



Projects with PPP programme allowance 2019

FOAMEX-II + DISCOVER-II

(CHEMIE.PGT.2018.016)

Organisation: Wageningen University & Research

FOAMEX-II: Advances in foam extrusion of PLA

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development of an environmentally friendly alternative to bituminous roofing systems, in which the fossil bitumen has been replaced by biobased raw materials.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.

Modular, designer polydopamine adhesives for facile and versatile surface conjugation of functional polyethylenes

(CHEMIE.PGT.2019.016)

Organisation: DPI

CPolydopamines (PDA) are a popular class of materials and promising candidates as adhesives for new fastening techniques. PDA layers can be formed on any substrate, as e.g. seen in marine environments. PDA sticks to plastic or natural waste, or even underwater constructions.

We developed a novel method for functionalizing PDA-based copolymer films. The PDA-based polymer macro-initiator is developed for grafting from a surface using surface polymerization or grafting to a surface using click chemistry. These ingredients have provided a platform through which a variety of substrates have been successfully functionalized. These functionalizations include antifouling or photonically engineering, creating a toolbox that can provide many different properties to many unlike surfaces.

Kristalheldere analyse voor spiegelbeeld moleculen

(CHEMIE.PGT.2020.001)

Organisation: Amolf

This TKI project has led to practical proof-of-concept and benchmarking of a new analytical technique to determine crystallization behavior of mirror image molecules using a new technique called Rapid Analysis of Phases (RAP). Using 4 different

compounds, we determine for two most common crystallization types with RAP (racemic compounds and conglomerates, partially provide by collaboration partner Syncom (now Symeres)) and compared these measurements with current state-of-the-art methods (classical ternary phase diagram methods as describe by Collet & Wilen Enantiomers, Racemates and Resolutions). For all cases we found that RAP gave comparable results as the state-of-the-art, but with the advantage that only fraction of material was required (350 mg instead of grams).

Energie-absorberende kern (Energy absorbing core)

(CHEMIE.PGT.2020.002)

Organisation: Hogeschool Windesheim

The waste streams that cannot be recycled to the original applications are still considerable. Examples of these waste streams are composites (e.g. rotorblades for wind milles), mixed plastics (heterogeneous thermoplastics waste) and old car tyres. Solutions for re-use must be developed for a circular society.

In the project energy-absorbing cores have been developed that can be used in structural applications. It is investigated how such cores can be made from mixed plastics or from old rubber car tyres.

The use of car resulted in successful solutions. In a demonstrator guiding beam for ships it was shown that an internal core made of folded rubber car tyre tread worked very well for energy absorption. Other parts or other shapes of parts from car tyres were not found applicable in the tests.

The use of mix-plastics to manufacture an elastic and energy-absorbing core was found not to be succesful. With a specially developed low-pressure extruder the resulting core material remained too dense and not suitable for energy absorption. With other techniques the density could be lowered but then the core material was too weak to use.

Kinase activation on the FGF pathway

(CHEMIE.PGT.2020.007)

Organisation: Utrecht University

When viruses infect host cells an intricate war between species is started, with the aim of the virus to replicate itself, whereas the host cell aims to survive this viral attack. It is well known that as part of this battle, these viruses modify host kinase activity during infection. To visualize these battles, we developed proteome-wide kinase activity assays providing a detailed overview of the (de)regulation of cellular kinases during picornavirus. This led to the identification of many of the kinase actors. Next, using pharmacological kinases inhibitors, we demonstrate that several of the activated

kinases are essential for the replication of EMCV, and thus our data provides a resource important for developing novel antiviral therapeutic interventions.

Improving analysis of (tool) compounds for treatment of cystic fibrosis to determine mode of action

(CHEMIE.PGT.2020.008)

Organisation: Utrecht University

Cystic Fibrosis (CF) is a lethal inherited disease caused by mutations in the CFTR gene. In the past 10 years, some small-molecule medicines have become available that modulate the defective CFTR protein, and offer all but a cure to a majority of CF patients. Trikafta is this current, highly effective therapy for many people with CF. It consists of two small-molecule corrector drugs and one potentiator. The correctors repair the defective CFTR protein, which allows it transport to the cell surface, where the potentiator boosts CFTR function as chloride channel. While Trikafta has turned many "CF patients" into "people with CF" who lead relatively healthy lives, an appreciable number of patients is not helped by Trikafta.

AbbVie identified a novel corrector that is potent in rescuing the most prevalent F508del-CFTR mutant from degradation by the cell. Using antibodies and assays we have developed (Im et al, Cell Mol. Life Sci 2022), we found that the new corrector compound rescued the F508del mutant to 85% of wild-type CFTR. This dramatic increase in transport to the cell surface with a single corrector has not been seen before. We discovered that the corrector improved late stages in the folding of CFTR in a unique manner involving the linker between two first domains of CFTR.

In follow-up work we are investigating whether the new corrector compound can act synergistically with other correctors, and we are zooming into the new compound's effects to get a better understanding of the precise mode of action.

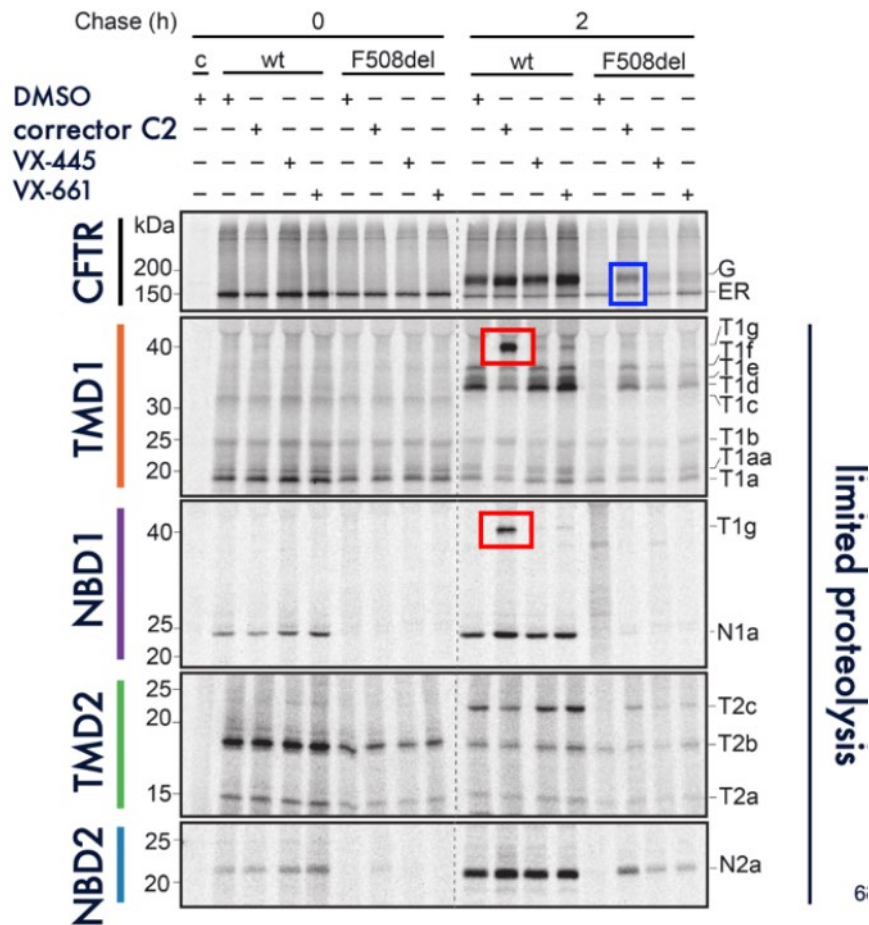


Figure legend; Upon viral infection host cells display alike kinome rewiring upon picornavirus infection by either CVB3 or EMCV

Cells expressing wild type CFTR or the CFTR F508del mutant were treated with clinical correctors VX-661 and VX-445 or experimental corrector C2. After a short labeling period with radioactive methionine/cysteine, cells were chased for 2 h or not in non-radioactive medium and lysed. Lysates were subjected to limited proteolysis with 10 µg/ml proteinase K, and fragments were immunoprecipitated with antibodies against the 4 different CFTR domains and analyzed by SDS-PAGE. Note 1) the conspicuous improvement of F508del signal in the presence of corrector C2 after 2 h of chase and 2) the stabilization of a T1g fragment in TMD1 and NBD1 immunoprecipitations, which is not seen with VX-445 and VX-661.

Fundamental studies on bifunctional catalysts and catalysis

(CHEMIE.PGT.2020.009)

Organisation: Utrecht University

Hydroconversion is a key step in the production of ultraclean fuels from renewable sources such as biomass and waste. However, this reaction is carried out with the use of an expensive and scares metal, platinum. In this project we showed how the amount of Pt that has to be used for effective conversion can be minimised, by controlling exactly

the spatial distribution of the small metal clusters. Additionally we found that to some extent it can be replaced by less scarce metals, such as nickel and copper, when mixed in the optimum ratio.

An Analytical Study of Biorefinery Lignin – part 2 / Wat is die lignine toch? Deel 2.

(CHEMIE.PGT.2020.010)

Organisation: Utrecht University

Universiteit Utrecht en Avantium werken aan het ontrafelen van de chemische structuur en samenstelling van een bijzondere bioraffinage lignine. Bioraffinage, het scheiden van de verschillende componenten van niet-eetbare biomassa, leidt vrijwel onvermijdelijk tot verandering in de structuur van een van de ligninecomponenten. De precieze verandering is afhankelijk van de bioraffinagemethode en moet per methode worden onderzocht. Fundamenteel inzicht in de structuur van lignine is nodig om processen te kunnen ontwerpen die deze omvangrijke stroom kunnen omzetten in waardevolle materialen.

Operando Characterization of Coke Deposits within Light Alkane Dehydrogenation Catalysts by Time-Gated Raman Spectroscopy

(CHEMIE.PGT.2020.011)

Organisation: Utrecht University

Propane dehydrogenation is an important method for the production of propylene, a key building block in chemical industry. This reaction is commonly facilitated by Pt-Sn based Al_2O_3 supported catalyst materials. Unfortunately, the catalyst is not (yet) perfect, especially with respect to its stability. Propane is not only converted into propylene, but also in unwanted side products. These side products form carbon deposits, also known as coke, on the surface of the catalyst material. The active sites at which propane is converted are covered and blocked by these coke deposits.

Therefore, the formation of coke deposits leads to the degradation of the performance of the catalyst material. The formation of coke can be studied with Raman spectroscopy. Unfortunately, Raman scattering is an intrinsically weak process that is often overshadowed by fluorescence. Time-gated Raman spectroscopy was developed in this project to suppress the fluorescence and record Raman spectra with a higher quality. We have applied the time-gated Raman technique to study catalysts in action during propane dehydrogenation. We tracked coke build-up over time on the catalyst material and showed that time-gating indeed yields Raman spectra with a weaker fluorescence background. The developed time-gated Raman spectroscopy results in a better understanding of the formation of coke during catalysis in industrially relevant conditions. More insights in coking behaviour gives new leads for the rational design of more stable light alkane dehydrogenation catalysts that are less susceptible to coking.

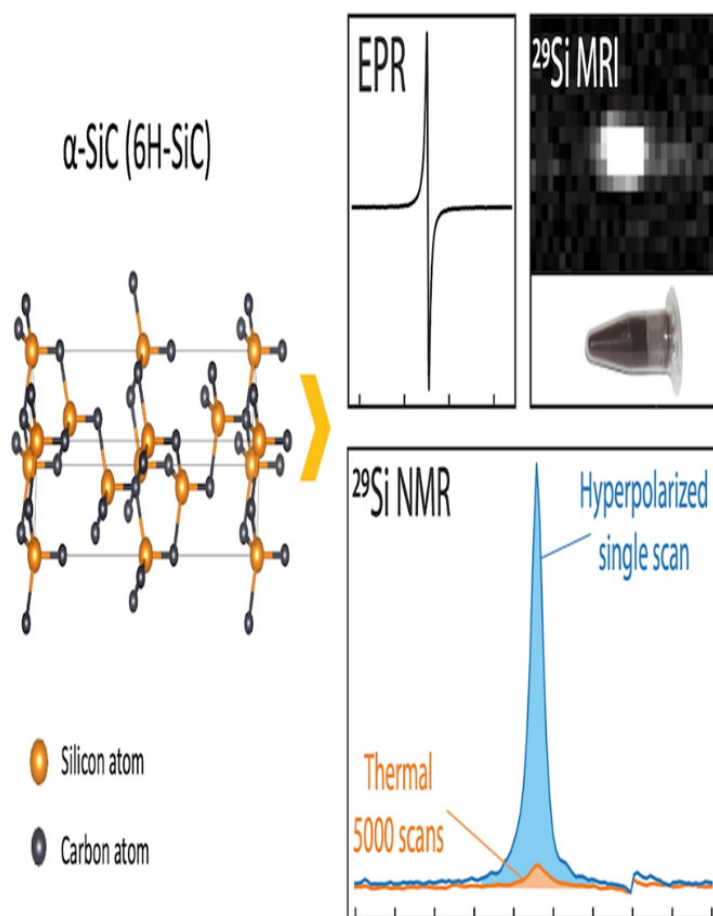
Hence, the efficiency of the propane dehydrogenation can be improved and the environmental impact of the process can be lessened.

Hyperpolarized Silicon Nanoparticles in Targeted Magnetic Resonance Imaging

(CHEMIE.PGT.2020.013)

Organisation: Universiteit Twente

Magnetic Resonance Imaging (MRI) provides excellent anatomical information, but severely lacks sensitivity, limiting its application potential. Hyperpolarization is a technique with which the signal intensity can be increased by orders of magnitude. This technique is already being used in the clinic, but a major downside is the very brief nature of the hyperpolarized state: the high signal intensity remains for only a couple of minutes. Owing to their unique isotope composition, silicon particles remain hyperpolarized for prolonged periods of time, up to hours. In this project we have successfully developed silicon nanoparticles for hyperpolarization MRI and developed strategies to ensure their stability in relevant media, as well as reducing their toxicity to a minimum.



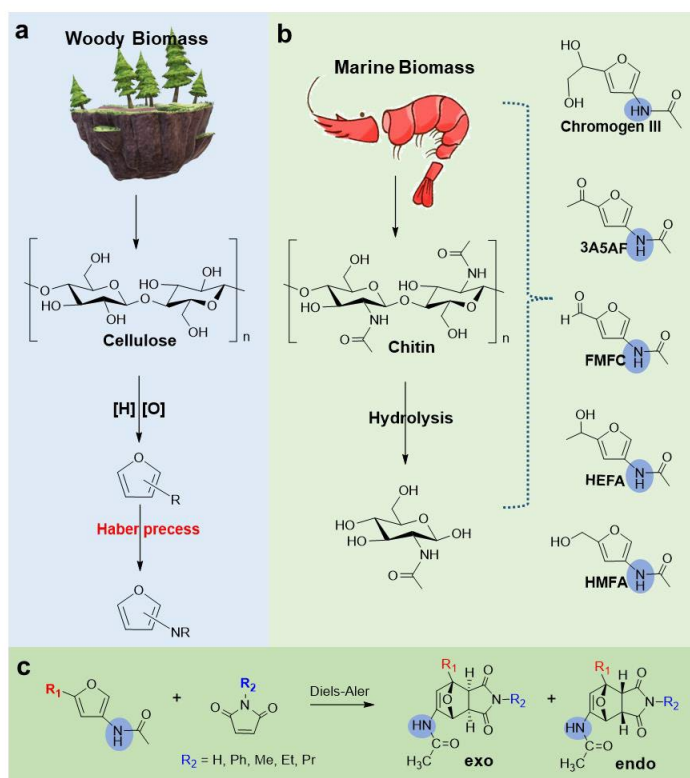
Gefunctionaliseerde aromaten uit garnalendoppen

(CHEMIE.PGT.2020.014)

Organisation: Rijksuniversiteit Groningen

Chitin, the second most abundant polysaccharide on earth and a component in 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 exoendo selectivity. The introduction of electron-rich groups (e.g., -OH) into furans led 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.



Hybrid semiconductor-insulator nanostructures for spectral conversion

(CHEMIE.PGT.2020.015)

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 life times 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.

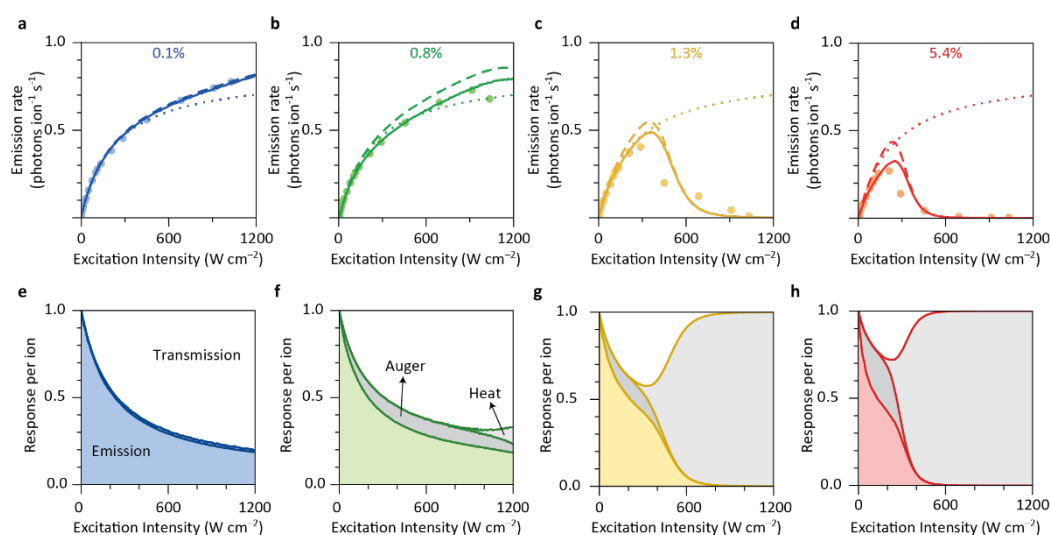


Figure 1 – Different processes limiting the brightness of Mn⁴⁺-phosphors with a long emission life time.

Preventing pollution by pesticides

(CHEMIE.PGT.2020.019)

Organisation: Universiteit Amsterdam

Pesticides are sprayed onto crops in the form of drops; how do we prevent these from polluting surrounding areas and the surface waters? A promising method is to add an environmentally friendly substance (a ‘tank-mix additive’) that influences the droplet size of the spraying agent, as well as improving coverage of the plants by the spray. The research done in this project is a collaboration between the University of Amsterdam

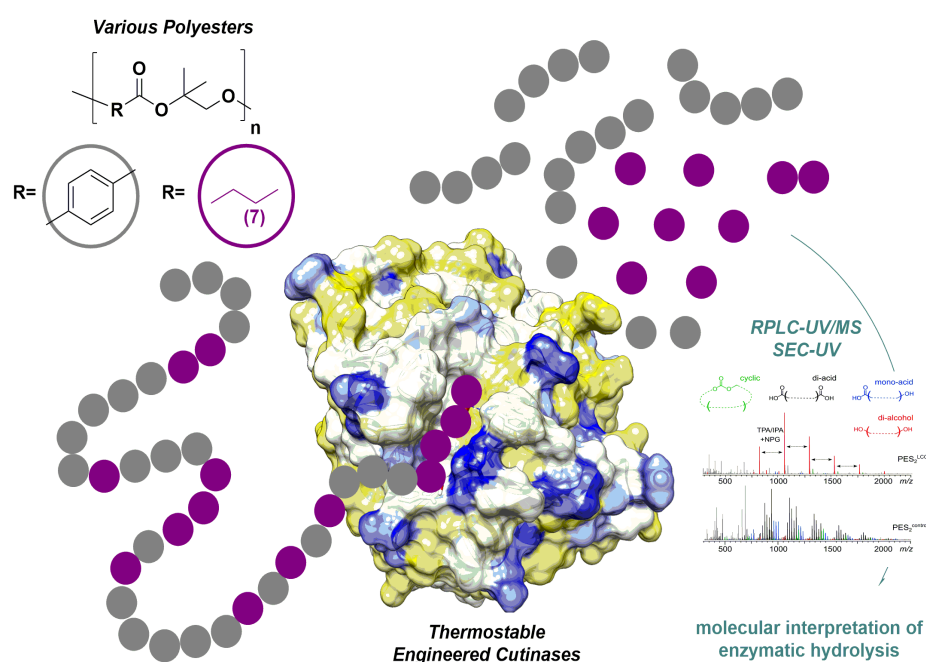
(Daniel Bonn, Institute of Physics) with the industrial partner GreenA (Maarten Klein, CEO) that successfully markets such an additive for tractor and backpack spraying. The project set the first steps to use the existing know-how and recent breakthroughs in understanding spray physics to see whether a similar additive can be developed for aerial spraying, which is still one of the main ways pesticides are sprayed.

Enzymatic Depolymerization of (synthetic) Polymers (EnDeP)

(CHEMIE.PGT.2020.020)

Organisation: Universiteit Amsterdam

The accumulation of plastic materials in the environment and their efficient recycling are essential challenges of today's society. Therefore, over the past decade, academia and industry have tried to develop new plastics that are biodegradable. However, the replacement of traditional plastic materials with biodegradable alternatives is not always possible. In fact, there are engineering applications that require conventional polymers because of the mandatory superior performance. Fortunately, it seems that the degradability of the traditional polymers can also be tuned. The biodegradability and performance of polymers are, however, related to their structural properties. Surprisingly, the performance properties of these polymers relative to degradability have not been elucidated in sufficient detail. Therefore, the TKI EnDeP project has developed new biocatalysts (enzymes) for the selective ("chemically controlled") degradation of polyesters homo- and copolymers of industrial importance. EnDeP also delivers an analytical work-flow for the determination of polymers sequences and composition that are the main factors influencing the degradability. In summary, EnDeP contributed to generating knowledge to understand the process of depolymerization of synthetic polymers, provides a toolbox of biocatalysts for polyesters recycling, and an analytical chemistry methodology for the analysis of synthetic polymers.



INTERACT (Interface Catalysis for Advanced Sustainable Chemistry)

(CHEMIE.PGT.2020.021)

Organisation: TU Eindhoven

NO_x, 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 could stem from transformation of inactive 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. After a steam treatment the performance remained almost unchanged. In contrast, catalysts treated in a custom built setup that can mimic realistic exhaust gas and conditions had a drastically reduced performance and characterization showed major changes in the catalysts structure.

Towards a circularity in recycling of polyurethanes

(CHEMIE.PGT.2020.022)

Organisation: TU Eindhoven

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: TU Delft

With the growing world population and the ease of international travel, the risk of global outbreaks of infectious diseases increases. To combat and prevent possible pandemics, vaccines are among the best options. This project focusses 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 for 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 from a molecular structure to chromatographic behavior. By predicting the behavior of the host cell impurities and the target antigen, an initial selection can be made for the purification process before 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 for different modes of chromatography. Additionally, parameters were predicted allowing accurate mathematical 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.

Real-Time Sensing

(CHEMIE.PGT.2020.024)

Organisation: TU Eindhoven

We have investigated a sensing technology for the continuous monitoring of biomolecules for food processing applications. The sensing method is based on the measurement of small particles that change their motion properties due to biomolecular binding. The chemical properties of the sensor were adapted so that specific biomolecular substances could be measured. Prototype sensors were developed for the continuous monitoring of a specific small molecule and a protein.

Process simulations were studied for real-time control concepts. Sensors were tested as a proof of concept that the sensing technology is applicable for food applications.

The impact of inhomogeneous electrode reactions on battery cycling

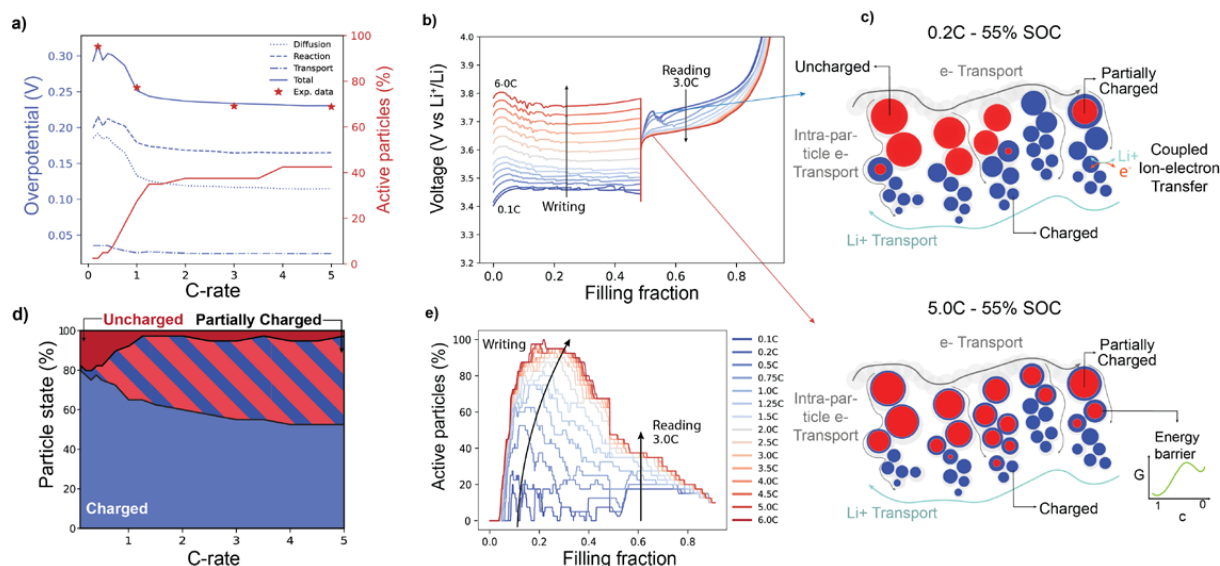
(CHEMIE.PGT.2020.025)

Organisation: TU Delft

In this project we focussed on the role of heterogeneous reactions in the performance of future Li battery systems focussing (1) on cathodes and (2) on next generation Li-metal anodes.

(1) Heterogeneities in commercial electrode materials were studied, including LFP, LTO, and NMC. The results reveal unexpected behaviors in materials undergoing phase separation, characterized by their thermodynamic tendency to form Li-rich and Li-poor phases. Remarkably, these materials exhibit an “activation” effect during faster (dis)charging pulses, resulting in a heterogeneous kinetic memory effect through an inverse correlation between overpotential and the prior (dis)charge rate. These results are directly applicable to practical battery operations and highlight the importance of accounting for phase separation phenomena when designing and operating lithium-ion batteries.

(2) High energy density Li-metal anodes induce a heterogeneous solid electrolyte interface (SEI) that largely determines the faith of the performance of these systems. Here we investigated the role of electrolyte composition on the SEI at Li-metal anodes. We discovered the synergistic role of specific additives, and developed a multi salt approach that has large potential to improve Li-metal performances.



Towards zero-emission processes in microbial biotechnology

(CHEMIE.PGT.2021.003)

Organisation: TU Delft

In industrial biotechnology, microorganisms convert predominantly sugars into a wide range of valuable products. Typically, about 50 % CO₂ is co-produced. This project, however, investigated microbial production from CO₂ using solar/wind electricity, to reach sustainable production. Various steps of this new production chain were developed in the laboratory and the overall chain was analysed using model calculations, showing promising options in case of modest electricity prices.

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

(CHEMIE.PGT.2021.005)

Organisation: Universiteit Leiden

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.

DREAMS: Derivatives of Renewable Estolides for Advanced Materials for Sustainability

(CHEMIE.PGT.2021.014)

Organisation: WUR

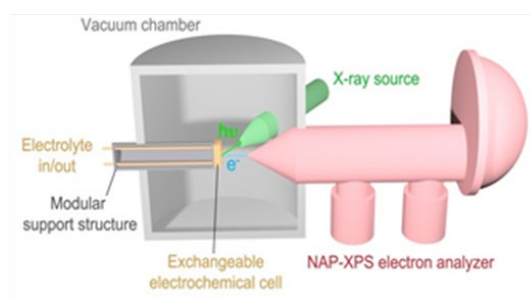
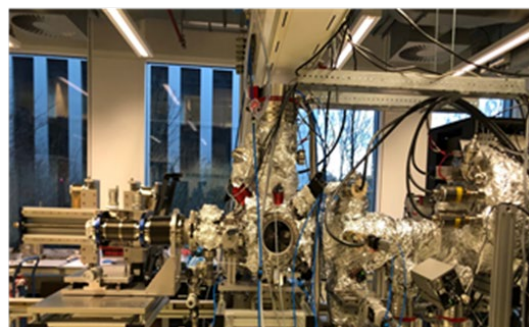
DREAMS aims to generate knowledge about bio-based alternatives for petrochemical polyurethane elastomers. Targeted applications include sports-/footwear, coatings and sealants. The project partners Wageningen Food & Biobased Research, Archer Daniels Midland, Will & Co, and Adidas aim to: - replace petrochemical elastomer building blocks with alternatives derived from vegetable oils - move away from toxic isocyanate chemistry and use more benign two-component reactivity: - improve elastomer performance in terms of mechanical/physical properties, carbon footprint, and recycling/reuse potential. Enzymatic catalysis plays a crucial role in the project. It will be used to convert vegetable oils to safe-by-design building blocks for the novel materials and to explore breakdown of the materials into reusable chemical building blocks, facilitating recycling. Matching the outstanding material performance of polyurethanes will be a challenge. Scientific knowledge will be generated on how the materials' chemical structure relates to performance attributes such as elasticity, strength, abrasion resistance and durability.

Near-Ambient X-Ray Photoelectron Spectroscopy for in situ studies of corrosion of platinum electrodes

(CHEMIE.PGT.2022.002)

Organisation: Universiteit Leiden

In this project, scientific instrumentation was developed that makes it possible to visualize the chemistry that occurs in electrochemical devices. We have demonstrated that the instrument is suitable to study the behavior of the electrodes used in devices ranging from batteries to fuel cells and electrolyzers. Here, however, the focal point was the study of Pt(alloy) electrodes. We have shown that these materials change their structure depending on the employed reaction conditions.



No longer ‘too hot to handle’: microscopy of heat-loving microorganisms

(CHEMIE.PGT.2022.006)

Organisation: Universiteit Leiden

In this project Leiden University and microscopy company Confocal.nl collaborated to visualize and study heat-loving organisms at high temperatures at high spatial and temporal resolution. A microscope combining Rescan Confocal Microscopy technology and high-temperature heating chambers was designed and constructed. With this microscope fundamental studies of the cell biology of such organisms under physiological conditions are now possible, aiding in establishing them as model organisms and industrial production vehicles. Furthermore, the established approach extends to application of super-resolution rescan confocal microscopy to other biological and non-biological systems (e.g. in materials science) that require high temperatures.

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

(CHEMIE.PGT.2022.012)

Organisation: TU Delft

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.

CIRCPET = 100% recyclable PET trays

(CHEMIE.PGT.2022.028)

Organisation: DPI

PET-trays are a major packaging type and is growing in use. The recycling of this type of packaging is problematic, because it is collected in the general post-consumer waste collection (source or subsequent separation) and the packaging is not designed for recycling; it consists of different types of plastics with a lidding film consisting of LDPE.

This project focused on the material aspects; design a 100% PET tray and investigate rPET application. Most of the research related to the design was focused on sealing properties of PET based lidding film. For meat-application a lock-seal (peel force $\geq 20\text{N}$) was needed. With a 100% PET lidding film this was not possible to reach; a lidding film

with a PU sealing agent gave a lock-seal, but this turned out not industrial applicable because of the needed sealing temperature-time combination. Modification of the PET-seal layer is needed; this research gave enough information to enable applicable results in a new research project.

Application of rPET was researched based on various post-consumer sorted PET streams. The short conclusion was that Magnetic Density Separated PET did not deliver a source for rPET, as this was too contaminated. In our research only rPET from bottles (Wellman) was perceived as good rPET for food application.



AquaSurf: Plastic waste stream characterisation methods for moisture & surface contamination

(CHEMIE.PGT.2022.029)

Organisation: NTCP

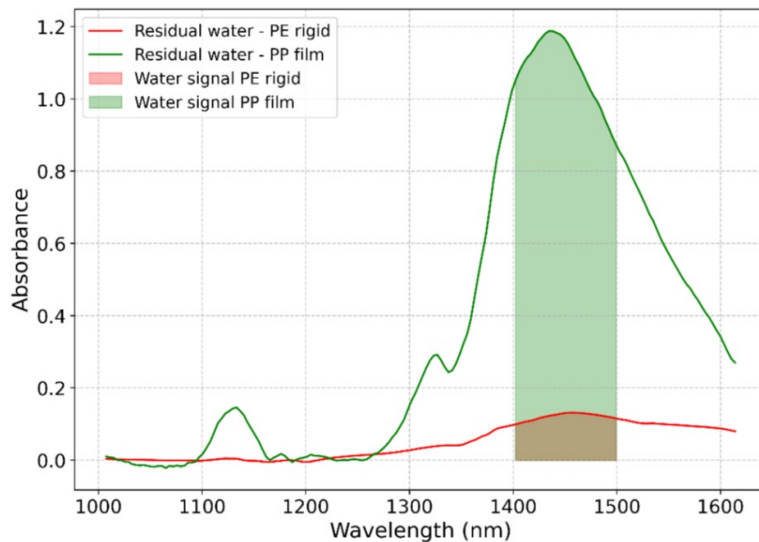
Surface contamination in plastic packaging waste

Recycling is increasingly recognized as the future of plastic waste management to meet the growing demand for plastics. However, the efficiency of recycling processes is significantly impeded by surface contamination on plastic waste. This contamination encompasses a wide array of materials, including biogenic substances, inorganic residues and other pollutants. Accurate quantification of surface contamination is essential to enhance the efficiency of plastic waste recycling. Despite its importance, there is a notable scarcity of quantitative data on surface contamination throughout the recycling chain. Furthermore, the complexity of surface contamination presents

substantial challenges in developing rapid, simple, and accurate quantification methods for various waste streams. Several approaches have been explored, namely HSI-NIR spectroscopy, Raman spectroscopy and electrical conductivity. Herein we show the development of a procedure to quantitatively assess surface contamination on household packaging plastic waste. The most promising method is by measuring the electrical conductivity of wastewater and correlating that with known levels of surface contamination across various plastic types (PE and PP films and rigids, and PET), we demonstrated a strong linear relationship, with R^2 values ranging from 0.87 to 0.96, suggesting conductivity as a reliable proxy. Moreover, the results showed that different types of plastic exhibited distinct conductivity responses based on their ion contamination profiles, as confirmed by ion chromatography. Inline conductivity measurements on PP rigid flakes in a pilot-scale washing facility validated the approach, showing dynamic adjustments to the washing process based on real-time contamination levels. Overall, the developed method is efficient, simple, and scalable for assessing surface contamination. Further research should focus on refining this model and exploring the interaction of contamination components with wastewater conductivity for broader application in recycling facilities.

Moisture content in plastic packaging waste

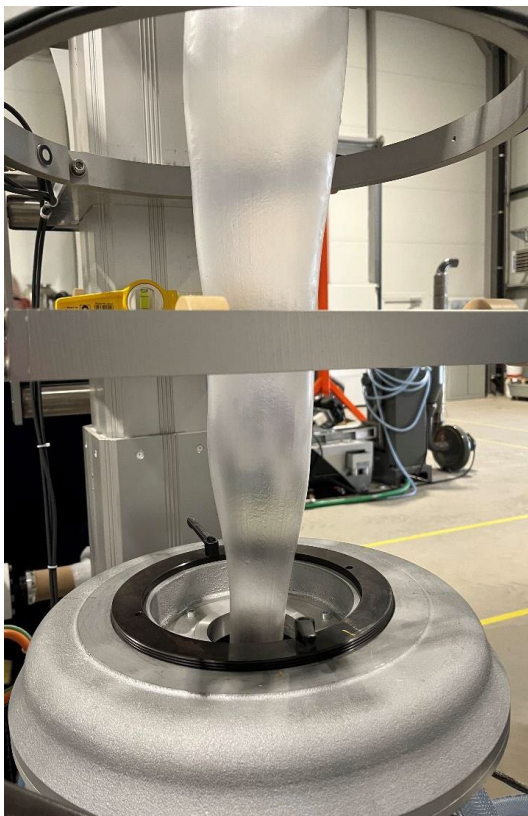
Quantifying moisture in plastic waste is crucial for optimizing recycling processes and improving the quality of recycled materials. Conventional methods, such as gravimetric analysis, are laborious and energy intensive, limiting their efficiency in high-throughput industrial environments. This study presents and validates the use of near-infrared spectroscopy hyperspectral imaging (NIR-HSI) as a rapid, non-destructive method for moisture analysis in household plastic packaging waste (i.e., PE and PP films and rigids, PET, mixed plastics). By utilizing a NIR-HSI camera on a data collection conveyor belt, samples with varying moisture levels were analyzed. The method employs univariate calibration, correlating NIR absorbance from water with moisture concentration determined by the standard gravimetric method. To ensure accuracy, the NIR absorbance from water was isolated by identifying and eliminating polymer-related absorbance through peak annotation. Principal component analysis (PCA) was subsequently applied to distinguish between rigids and films. Further refinement was achieved by normalizing the spectra and subtracting a dry reference spectrum, effectively eliminating the polymer signal. This approach enabled accurate quantification of moisture content and provided spatially resolved information on moisture distribution, including subsurface moisture. The method was successfully implemented in a pilot-scale sorting facility, where 95% of measurements achieved an accuracy within 2.6 percentage points. This integration underscores the significant potential of NIR-HSI for inline analysis and real-time feedback in recycling operations, offering significant advancements for future research and industrial applications in plastic waste recycling.



Multiflex

(CHEMIE.PGT.2022.030)

Organisation: Universiteit Maastricht / NTCP



In this study we started from a commercially available sorted PP film streams from household packaging waste to investigate the potential for mechanical film-to-film recycling. In our manual composition analysis we showed that the stream consists of approximately 30-40% monolayer and transparent PP film material that we considered suitable for this recycling route. By using optical sorting, we were able to create a stream of almost 80% transparent PP film on object basis. Taking the sorted materials, we assessed the mechanical properties of films produced by film blowing after compounding with a certain amount of virgin PP. The presence of contaminants such as ink, metals and paper present in the compound drastically impacts the processability for film blowing. The highest achievable yield (from sorting to a blown film) to realize film-to-film by

means of film blowing is not higher than 10%. This does not yet include the yield achieved from collection to sorting. Knowing that this leads to a film with poorer mechanical properties than virgin material, film-to-film recycling of PP seems not yet a viable option.

HOPY

(CHEMIE.PGT.2022.033)

Organisation: Universiteit Twente

The Headstart on Pyrolysis project (HoPy) focused on two main areas. First, DKR350-like plastic streams from a previous Circular Plastics Initiative project were pyrolyzed using a fluidized bed reactor, investigating amongst others the effect of hot vapor residence time. This oil was analyzed for composition and this information, along with publicly available data, was incorporated into a modular economic decision model. The development of this Excel model, the second main area of this project, was supported by public information and expert insights (for example on specifications). The model provides the user insight into optimizing the recycling pathway for DKR350 between pre-treatment of the plastic feed, pyrolysis, and post-treatment of the oil. Initial results suggest that costs could be reduced when more emphasis is placed on post-treatment. The model can potentially be adapted to other waste streams and custom inputs.

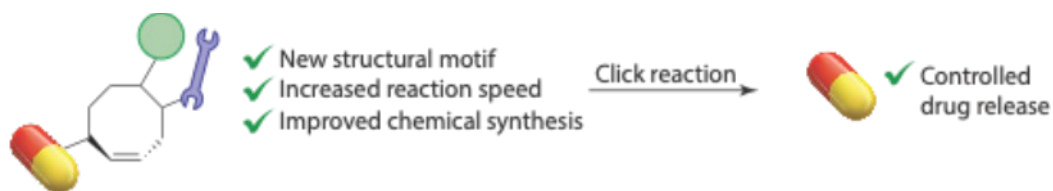
Novel click-to-release strategies with trans-cyclooctenes

(CHEMIE.PGT.2024.002)

Organisation: Radboud University

The Nobel Prize in Chemistry 2022 was awarded to Carolyn Bertozzi, Morten Meldal and Barry Sharpless for the development of click chemistry and bioorthogonal chemistry. These types of elegant and efficient chemical reactions bind two molecules together.

The most promising click reaction partners involve the coupling of trans-cyclooctenes (TCOs) to tetrazines. These TCOs can be functionalized to release a third molecule after its click reaction with tetrazine in a so-called click-to-release reaction. These types of molecules open up a whole new field of applications, building forth on the current use of regular click chemistry in medicinal & material sciences. In this project, novel click-to-release strategies with TCOs are studied to create molecules with better properties for reaching the full potential of click-to-release applications. This was done by synthesizing new TCOs having a different structural motif and testing its click-to-release capabilities.



Wood to Wheels: Bridging Biomass and 1,3 butadiene in flow-chemistry

(CHEMIE.PGT.2024.027)

Organisation: Universiteit Maastricht

Our research explores a sustainable way to produce butadiene, a key material for rubber and plastics, from a plant-based compound called GVL. Instead of traditional energy-intensive methods, we investigated a light-driven process. While our initial approach showed limited success, an alternative method effectively broke down the compound but produced a complex mixture. Encouraged by this, we optimized the process using visible light and confirmed the formation of reactive radical intermediate, which behaved as expected. These findings provide valuable insights for developing a greener butadiene production method.

