Projects with PPP programme allowance 2018

NWO-projecten

(CHEMIE.PGT.2018.013 NWO)
Organisation: NWO

Infrared Ion Spectroscopy: development and application in drug metabolism
Bij de ontwikkeling van nieuwe medicijnen is het niet alleen van belang te weten wat het effect van het nieuwe molecuul is, maar ook wat die van zijn gemetaboliseerde producten zijn. Hiervoor dient de moleculaire structuur van deze van het medicijn afgeleide metabolieten nauwkeurig in kaart gebracht te worden. In labtests worden de nieuwe moleculen daarom geïncubeerd in levermicrosomen, en deze worden daarna met massa spectrometrie (MS) onderzocht op de aanwezigheid van medicijn metabolieten. Het is echter moeilijk om op basis van deze MS data de precieze structuur van de metabolieten vast te stellen; metabolisering, bijvoorbeeld door oxidatie, kan op veel verschillende plaatsen op het molecuul hebben plaatsgevonden en al deze producten zouden dezelfde massa hebben. In onze methode onderzoeken we de in de massaspectrometer geselecteerde producten met IR spectroscopie, door gebruikmaking van de vrije-electronenlaser FELIX.

Visible light-driven hydrogen production from the humidity of ambient air
The prospect of solar hydrogen as a sustainable energy source is the driving force for the steady progress toward efficient water-splitting materials. While current systems run on liquid water, the idea of capturing water from ambient air in a solar watersplitting device is appealing. The focus of the Air2Hydrogen project was to overcome the technical challenges of the direct conversion of sunlight and humidity from the ambient air to hydrogen. In the frame of this project, we have not only developed efficient water absorption coatings and photoelectrodes material but we have also scaled up their fabrication processes beyond state-of-the-art.

Sustainable production of biobased aromatics by selective furan activation
In this project we studied how aromatics, building blocks of products we use daily (e.g. plastics, coatings, medicine), can be made from biomass rather than from fossil resources. Those compounds that can directly be obtained from biomass and that should serve as the starting point for aromatics production, don't work well, however, in the key conversion step of the proces. In this project we studied a clever method to get this reaction to run efficiently, in order to increase the viability of biorefining. The research provided insight into the potential and the limitations of this approach.

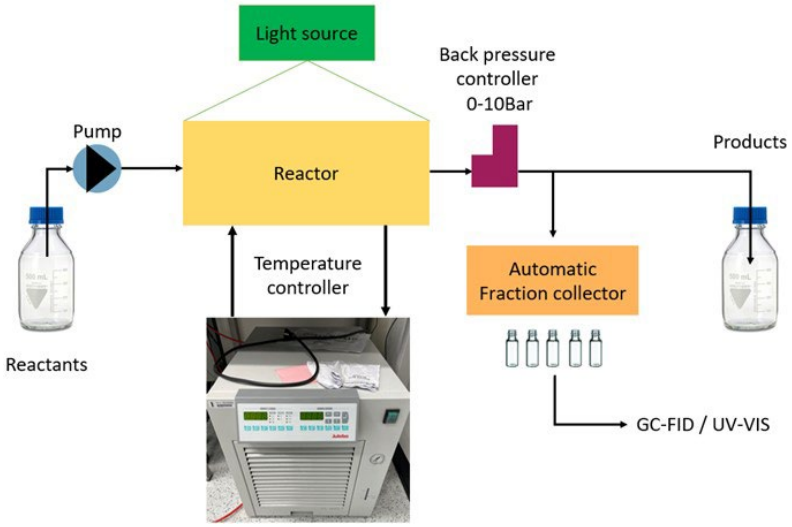
TNO-projecten

(CHEMIE.PGT.2018.014 TNO)
Organisation: TNO

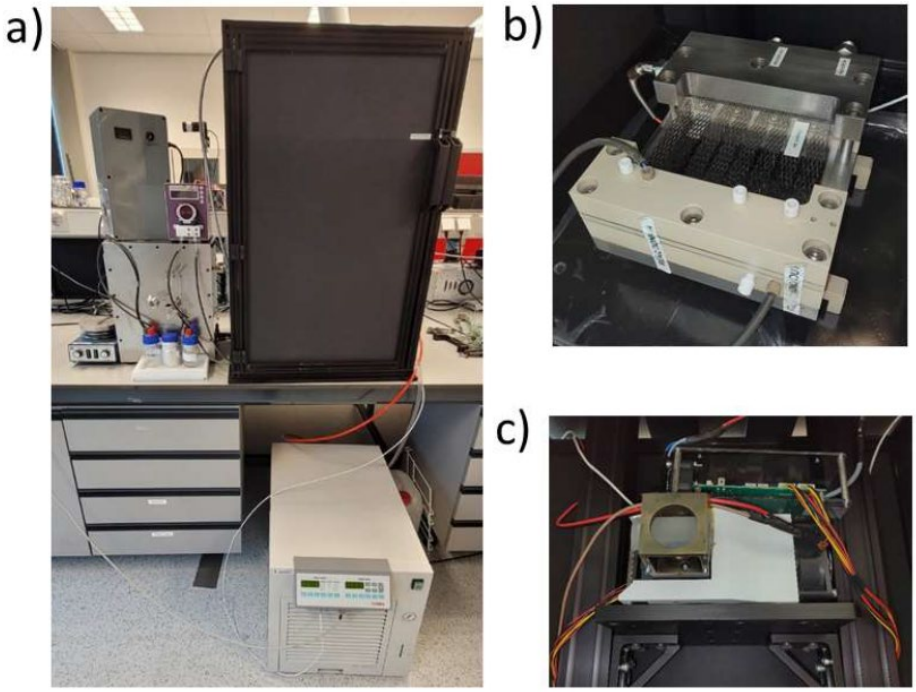
FLuxCHEM: Integral optimization of Flow reactor and Light source for photoCHEMical conversions
In recent years, many different photochemical reactions have been developed in academia. In spite of that, uptake of photochemistry in industry is lagging behind. This slow uptake is mainly due to:

- the limited availability of suitable photochemical reactors for (larger) scale reactions;
- the absence of suitable high intensity light sources for photochemistry;
- the absence of integrated systems combining light source and tailored reactor.

In the FLuxCHEM project we aimed to enhance the uptake of photochemistry by industry through the integral development of a prototype photochemical A first design of a system using an existing (prototype) Signify LED light source and an existing (prototype) Chemtrix flow reactor was developed. A light intensity measuring device has been designed, manufactured and validated. The system was setup and validated optically at the TNO laboratories in Eindhoven by measuring the light intensity based on fibre optics in the flow channels and chemically via prototype photochemical conversions. The validation reaction showed 16 times higher light flux with moderate light intensity as compared to a literature reference. This reflects the gain in optical and energy efficiency compared to the state of the art. This enables faster and more efficient photochemical conversions, underlining the relevance of further integration of light source and reactor design.



Schematic representation of the flow photochemistry reaction set-up



Images of the FluxChem set-up a) Full set-up within an optical cabinet; b) Chemtrix KiloFlow® reactor; c) Signify high lumen density (HLD) light engine (green light).

MAT4CAT

One of the biggest challenges we currently face as a society is securing our future energy supply. This requires a transition from fossil fuels, such as oil and natural gas, to renewable energy sources such as solar and wind. In addition, there is a second major challenge: reducing the emission of the greenhouse gas carbon dioxide (CO2). The so-called “low carbon economy roadmap” of the European Union has the ambitious goal of reducing emissions by 2050 to 80% below 1990 levels. In the MAT4CAT project we have developed catalysts that convert CO2 with green hydrogen (H2) to methane (CH4) as fuel or carbon monoxide (CO) as component of syngas; a commonly used intermediate product for the chemical industry. For both conversions, we aim at using sunlight directly as a sustainable energy source. This way, both the energy challenge and the reduction of CO2 emissions can be simultaneously addressed. Within this project we have shown that mineral materials of natural origin, which are exploited by Sibelco, can be successfully used as support materials for plasmonic metal nanocatalysts developed by TNO. The outcome of the project is a library ofcatalyst materials, consisting of combinations of different natural mineral support materials and metal nanoparticles, that can be used for the selective conversion of CO2 to CH4 or CO using sunlight as sustainable energy source.

For the sunlight powered conversion of green H2 and CO2 to CH4 or CO, plasmonic catalysts are used. These catalysts consist of small metal nanoparticles that are applied to a support material. Based on the localized surface plasmon resonance (LSPR) of the supported metallic nanoparticles, the catalysts absorb a large share of the sunlight spectrum from the ultraviolet part up to the infrared radiation, and in this way efficiently use the solar energy for the conversion of CO2. In this project we have used support materials from natural sources supplied by Sibelco and evaluated how the type of metal, the size and

shape of the metal particles, and the characteristics of the support influence the efficiency of the production of CH4 and CO.

The MAT4CAT project milestone, a higher catalytic activity of plasmonic metal nanocatalyst using Sibelco natural support material than similar metal nanocatalyst on synthetic support materials, was partly achieved. For Sabatier reactions, the achieved catalytic activity was proven to be similar to the ones previously achieved by TNO using plasmonic nanocatalysts comprising synthetic alumina support materials. For the rWGS reaction, the developed photocatalyst formulations did not show catalytic activity, despite the successful preparation of small Au nanoparticles on mineral supports.

Synthetic procedures to deposit Ruthenium (Ru) nanoparticles on kaolins, metakaolins and mixtures thereof as support materials were successfully developed. The produced catalysts were characterized to determine their chemical composition, their nanostructure and their optical properties. The Metakaolin supported Ru nanocatalysts yielded a catalytic performance similar to the Ru/Alumina benchmark.

Synthetic procedures to deposit gold (Au) nanoparticles on kaolins, metakaolins and mixtures thereof as support materials have been developed. The chemical composition and nano-/microstructure of the supported Au nanocatalysts was successfully characterized. Metakaolin supported Au nanocatalysts yielded no catalytic activity. Most likely, codeposition of multiple components (e.g. Au and semiconductor, or Au and ionic liquid) is needed to achieve a well performing catalysts for the rWGS process. This investigation will be part of a joint follow up project.

Three Deliverable reports were prepared describing the outcome of materials inventarisation, synthesis procedures of selected catalysts and results of the validation experiments of the materials in the catalytic conversion of CO2 and H2 to CO and CH4 using (concentrated) artificial sunlight as the energy source.

Optimization and scale-up of production of thermochromic nanopigments, for use in solar control coatings for architectural building skin (THERPA)

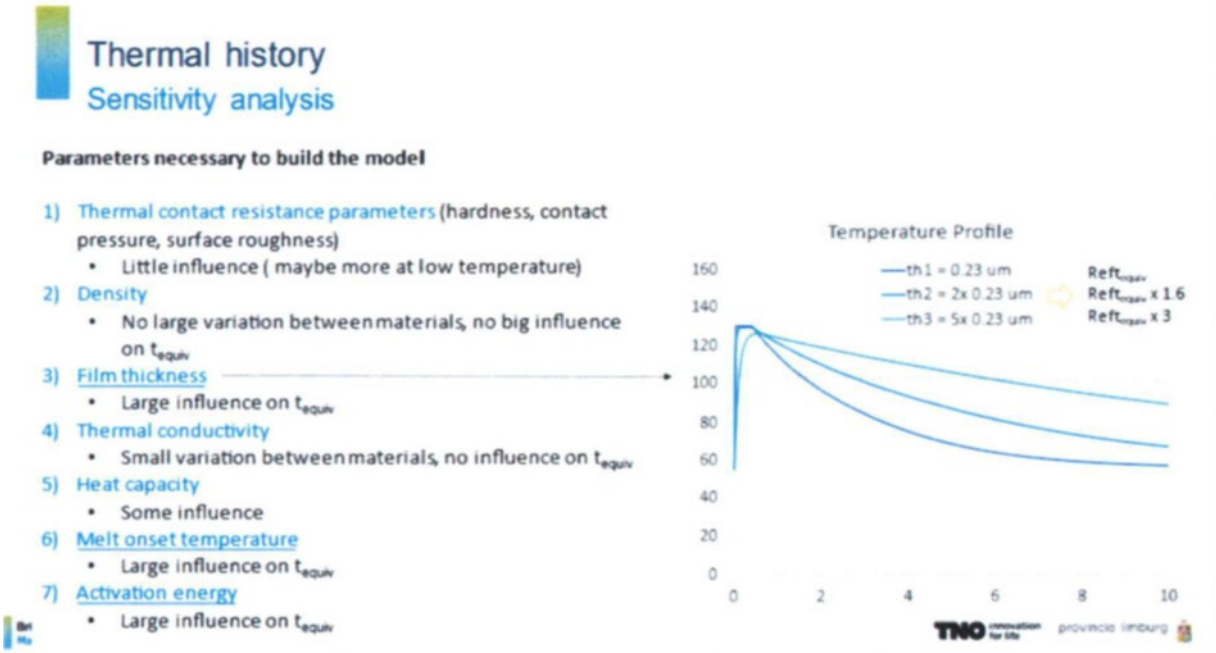
In Europe, more than one third of the total energy consumption and CO2 emission result from the built environment, with energy for heating and cooling of buildings as a major share. Adaptive glazing solutions can have a significant impact on a buildings energy demand, making optimal use of sunlight and solar heat. Thermochromic materials, such as vanadium dioxide (VO2), can be used for adaptive glazing since they can autonomously switch their solar infrared (IR) transmission depending on the glazing temperature. VO2 displays thermochromic properties based on its structural phase transition from monoclinic VO2 (M) to rutile VO2 (R) and vice versa, and the accompanying reversible metal-insulator transition. In this project we developed a hydrothermal procedure to synthesize VO2 nano-pigments to be used in coatings and pigmented polymer films for smart glazing solutions. We optimized the process to realize high purity and crystallinity of the pigment material. Furthermore, we used dopants to reduce the phase transition temperature to application oriented values between 20 – 30°C and reduced the average particle size to <100 nm to reduce scattering and improve properties for optical application. In addition, we started transferring the lab scale procedure towards pilot scale.

TKI Bubble Foil

Thermoplastic polymer foils are key elements of many packaging materials. Protective inflated films are a large class of thermoplastic polymer foil based packaging materials. Their major use is for void filling

in delivery of packages, like Amazon of Bol.com. The quality of these protective films depends highly on a good seal to ensure air retention. Due to the increasing demands to supply sustainable products, the market wants to increase its share of post-consumer recycled material (PCR, according to ISO 14021) in its films. This may influence the performance properties of inflated films, in particular the sealing quality.

The aim of this project is to gain an improved understanding of the sealing process and its relation to the properties of the thermoplastic polymer used. Based on this understanding it is expected that we can design new thermoplastic polymer compounds with increased content of PCR at equal or better performance in an economically viable way.

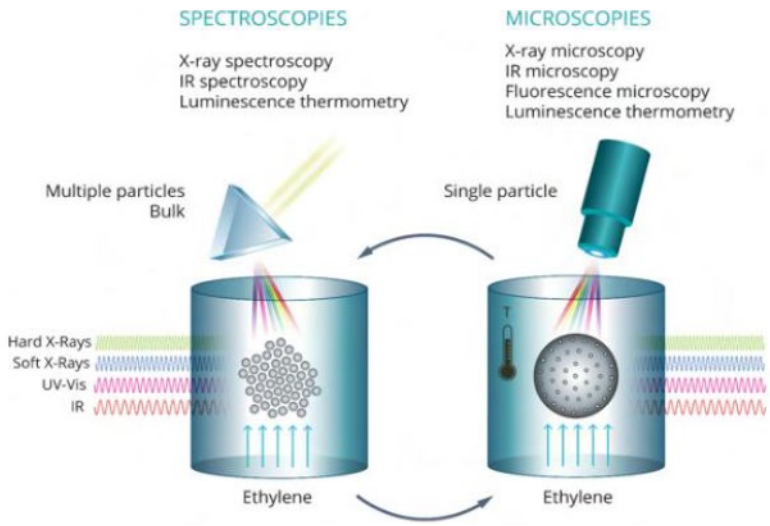


The material model developed in WP6 qualitatively shows the effect of different film physical property on the sealing strength

Call for Proposals Technology Areas Polyolefins en Performance Polymers

(CHEMIE.PGT.2018.015)
Organisation: DPI

Despite their long-term use and many efforts to disclose their properties, the olefin polymerization catalysts are still black boxes concerning the understanding of their molecular level properties and structure-activity relationship. The work of this project describes how an analytical toolbox, consisting of various microscopy and spectroscopy techniques, was explored to study the structure, composition and temperature of industrial grade silica supported ethylene polymerization catalysts, such as supported metallocene based and Ziegler-Natta catalyst materials.



Both families of heterogeneous catalysts were characterized in the early stages of active site genesis and polymer formation to elucidate structure-composition-performance-morphology correlations at the single particle level. An experimental methodology was developed based on time-resolved IR spectroscopy with insertion probes, which allows to obtain simultaneously information on the catalyst properties at molecular level and on their polymerization ability. This was achieved by the synergetic use of insertion probe molecules and monomers. In particular, by performing systematic experiments on different catalysts in the same experimental conditions, this approach allows to determine the relative fraction of accessible sites, The acquired insights can ultimately contribute to the optimization of established catalyst systems, thereby improving both the catalyst productivity and the product quality. With the recycling of polymers gaining momentum, the potential of the previously mentioned analytical toolbox for heterogeneous catalysts in the field of chemical polyolefin recycling is also discussed.

FOAMEX-II en DISCOVER-II

(CHEMIE.PGT.2018.016)
FOAMEX-II: Advances in foam extrusion of PLA
Organisation: Wageningen University & Research

Poly (lactic acid) PLA is one of the most attractive biopolymers. It combines a low ecological footprint with good material properties and biodegradability. Moreover, PLA is one of the most affordable biopolymers. Nowadays PLA can be processed via several techniques including film casting, injection moulding and thermoforming making it applicable in several products in the market. However, some inherent properties of PLA have limited its use in commercial extrusion foaming. Within the FOAMEX-II project, the participants have taken the production of PLA based extrusion foams to a next level where its applicability in foamed products has become possible. For a commercial breakthrough, improvements were still needed with respect to rheology and crystallinity of the proposed formulations and materials. In the project, formulations and (more important) concepts were optimized in order to make them even more commercially interesting. The optimization of the materials focused on the requirements of the market, i.e. a broad and stable process window, sufficient crystallinity, melt strength and an interesting cost price.

DISCOVER-II: Development of an innovative, sustainable roofing system

The DISCOVER-II project aimed at the development of a biobased alternative to conventional roofing membranes, such as bituminous or synthetic roofing. In this project, Wageningen Food & Biobased Research worked together with roofing producer BMI (formerly Icopal) and Stora Enso.

Conventional flat roof covering systems such as bitumen or synthetic polymer based membranes are of high quality and have a long service life, however, they are mainly made from petroleum resource. Since this fossil resource is finite and its extraction, refining and use contributes to climate change, there are ample reasons to consider more sustainable alternative materials while retaining the required technical and functional characteristics of roofing membranes.

Biobased roofing

The ultimate goal of the project was the development of an environmentally friendly alternative to bituminous roofing systems, in which the fossil bitumen has been replaced by biobased raw materials. In the DISCOVER-II project a large range of biobased streams was evaluated. One important issue is that biomass derived streams are less hydrophobic and more reactive than bitumen. Focus was given to side streams which are available in large quantities from the pulp&paper and agri&food industries.

Results on the evaluation

Binder mixes were designed based on fully biobased components comprising for example lignin and vegetable oils. These binders were manufactured at lab scale up to around 1kg and evaluated for its main characteristics such as mixing ability, homogeneity, visco-elastic and rheological behavior, penetration value and stability. The results are close to the desired range of properties for sustainable roofing systems. Industrial applicability with current manufacturing principles seems possible with these innovative materials. LCA results indicate that the use of biobased streams can have a significant benefit, giving a lower carbon footprint, especially if the biogenic carbon sink function is taken into account.

ReoSim: Het modelleren en simuleren van de reologie van grensvlaklagen

(CHEMIE.PGT.2019.003)
Organisation: Eindhoven University of Technology

Plenty of soft materials all around us consist of drops or bubbles of one fluid distributed in another fluid. These fluids do not mix, unlike sugar or salt that do dissolve in water. For example, when you try to mix oil and water, after leaving the fluid at rest you will see that the oil floats to the surface and forms a layer on top of the water. Oil and water are said to be immiscible.

The chemical and mechanical properties of immiscible fluids are taken advantage from in a lot of applications varying from everyday consumer care products and foods to pharmaceuticals, petrochemicals, and polymer blends. The presence of an interfacial layer in between the immiscible fluids yields a completely different structure on very small length scales in the mixture than in the constituent fluids separately. The holy grail is synergy of properties: the mixture has more beneficial/desired properties and performance than the fluids separately.

The goal of this project is to study the flow behaviour of immiscible fluids using computer simulations. By varying the mechanical properties of the interface in between a single drop suspended in another fluid, we gain insight into the influence of the interface on the flow of the mixture. This enables to predict and control final properties and performance of products by providing design rules in material choice and processing. For this purpose, a computational modelling framework has been developed which has been shown to describe the stress-strain behaviour of interfaces as observed in the

literature. Conclusions so far: by including elasticity to the interface, meaning that it can store more and more energy upon deformation, you need to apply a stronger flow to deform the drop.

New insights into the working principles of metal-alkyls as co-catalysts in Cr/SiO2 Phillips catalysis

(CHEMIE.PGT.2019.004)
Organisation: Utrecht University

Single-site heterogenized catalysts fulfil a prominent role in ethylene polymerization. In our research we combined the ethylene polymerization properties of chromium and the tunability of Metal-Organic-Frameworks (MOFs) and studied Cr-based MOFs in ethylene polymerization. We found that the activation procedure by the metal-alkyl co-catalyst is critical for obtaining appreciable ethylene polymerization activities. While it was postulated that this activation procedure is related to total collapse of the MOF, pore structure and morphology analysis has revealed that although part of the pore structure is lost, the morphology of the material remains intact, inferring that total collapse of the MOF does not occur, and indeed the activated MOF materials act as polymerization catalysts. Spectroscopic efforts towards revealing the active-site structure revealed that despite the pristine MOF being a heterogenized single-site material, the active catalyst cannot be considered as such. We found that a multitude of different Cr(III) surface structures are formed upon activating the MOF with the co-catalyst, which is further corroborated by investigating the polyethylene (PE) product properties and is strongly emphasised in the materials' broad Dispersity Indices (DI). Analysis of the PE product morphological properties demonstrated that with benefits of MOFs also additional challenges arise: this work revealed that a too-narrow active-site spacing results in products with worm-like morphological features, that are often associated to reactor fouling, whereas appropriate active-site spacing resulted in favourable spherical morphologies. Conclusively, we have shown that Cr-based MOFs can be considered suited candidates for ethylene polymerization, however additional research is still required for increasing understanding of these systems, even more so if they at some point are desired to be more mainstream catalysts.

Additive Manufacturing in lndustrial production

(CHEMIE.PGT.2019.005)
Organisation: Hogeschool Windesheim

The main goal of the overall project was to define the opportunities and challenges to integrate Additive Manufacturing (AM) in industrial, profitable processes for singular as well as serialproduction and to generate the required knowledge for implementation. The aim was the production of final products instead of prototypes, which is the main focus of many AM users.
Different AM technologies were compared for their potential to produce loadbearing end-use parts as well as for the production of small series. Some technologies were found more suitable, and focus was narrowed down to 2 technologies: SLS (PA12) for its potential to produce load bearing parts, its high production capacity and simpler design rules and FDM, as it proved the
most accessible, affordable and up to that point most widely adopted technology.

For SLS printed PA12 it is clear that the prerequisites for series production are met. Production capacity is high, parts are accurate and generally strong, allowing the use in load bearing applications. However the failure mode is brittle, thus limiting practical usability. In-depth research was conducted to find solutions to obtain a ductile and safe failure mode of PA12

parts processed by means of SLS printing. It was found that although this cannot be achieved within the state-of-the-art printing process itself, ductility can be increased greatly by heat treatment around (and preferably above) the melting temperature after the printing process. It does however reduce part accuracy; methods to support the parts during heat treatment could be a means to overcome this problem in future. For FDM it was found that its suitability for serial production and load bearing parts is highly dependent on aspects such as part size, geometry, complexity and material choice. The technology requires considerable knowledge for both design and production and this can limit applicability for end use components and serial production, especially as part size, complexity and mechanical demands in the end application increase.

A demonstrator object was designed and produced to demonstrate learnings from this project: a non-conventional bicycle called the MesoCruiser, containing a frame completely produced using different AM technologies. Every part of the frame is designed and produced to use specific advantages of a specific combination of AM-technology, material and finishing, while the complete frame provides insights in design for AM, specific design rules and examples of using efficient connections and assemblies of FDM printed parts.

Hybrid semiconductor-insulator nanostructures for spectral conversion

(CHEMIE.PGT.2019.006)
Organisation: Utrecht University

White light LEDs rely on the efficient partial conversion of blue LED light to green and red emission. Luminescent lanthanides are ideal emitters based on their efficient and narrow line emission. However, the absorption of blue light is weak and the emission life time is long. In this project we explored new routes using strongly absorbing semiconductor halide nanocrystals doped with lanthanide ions to solve the absorption problem and to study the light output for high excitation powers to understand how long emission lifetimes limit brightness of LEDs. For the lanthanide Yb3+ incorporated in bromide semiconductor nanocrystals, energy transfer was observed and the transfer mechanism was elucidated. Experiments on Mn4+-doped materials revealed the contributions of different processes limiting LED brightness as well as possible solutions.

Electrochemical Hydrogen Peroxide (EHP) production

(CHEMIE.PGT.2019.007)
Organisation: Twente University

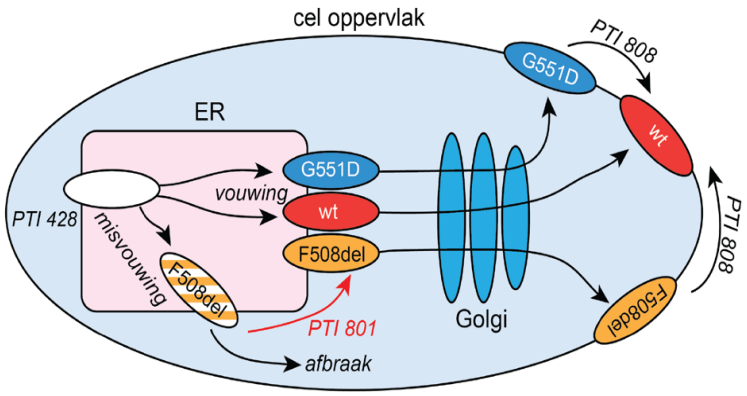
Hydrogen peroxide is considered an important environmentally friendly oxidant that is employed as disinfectant for water/air treatment, in agriculture and food industry or as soft oxidant in chemical industry. Compared to the currently employed anthraquinone process, electrochemical hydrogen peroxide production provides substantial advantages, such as the ability for decentralized production, and a reduced dependence on fossil resources. This project aimed at the development of hydrogen peroxide production processes utilizing abundant materials and renewable energy sources to facilitate implementation of green hydrogen peroxide into the value-chain of the chemical industry. To achieve this goal the development of materials and evaluation of process conditions allowing for the production of hydrogen peroxide with high selectivity is required. Here, boron-doped diamond electrodes as a new class of selective and stable electrode materials for the production of hydrogen peroxide has been thoroughly investigated. After process optimization high selectivity for hydrogen peroxide > 30% were obtained in a reproducible manner using an attractive electrochemical process requiring only liquid phase reactant. The established understanding of selective hydrogen peroxide production from water will be utilized in follow-up work to target operation at industrially relevant conditions.

Characterizing new candidate drugs for treatment of cystic fibrosis

(CHEMIE.PGT.2019.008)

Organisation: Utrecht University

Cystic Fibrosis (CF) is an inherited disease caused by mutations in the CFTR gene that lead to absent or defective CFTR protein. Since 2012, some drugs have become available to CF patients that can improve defective CFTR protein, enhancing CFTR function. While effective for the majority of CF patients, they are not for many others. A large unmet need therefore still exists for effective medication for many CF patients.



The industrial partner has developed candidate medicines with at least four different activities. We advanced and enhanced the conformational assays in the academic lab and combined these assays with functional assays to characterize the candidate medicines. Mode of action of one of these appeared similar to one of the available drugs, while the others displayed a novel mode of action, which we aim to further uncover in a follow-up grant awarded to the consortium.

Unravelling the ubiquitin ligase binding landscape

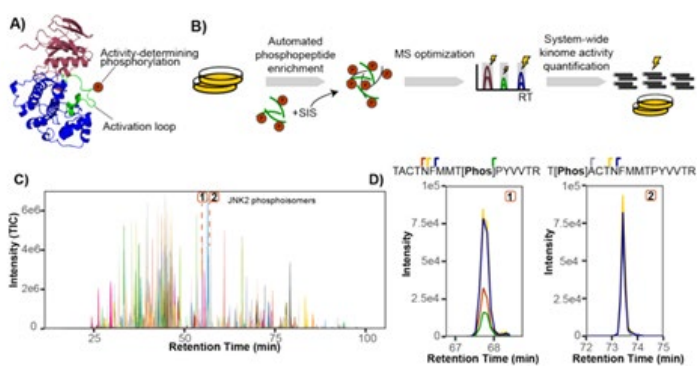
(CHEMIE.PGT.2019.009)

Organisation: Utrecht University

This project aimed at deepening our understanding of the three-dimensional structure of E3 protein ligases. This class of proteins is involved in our own protein degradation pathway and are emerging as a new drug discovery paradigm. By tricking our protein degradation machinery to target a protein of choice it is possible to clear from our cells harmful proteins involved in a variety of diseases. In this project, as a first step to achieve this general aim, we developed a computational protocol to predict the E3 ligase binding site for their target proteins. This is a necessary first step in the design of PROTACS, small molecules that can link a protein to be degraded to a specific E3 ligase.

Rapid assessment of kinome-wide activation to characterise defined cell states

(CHEMIE.PGT.2019.010)
Organisation: Utrecht University



Cellular signalling plays a vital role in maintaining our overall health. Through intricate networks of communication, these signalling pathways orchestrate harmonious interactions to sustain our well-being. However, there is no guarantee that cellular signalling remains untainted. Dysregulation can arise from various sources, including pathogens like viruses or toxins, internal factors such as genetic errors, or a combination of both. Consequently, there is a key need to find treatments for diseases to restore healthy cellular signalling. To address this need, we must comprehend the rules and complexity of cellular signalling. The research performed in this project aimed to precisely do that.

Syngas reaction with light olefins to produce high value products

(CHEMIE.PGT.2019.011)
Organisation: Utrecht University

New catalysts for new conversion routes It is crucial to produce our fuels and chemical building blocks from renewable and circular resources instead of relying on fossil resources. An important quest is for routes to couple smaller units/molecules to make longer and more complex ones. We investigated the possibility to do so, and found promising leads to catalyse this reactions with sustainable catalysts, based on stable solids, instead of the now common liquid-based catalysts.

An Analytical Study of Biorefinery Lignin

(CHEMIE.PGT.2019.012)
Organisation: Utrecht University

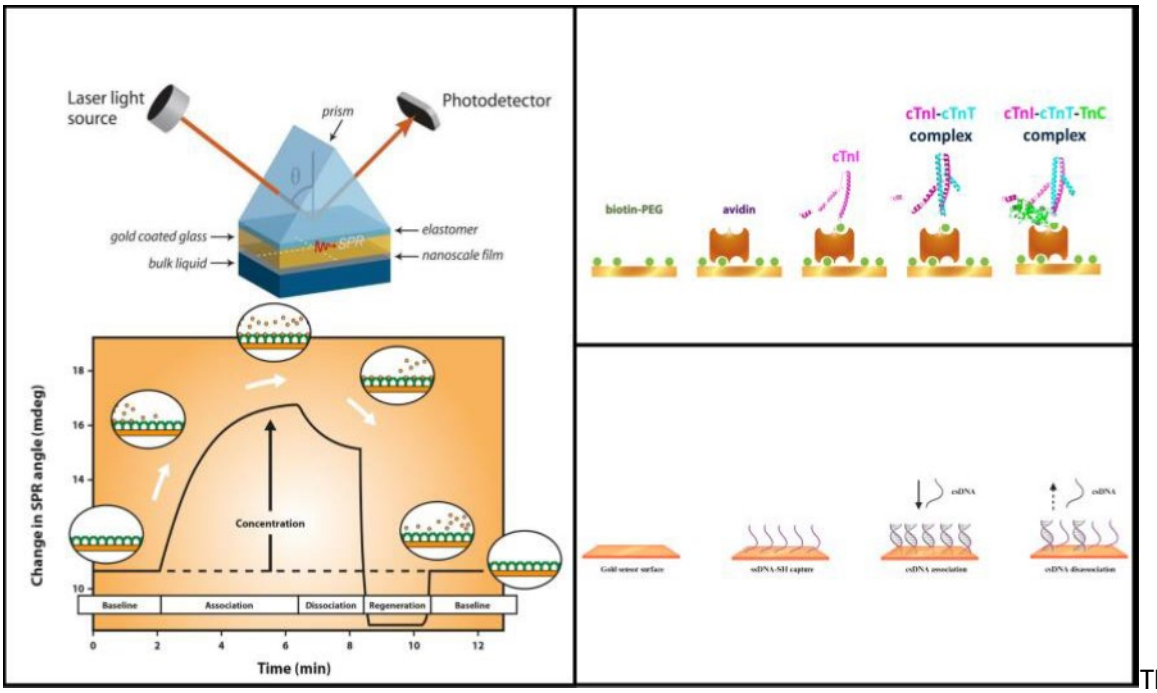
Lignin is a complex material, a part of woody biomass that changes extensively upon biorefining. These studies provided more insight into the molecular structure of a certain lignin, aiding further valorization of this biobased material.

Smart Materials: assessment of biology-materials interactions with advanced Surface Plasmon resonance

(CHEMIE.PGT.2019.013)
Organisation: Maastricht University

Biomedical materials Research and Development is primarily focused on the design, development, and application of smart materials, aiming to mimic biological responses and enhance cell adhesion and proliferation. The interaction between materials and biology is crucial for creating intelligent, dynamic supramolecular materials. However, the current understanding of these materials is insufficient in

characterizing their chemical functionality and establishing correlations with key biological processes. Bridging this knowledge gap is essential to unlock the full potential of smart materials in biomedical applications.



The "Smart Materials" project aimed to characterize supramolecular biomaterials and engineer structures that closely simulate natural formations. Molecular interactions between biomolecules and the designed biomaterials were explored to exert precise control over surface properties, guiding cell responses and influencing tissue growth. The project utilized Multi-Parametric Surface Plasmon Resonance (SPR) as the analytical method of choice, leveraging the advanced capabilities of a newly developed instrument by Bionavis. This technology allowed the scanning of multiple wavelengths and generating complete SPR curves, providing novel insights into sample properties and interactions.

The project's findings in the Myocardial infarction model demonstrated conformational changes in cardiac proteins, indicating that our functionalization approach successfully enables studying the dynamic nature of proteins. Additionally, insights into DNA interactions revealed a correlation between the length of sequenced DNA and the strength of interactions. This trend facilitated the control and direction of stem cell adhesion or migration, showcasing the potential applications of smart materials in manipulating biological responses for therapeutic purposes.

Spatiotemporal operando studies of automotive catalytic reactors

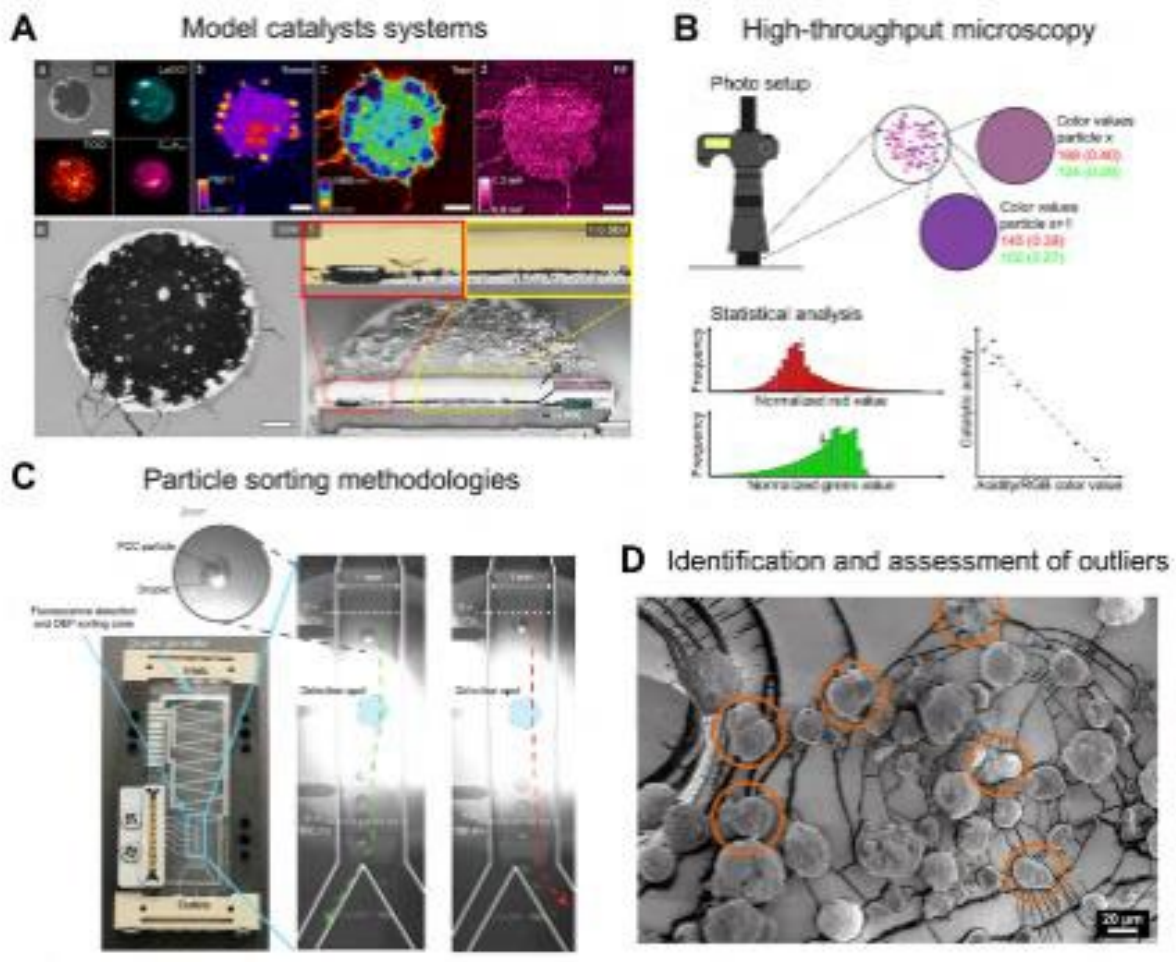
(CHEMIE.PGT.2019.018)
Organisation: Delft University

The design of catalysts and functional materials in modern devices is largely dependent on empirical trial-and-error approach. Useful empirical relationships between catalyst material and performance may be possibly established; however, this approach needs a large amount of time and manpower to reach desired performance, and for this reason the current functional devices are often the results of serendipity and intensive optimization of extensive experimental parameters. Once an empirical material structure vs. performance relationship is established, rational design of functional devices can be in principle facilitated. However, this is not fully true as represented by the case of automotive catalytic converters where large gradients of material structures, oxidation states, concentrations (gas phase and surface/bulk species) and temperature exist as a consequence of chemical conversions processes. Even worse, in practice the gradients fluctuate and vary with time within the catalytic converter. Reflecting the background, this project identified the nature of active surface chemical species, surface/bulk structures of catalyst, gas phase species, temperature and their spatial gradients within catalytic reactors of high relevance for the automotive industry. The state-of-the-art spatiotemporal analytical tools such as gas sampling and temperature detection were developed to enhance the quality and complementarity of physicochemical information within catalytic reactors. Through the information, the mechanistic details and support effects of CO oxidation over Pt were elucidated. Furthermore, the gained information was used as an input for simplified yet practical kinetic modelling of catalytic processes to extract intrinsic kinetic parameters to precisely express chemical reactivity and redox properties of catalyst materials on the reactor scale.

Green Foams

(CHEMIE.PGT.2020.005)
Organisation: University of Groningen

The project aimed at providing a toolbox for the industrial sponsor regarding the kind and intake of a crucial additive for the production of “green foams”. The latter are meant to replace current oil-based materials for a variety of applications (e.g. comfort foams used in furniture, automotive or aviation applications). This of crucial importance at academic, industrial and societal level. The foams currently used in our society are all oil-derived and factually impossible to recycle, if not with severe loss of properties or downcycling. The ones produced in this project are biobased and produced via an environmental friendly process. Furthermore, they are recyclable in a cradle-to-cradle manner (i.e. a new foam can be made out of the old one) and also biodegradable.



A summary of results is depicted, the blue datapoints represent an unmodified sample. What is clear is that respective to the blue data points both elastic modulus and dinamic viscosity can be increased and decreased. These values are known to have a large influence on the applicability of materials for foaming.

CARe – Contaminant and Ash Removal from pyrolysis liquids

(CHEMIE.PGT.2020.006)

Organisation: University of Groningen

Biomassa kan een belangrijke rol spelen in de transitie van petro- naar bio-gebaseerde economieën. Thermochemische conversies van biomassa naar vloeibare energie dragers en groene chemicaliën die verder omgezet kunnen worden naar bijvoorbeeld groene kunststoffen zijn goede opties voor het vergroenen van de economie. Een zeer veelbelovende technologie is pyrolyse, een technologie die momenteel beschikbaar is op semi-commerciële schaal. In dit project werken de Rijksuniversiteit Groningen en BTG BV samen aan het verwijderen van contaminanten in pyrolyse oliën. Indien succesvol zal dit een belangrijke bijdrage leveren aan het verbeteren van de kwaliteit van de pyrolyse oliën waardoor de techno-economische haalbaar voor een breed scala aan toepassingen verbeterd wordt. Een voorbeeld is de omzetting van pyrolyse oliën met behulp van waterstof en een geschikte katalysator tot een product dat samen met de huidige fossiele stroom gevoed kan worden in een bestaande olie raffinaderij. Zo kan (een deel) van bijvoorbeeld de chemicaliën uit een raffinaderij (olefinen, aromaten) groen geproduceerd worden. Echter, contaminanten in de vorm van b.v. zwavel en chloor hebben een negatief effect op de gebruikte katalysatoren en maken dat het proces economisch

minder aantrekkelijk is. In dit project gaan we het verwijderen van deze contaminanten uitgebreid bestuderen. Hoofddoelen van het project zijn i) een beter begrip van hoe de contaminanten aanwezig zijn in de pyrolyse oliën en ii) het verwijderen van de contaminanten met simpele en goedkope technologie.

Gefunctionaliseerde aromaten uit garnalendoppen

(CHEMIE.PGT.2020.014)
Organisation: University of Groningen

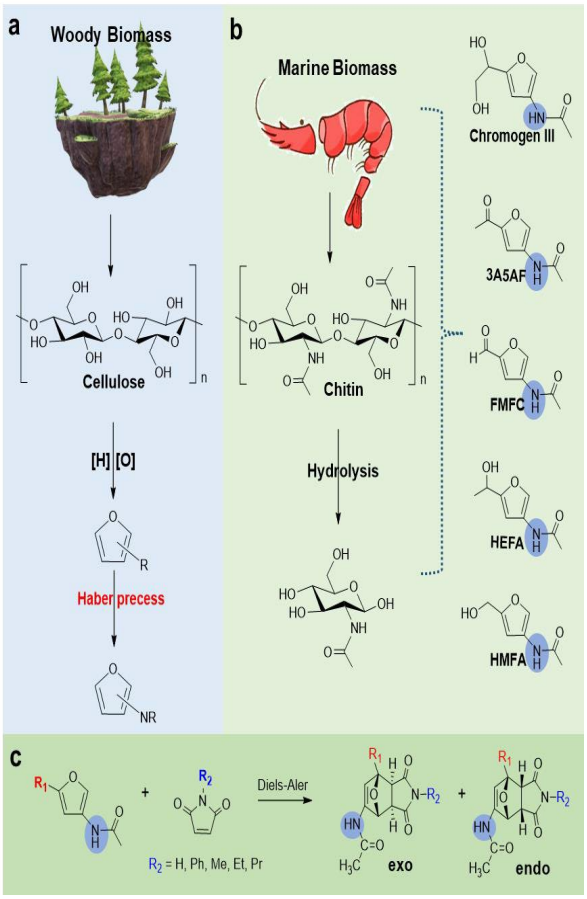
Chitin, the second most abundant polysaccharide on ear and a component in of the exoskeleton of arthropods such as shrimps represents an abundant source of nitrogenous polysaccharides that can be a suitable feedstock for organonitrogen platform chemicals. Especially furan compounds such as 3-acetamido-5-acetylfuran (3A5AF) can be readily obtained. Such furans can be further as dienes functionalized using Diels–Alder (DA) cycloaddition.

Herein, we report on the DA of 3A5AF, chromogen III and its aldehyde and alcohol derivatives with maleimide dienophiles. Exo or endo isomers are identified using computational tools and trends in their formation are monitored in detail. A reaction network is established and rates are calculated by performing reactions at different temperatures. The influence of electronic properties of different substituents on the five maleimides and NAG-derived dienes show significantly affect the cycloaddition rates and exo endo selecitivity. The introduction of electron-rich groups (e.g., -OH) into furans leaded to the stereoselectivity transformation from exo-selectivity to endo-selectivity. DFT calculations have also been performed to interpret the experimental results and gain more insights into the reactivity and selectivity trends.

4TU PDEng support programme TKI Chemie TUD part

(CHEMIE.PGT.2020.018)

Organisation: Delft University



Three industrial partners with activities in the fields of life sciences and health and energy transition (Tetrapak Cheese and Powder, Pertracta and LenioBio) cooperated in 4 PDEng (Professional Doctorate in Engineering) projects in these fields. These 4 projects were executed in the period 1 February 2022 to 30 September 2023. These projects were novel, innovative developments in which the activities focused on the best design options and recommendations to further improve the product/process for a sustainable application.

Devise and execute a workplan as suggested by the (bio)chemical product and process design methodologies as developed at TU Delft (Delft Design Map) taught to PDEng trainees at TU Delft.

The product and process to be designed were clearly pre-defined by looking at stakeholder analysis and product/process specifications and targets. Especially with a large number of stakeholders. The needs very much steered the development and further refinement of the technical solution(s).

INTERACT (Interface Catalysis for Advanced Sustainable Chemistry)

(CHEMIE.PGT.2020.021)

Organisation: Eindhoven University of Technology

NOx, CO and hydrocarbon emissions from combustion processes are major contributors to air pollution. Selective catalytic reduction (SCR) and three-way catalysis (TWC) are commercially used methods for removing such pollutants from exhaust. This project uses advanced characterization methods to study the catalysts used in these processes and how they change under operating conditions.

Iron exchanged small-pore zeolites used for SCR showed improved catalytic performance after a steam treatment. This stems from transformation of lesser active isolated Fe(II) species into more active Fe(III) species (e.g. dimers, oligomers), as observed by Mössbauer spectroscopy.

Palladium and platinum supported on cerium oxide were studied as model TWC catalysts. High temperature steam treatments have a minor effect on the structure of the catalysts but still modify their reactivity. In contrast, catalysts treated in simulated exhaust under realistic conditions underwent major structural changes, which are dependent on gas atmosphere and temperature.

Towards a circularity in recycling of polyurethanes

(CHEMIE.PGT.2020.022)
Organisation: Eindhoven University of Technology

Polyurethane (PU) represents one of the most important classes of polymers with versatile chemical and physical properties that has been widely used in a variety of industries, such as in the construction, automotive, footwear, furniture and clothing industry. However, despite the universal use of polyurethanes, the recycling of PU waste remains a challenge. In this project, we demonstrate that the recyclability of PU materials can be achieved by introducing new monomers containing cleavable bonds. We first developed a sustainable process for the synthesis of acetal-containing polyols under solvent-free conditions using heterogeneous catalysts and enabling reuse of the recovered catalyst. The acetal-containing polyols were used to prepare various acetal-containing PU materials which can be depolymerized under mild conditions, allowing recovery of the monomers in high yields and purity. These monomers can be reused for producing fresh and identical polymers in a manner of closed-loop recycling.

Advanced Molecular Modeling for Improved Chromatographic Separations – AMMICS

(CHEMIE.PGT.2020.023)
Organisation: Delft University

With the growing world population and the ease of international travel, the risk of global outbreaks of infectieus diseases increases. To combat and prevent possible pandemics, vaccines are among the best options. This project tocusses on the development of recombinant antigen subunit vaccines, which are specific parts of the pathogen recognized by the immune system. These antigens are produced using modified host cells in a fermentation process and at harvest, the host cells are commonly disrupted, releasing the antigen plus host cell impurities produced inside the cell. Efficient removal of these impurities is essential to ensure quality and safety of the final vaccine, and is performed in downstream processing, most commonly by multiple chromatography separation and purification steps. Chromatography uses binding of molecules based on physicochemical properties like charge, hydrophobicity and size, allowing tor very specific separation. Optimizing this separation currently requires time and resource intensive experimental screenings, making the process expensive. This project aims to provide computational methods allowing the screening of different possibilities limiting otherwise required experimental resources.

Quantitative Structure Property Relationship models can identify and relate specific properties trom a molecular structure to chromatographic behavior. By predicting the behavior of the host cell impurities and the target antigen, an initia! selection can be made for the purification process betore doing any experiments. Dedicated software was developed in this project to calculate specific protein descriptors tailored to the prediction of chromatographic behavior. Using this software, successful models were trained to predict protein binding tor different modes of chromatography. Additionally, parameters were predicted allowing accurate mathematica! simulations of protein chromatography separation and purification. Finally, the prediction of host cell protein behavior in a complex mixture was achieved, bringing fully computational process development and optimization of vaccines closer to reality.

Unravelling Fabry disease: establishing toxicity of lysoGb3 and identifying additional toxic storage compounds

(CHEMIE.PGT.2021.005)
Organisation: Leiden University

Fabry disease is the most common lysosomal storage disorder caused by a defective enzyme α-galactosidase A (GLA). The enzyme GLA has been thought to only degrade the lipid Gb3. The symptoms of FD are still poorly understood and do not fit with those of patients with a comparable lipid accumulation. The project attempted to get further insight using a generated model of FD in zebrafish (knock-out of the gla gene). The study has provided indications that a second substrate for the enzyme GLA exists beside the lipid Gb3. This finding provides arguments for the best choice of treatment of FD. That means, providing patients with enzyme to allow degradation all accumulating substrates. This can be achieved by enzyme infusion or by AAV5-based gene therapy.

Iron fuel: a clean and circular energy carrier (MEC II)

(CHEMIE.PGT.2022.005)
Organisation: Eindhoven University of Technology

To develop a new iron powder based (Iron Power Cycle) energy carrier, the technologyis is shown at TU/e lab scale but needs to be developed at larger (size and TRL) scale.

This technology deals with a combustion system D26for producing steam from iron powder and a (rotating-drum based) iron-oxide conversion system back to iron powder using (green) hydrogen.

The combustion system has been improved significantly, recoverability improved, partly automated and long duration test executed with success (see first figure below for the current system).

The rotating drum (second figure below) is developed, built and tested recently, but not completely operating well enough yet at high temperatures in hydrogen atmosphere. This needs to be addressed before cyclic tests will be performed in the remaining part of the program the coming year.

The CO2WA program: the development of new technology for water electrolysis and the capture, compression and conversion of CO2

(CHEMIE.PGT.2022.012)

Organisation: Delft University

The aim of this project is to develop technologies to turn renewable electricity into useful fuels and chemicals. One part of the project is to make a leap forward in the conversion of water into hydrogen. This happens in equipment using a membrane, where this membrane is typically the weak spot for efficiency and lifetime. We seek to improve this significantly. Also other ways to increase the efficiency - for example using magnetic fields – will be investigated. The second part is to convert CO2 into useful chemical using electricity. We seek to efficiently integrate this process with capturing CO2 from the air.