over Pt supported catalysts Harry Bitter, 9th International Symposium on Carbon for Catalysis (CARBOCAT), Zaragoza, Spain, 28/06/2022 -30/06/2022

Designing elastoplastic edible 3D printable material using jammed emulsions stabilized with pea proteins Costas Nikiforidis, International Colloids Conference, Lisbon, Portugal, 12/06/2022 - 15/06/2022

Faculty-based design of Virtual Laboratory applications for Large-Scale Use Harry Bitter, Educational Pioneers and Innovators Conference – EPIC, Rotterdam, Netherlands, 30/05/2022 - 1/06/2022

Steering the Oxophilicity and Hydrogenation Ability of Transition Carbide Catalysts for Deoxygenation of Stearic Acid

Marlene Führer, North American Catalysis Society Meeting (NAM27), New York, United States, 22/05/2022 - 27/05/2022

On the role of support oxygen-groups in the electrochemical oxidation of glucose over Pt/Carbon nanofiber catalysts

Harry Bitter, North American Catalysis Society Meeting (NAM27), New York, United States, 22/05/2022 - 27/05/2022

Electrocatalytic oxidation of glucose and starch over Pt based catalysts Harry Bitter, International Symposium on Green Chemistry, La Rochelle, France, 16/05/2022 - 20/05/2022

Tuning the oxophilicity and hydrogenation ability of transition carbide catalysts for deoxygenation of stearic acid

Marlene Führer, NCCC The Netherlands' Catalysis and Chemistry Conference (2022), Noordwijkerhout, Netherlands, 9/05/2022 - 11/05/2022

Designer edible materials using oleosomes Costas Nikiforidis, Aristotle University of Thessaloniki, Greece, 2/04/2022

Designer edible materials using oleosomes Costas Nikiforidis, Nanyang Technological University, Singapore, 9/02/2022

Biobased Soft Materials Costas Nikiforidis, Agency for Science, Technology and Research (A\*STAR), Singapore, 8/02/2022

Facile and efficient exploitation of plant materials Costas Nikiforidis, Universidad de las Americas Puebla, Mexico, 16/01/2022

## **Poster presentations**

'Competition of rapeseed proteins and oleosomes for the air water interface' Yang, J, Berton-Carabin, CC, Nikiforidis, K, van der Linden, E & Sagis, LMC, Annual European Rheology Conference (AERC 2022), Sevilla, Spain, 26/04/22 - 28/04/22

'Elucidating the reaction pathway for the electro-catalytic oxidation of glucose over platinum' van Keulen, E, van der Ham, MPJM, Asadi Tashvigh, A, Koper, MTM & Bitter, JH, NCCC The Netherlands' Catalysis and Chemistry Conference (2022), Noordwijkerhout, Netherlands, 9/05/22 - 11/05/22

'Electrocatalytic oxidation of glucose over Pt on carbon nanofibers: effect of support oxygen groups' van der Ham, MPJM, van Haasterecht, T, Koper, MTM & Bitter, JH, 32nd Topical Meeting of the International Society of Electrochemistry, Stockholm, Sweden, 19/06/22 - 22/06/22

'Electrocatalytic oxidation of glucose over Pt on carbon nanofibers: effect of support oxygen groups' van der Ham, MPJM, van Haasterecht, T, Koper, MTM & Bitter, JH, NCCC The Netherlands' Catalysis and Chemistry Conference (2022), Noordwijkerhout, Netherlands, 9/05/22 - 11/05/22

'Hydrodeoxygenation reaction mechanism of butyric acid over Mo2C: A combined DFT and MKM study' Meena, RM, Bitter, JH, Zuilhof, H & Li, G, International Conference on Theoretical Aspects of Catalysis (ICTAC) 2022, Lyon, France, 13/06/22 - 17/06/22 'Insights into the reactivity of transition metal carbides for biomass conversion: A DFT study' Meena, RM, Draijer, KM, Bitter, JH, Zuilhof, H & Li, G, NCCC The Netherlands' Catalysis and Chemistry Conference (2022), Noordwijkerhout, Netherlands, 9/05/22 - 11/05/22

'Fermentability of resistant starch type 3'

Klostermann, CE, Quadens, TMC, Endika, MF, Ten Cate, E, Silva-Lagos, LA, de Vos, P, Schols, HA & Bitter, JH, 8th International Conference on Dietary Fibre 2022, Leuven, Belgium, 16/10/22 - 18/10/22

'Specific Resistant Starch type 3: a bioactive ingredient' Klostermann, CE, Silva-Lagos, LA, Buwalda, PL, de Vos, P, Schols, HA & Bitter, JH, Carbohydrate Competence Center Lente Symposium 2022, Groningen, Netherlands, 31/05/22 - 31/05/22

'Synthesis of carbon supported bimetallic MoW-carbide catalysts' Führer, M, van Haasterecht, T, Boed, de , J, de Jongh, PE & Bitter, JH, CHemistry As INnovating Science (CHAINS) 2022, Veldhoven, Netherlands, 21/09/22 - 22/09/22

'Zooming in: measuring micro-gradients of H2 and pH in (bio)electrochemical 3D electrodes' de Smit, SM, Bitter, JH & Strik, DPBTB, 7th Young Water Professionals BeNeLux conference 2022, Delft, Netherlands, 4/04/22 - 6/04/22

## Press/Media

New membrane for portable artificial kidney Resource jrg. 17 nr. 8 p. 7-7 <u>https://edepot.wur.nl/583405</u> Akbar Asadi Tashvigh 15/12/22

3D printed pea proteins and oil to mimic lard in veggie burgers raiplay.it https://www.raiplay.it/video/2022/08/Sostituti-del-latte-e-della-carne---Superquark-03082022-227541df-0c28-4e15-b351-85626b21e0e2.html Costas Nikiforidis 3/08/22

Hoe vervang je het romige mondgevoel van dierlijk vet Food Inspiration <u>https://www.foodinspiration.com/nl/hoe-vervang-je-het-romige-mondgevoel-van-dierlijk-vet-/</u> Costas Nikiforidis 6/03/22

Erwteneiwit uit 3d printer vervangt dierlijk vet De Ingenieur <u>https://www.deingenieur.nl/artikel/erwteneiwit-uit-3d-printer-vervangt-dierlijk-vet</u> Costas Nikiforidis 17/02/22

3D printed pea proteins to mimic lard in veggie burgers ENP Newswire Costas Nikiforidis 10/02/22 3D printed pea proteins to mimic lard in veggie burgers Mirage News https://www.miragenews.com/3d-printed-pea-proteins-to-mimic-lard-in-veggie-721413/ Costas Nikiforidis 9/02/22

Zonnebloem levert duurzaam vet VMT Costas Nikiforidis 6/02/22

## Organising a conference

2nd Edible Soft Matter Conference Jack Yang (Organiser), Elke Scholten (Organiser), Renko de Vries (Organiser), Wageningen, Netherlands, 11/07/2022 - 13/07/2022

## Prizes

Best PhD award: The beauty of RS-3 degradation by gut microbiota Klostermann, Cynthia (Recipient) 8th Symposium on the Alpha-Amylase Family - ALAMY\_8 (2022), Smolenice, Slovakia, 10/10/2022

Rudy Rabbinge Prize best poster CCC Spring Symposium Klostermann, Cynthia (Recipient) Granting Organisations: Carbohydrate Competence Center (CCC) Carbohydrate Competence Center Lente Symposium 2022, Groningen, Netherlands, 31/05/2022