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TNO-rapport

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Meerjarenprogramma 2018-2021 Topsector Chemie Activiteitenplan 2018

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1.1 Summary

In line with the needs of the industry and the ambitions of the Topsector Chemie TNO's program Sustainable Chemical Industry focuses on developing technology and new business models in three mission-driven Public Private Partnerships being Biorizon, VoltaChem and Brightlands Materials Center, whilst exploring novel topics like digitization and recycling in relation to these partnerships.

We will, for the period 2018-2021, continue to strengthen these partnerships and further embed them in regional, national and international innovation ecosystems:

1. **Biorizon** targets the development of aromatic molecules, an important building block for polymers, out of biomass and the connected values chains where scale up of the processes is the key focus in order to demonstrate the technologies in close cooperation with the industry and the ecosystems. At the end of 2018 the waste to aromatics technology should reach the TRL 5 and the Diels-Alder chemistry will be further expanded for bi- and trifunctional aromatics. At that time will be able to provide 1-5 kg samples to the partners for application development.

2. The focus of **VoltaChem** is electrification of the chemical industry. Key intermediates in the plastics, fuels and fertilizers value chains are the target for electrification system studies and application of electrochemistry, electrocatalysis and electrochemical engineering together with downstream processing. These activities will be business case driven and piloting activities will be a key element in close cooperation with regional chemical clusters. Technologically we aim to have demonstrated by 2021 paired electrosynthesis of key plastic intermediates and high value chemicals together with industry and academia. Therefore proof-of-principle regarding paired electrosynthesis, further expansion of the network and the equipment and know-how base are the key elements for the program next year.

3. **Brightlands Materials Center** will provide solutions in its Sustainable Buildings line to improve the energy efficiency of buildings with novel materials for the building envelope that can regulate the energy in- and output in an adaptive manner. These solutions will contain coating technology or polymer films with nanoparticles to create nanocomposites. Synthesis, characterization, functionalization and controlled integration of these particles and the demonstration of the functionality in the actual application will be the goal of the program. In 2018 the focus will be on the development of infrared regulating coatings and polymer foils at temperatures at around 35 °C. Furthermore, it will provide solutions to the automotive value chain in its Lightweight Automotive line where predictive material performance, the use of recycled materials and design to recycle of thermoplastic composites play a central role.

These activities fit within the newly identified Topsector themes "Waarde uit Biomassa", "Electrochemical Conversion & Materials" and "Soft Advanced Materials" and are fully compliant with the societal challenges, key enabling technologies and NWA-routes in which the chemical sector will play a crucial role.

1.2 Introduction

The challenge of the Dutch Topsector Chemie is to contribute to the societal transition towards a carbondioxide neutral circular economy with sustainable energy sources in the coming 30 years, whilst remaining competitive during this transition. Therefore, the goal that the Topsector has set itself in its KIA is: “in 2050 the Netherlands is known as *the* country for green & sustainable chemistry” and “smart materials with high added value whilst providing smart solutions”. This context and goal, the continuous discussion with our stakeholders and our competences and facilities together determine the focus of the program Sustainable Chemical Industry at TNO.

Recently, the Topsector has identified new high-level focal themes that will contribute to its goals, based on existing roadmaps, societal challenges and key enabling technologies. This renewed focus will most likely further facilitate growth and interaction between public private networks and thereby accelerate innovation. The themes that were identified (especially “Waarde uit Biomassa”, “Electrochemical Conversion & Materials” and “Soft Advanced Materials” and the “Go-Chem” initiative) form a perfect landing platform for the three mission-driven Public Private Partnerships that TNO, with public and private stakeholders, has initiated successfully in the previous period.

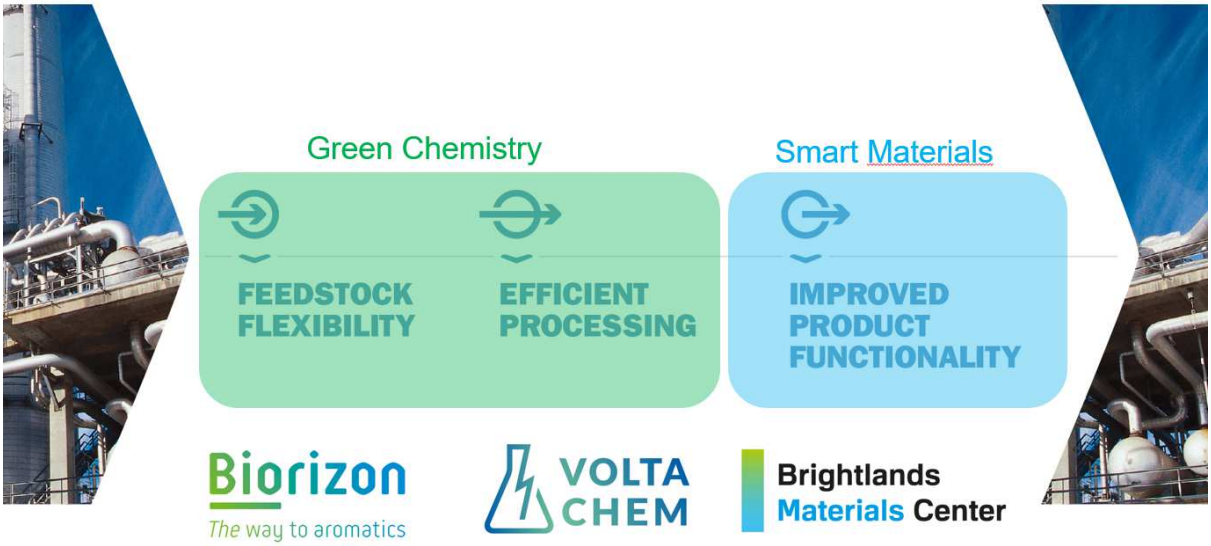
The program of Sustainable Chemical Industry will therefore, for the period 2018-2021, continue to strengthen and expand these three existing mission-driven Public Private Partnerships (PPPs), further embed them in regional, national and international innovation ecosystems, and at the same time explore new or enabling topics that will add to their strengths:

1) **Biorizon** targets the development of technology and value chains that convert biomass into aromatics. Here, TNO is focused on “Sugar-2-Aromatics” using Diels-Alder chemistry for the production of functionalized bio-aromatics from biomass-derived furanics.
2) **VoltaChem** targets the development of technology for and ecosystems around the electrification of the chemical industry. Here, TNO is focused on using electrochemistry for the production of chemical building blocks that can be used in plastics, fuels and fertilizers.
3) **Brightlands Materials Center** targets the development of advanced materials that regulate the energy consumption and generation within the building envelope as well as the improvement of thermoplastic composites for automotive applications.

Within the context of these PPPs the program will explore topics such as digitization and (chemical) recycling of plastics/composites and energy storage in chemicals.

1.3 Description

In the below diagram the relationship of the three PPPs within the program Sustainable Chemical Industry, the goals of the Topsector and the needs of the chemical industry are shown.



The overall goals of this program for the period 2018-2021 are to contribute to:

a) Intensified ***triple-helix collaborations*** with industry, academia, RTO's and regions in Joint Innovation Centre's, one for each PPP.
b) Realization of ***piloting infrastructure*** (TRL 5-6) for the key technologies (electrochemistry, Diels-Alder chemistry and nanoparticle synthesis & surface functionalization).
c) Delivery of prototypes of ***sustainable chemical building blocks and smart materials***.
d) ***Strengthened knowledge & IP position*** in the fields of green & sustainable chemistry and smart materials in order to provide industry with competitive solutions.

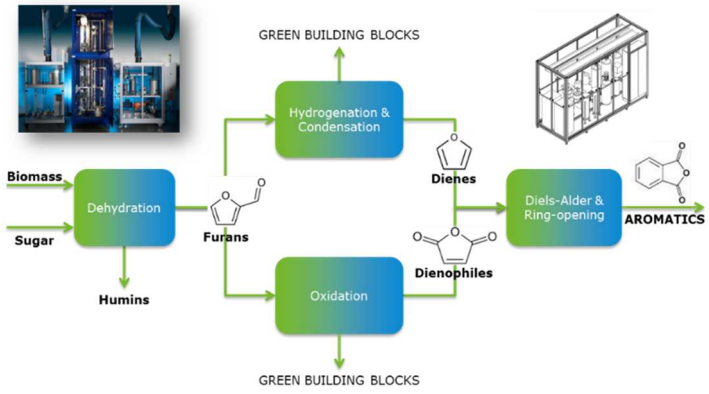
The deliverables and required activities are described in more detail for each of the three PPPs:

1. Biorizon Sugar-2-Aromatics

Biomass is a promising source for sustainable chemical building blocks. Aromatic compounds make up 40% of all chemicals produced. Full transition to a biobased economy requires bio-aromatics. Producing aromatics from biomass is a challenge, both technologically as economically. Several companies and research institutes have developed technology at TRL5-7 to produce drop-in aromatics (BTX). Unfortunately, drop-in aromatics must compete with their fossil counterparts, whilst there is no green premium. Especially with today's oil prices, business cases for drop-ins are difficult.

To overcome this issue, Shared Research Centre Biorizon focuses on the development of technology and value chains for the conversion of biomass into functionalized aromatics. These encompass drop-ins (e.g. vanillin, hydroxybenzoic acid) and molecules with 'novel' functionality (e.g. alkylphenols, hemi-mellitic acid). TNO is responsible for the Horizon (program line) entitled "Sugar-2-Aromatics", that focusses on the development of technology for the production of functionalized

aromatics from biomass-derived furanics (e.g. furfural, methylfuran). The following scheme depicts the chemistry and technology for the production of bio-aromatics.



Focus of TNO – Sugar based aromatics and piloting of technologies.

The basis for the current excellent knowledge & IP position has been developed in the previous period (2015-2017). Furthermore, several technological breakthroughs have been accomplished, samples for application testing have been produced and two process installations at TRL5 have been realized (see figure above). In the coming period (2018-2021), the technology will be further developed and scaled up to a full pilot plant (TRL6-7). For this purpose, the following activities are required:

- Process development at lab-scale for those components that are currently at TRL3-4.
- Design, construction & commissioning of TRL5 pre-pilots.
- Proof-of-concept of key technologies (dehydration, hydrogenation, condensation, oxidation, Diels-Alder, ring-opening) at TRL5.
- Expansion of scope of chemistry (from 5-10 targets currently, to 15-25).
- Production of samples (200 gram, 1 kilogram, 5 kilogram) to facilitate application testing by industrial partners (especially in case of aromatics with novel functionality).
- Design, construction & commissioning of the fully integrated pilot plant (TRL6-7).

Altogether, the knowledge & IP position will be strengthened, also in collaboration with other research institutes. In 2017, TNO started collaborating with Utrecht University on catalysis. TNO will strive to expand its running collaboration with TU/e on process design and will seek new partnerships as well.

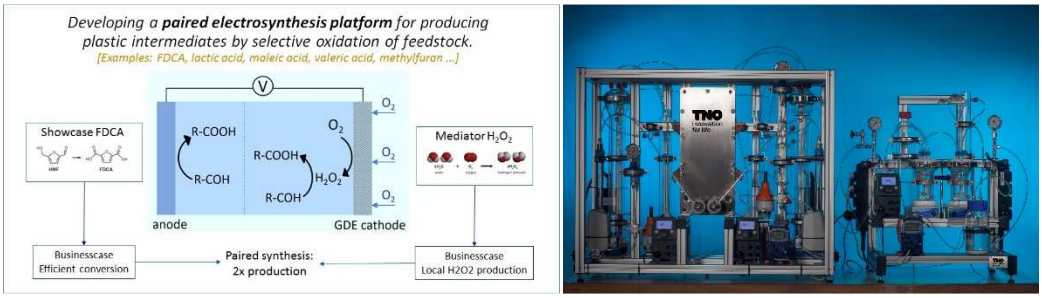
2. VoltaChem industrial electrification using electrochemistry

With more solar and wind energy being produced, sustainable electricity supply in North West Europe will be constantly increasing in the coming decades. This development in the energy market offers great opportunities for the chemical industry, especially in areas where renewable energy will be abundantly available and where industrial activities are nearby, e.g. in harbor industrial areas. Using novel electrochemical technologies to utilize the supply of this sustainable electricity in production processes as renewable energy source and feedstock can bring reductions in energy costs. And it can also offer numerous opportunities to develop new, high value products and lower the carbon footprint of production.

The chemical processes with the highest environmental and economic impact in the Netherlands are the production of Plastics, Fuels and Fertilizers. Electrification of

these processes can be done by implementing power-2-X technologies (where X can be heat, hydrogen, specialties and commodities), as has been shown in the whitepaper “Empowering the chemical industry – Opportunities for electrification” in 2016. Collaborative development and piloting of these technologies is the aim of the shared innovation program VoltaChem, that has been initiated by Topsector Chemie, TNO and ECN in 2015. In the period 2015-2017 the focus of this program was on the scouting and further development of early business cases and technologies together with partners from industry and academia. Recently, VoltaChem has entered into the next stage of development, implementing first pilot collaborations in regional clusters together with local, national and international partners.

In 2018-2021 TNO Chemicals will further contribute to these activities with specific focus on electrification system studies in the chemical sector and on production of key intermediates for plastics and high value chemicals using electricity as energy and feedstock source, applying electrochemistry and electrochemical engineering as main expertise. Within the TNO ERP “Energy Conversion & Storage” and within the partner ECN the focus will be on different end products and routes, like fuels and fertilizers using indirect (power-2-hydrogen) and direct (power-2-commodities) conversions. Furthermore, the overall program management of VoltaChem will be hosted by the TNO Chemicals VP. Further integration of activities regarding energy conversion and storage in to chemicals by electrochemistry and photochemistry will be explored in regards to processes, materials and industry needs.



Focus of TNO - Paired electrosynthesis (left) and development via bench-scale (right) towards pilots.

While the product focus of the activities will be primarily on the production of intermediates for plastics, the scientific focus will be on the development of paired electrosynthesis as a platform technology for highly efficient production of chemical compounds at both cathode and anode, see above figure. The main expertise’s to be further developed together with the academic and industry partners are electrochemistry, electrocatalysis, electrochemical reactor technology, membrane technology, electrochemical engineering, downstream processing integration and system design. Furthermore, industry system analysis and business case analysis are key enablers to continuously put focus on the rights topics.

Our main aims for the program 2018-2021 are to:

1. Expand and enrich the electrification community to increase industry involvement.
2. Closely collaborate with academia and industry labs to accelerate knowledge exchange.
3. Set-up complete screening to piloting testing infrastructure to accelerate development.
4. Integrate regional piloting activities in chemical clusters to accelerate implementation.

By the end of the program period we want to have implemented as one of the first in Europa at least two pilots at industrial scale in regional clusters showing the value and potential of paired electrosynthesis for plastic intermediates and high value chemicals production.

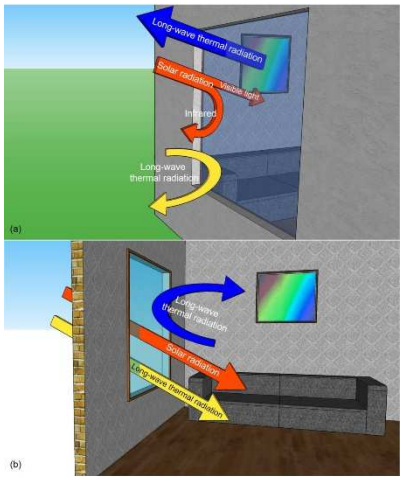
3. Brightlands Materials Center (BMC)

3a Shared Research line Sustainable Buildings

To facilitate the transition from a fossil fuel based energy system to a renewable one, we need to (1) efficiently harvest renewable energy such as solar and wind and convert it to a useable form of energy (e.g. electricity), (2) store energy to cover the inconsistency in supply of renewable energy (e.g. in form of fuels) and (3) reduce the energy consumption. Analyzing the energy consumption per sector, we conclude that buildings are the largest energy consumer with a share of 38% in Europe (EU-28, 2014) and 48% in the US (2013). To realize the goals set in the Paris Climate Pact, and fulfil the ambition of cities and regions such as Utrecht and Parkstad to become energy neutral in 2030 and 2040, respectively, we need to reduce the energy consumption for heating and cooling of buildings. Within BMC's Shared Research Program Sustainable Buildings, the ambition is to convert buildings from energy consumers to net energy suppliers. For that purpose, we apply a two-step strategy: improve the energy efficiency of the building, and cover the remaining need for energy with sustainable energy generated at location.

To improve the energy efficiency of the building, we focus on the development of novel materials for the building envelope. This envelope forms the primary barrier between the interior of the house and the outside environment, and plays a key role in comfort, natural lighting, ventilation and energy consumption for heating and cooling. The building envelope consists of non-transparent parts (e.g. façade element) and transparent windows.

In the period 2018-2021, the program will focus on the development of advanced materials to improve the energy efficiency of buildings, being (1) infrared regulating window coatings that provide optimum heat regulating properties both in summer and in winter, (2) infrared regulating polymer foils that can be laminated to glass windows and provide optimum heat regulating properties both in summer and in winter, (3) infrared regulating paints and polymers for non-transparent building elements. Most of these materials and coatings will be nanocomposites. Synthesis, characterization, surface functionalization, and controlled integration of the functional nanoparticles in (polymer) matrices will be key elements of the activities.



Furthermore, in the same period the program will focus on local energy generation. For that purpose, novel advanced materials will be developed that facilitate efficient and aesthetic integration of photovoltaic modules in the building envelope. Examples of such materials that will be developed are: (1) coatings/polymers that collect light on large surface areas and guide it to photovoltaic modules, (2) coatings/polymers for heat regulation in solar PV panels, (3) coatings/polymers for better photon collection in photovoltaic modules to improve the device efficiency (more current), (4) coatings/polymers for improvements of PV module aesthetics (e.g. coloration). Most of these materials and coatings will be nanocomposites. Synthesis, characterization, surface functionalization, and controlled integration of the functional nanoparticles in (polymer) matrices will be key elements of the activities.

3b Shared research line Lightweight Automotive
Major driver in the automotive world is to reduce emissions such as CO_2 and NO_x guided by EC directives to enforce meeting set goals. Different routes exist to reduce emissions such as a shift to electric vehicles or hybrid vehicles as well as improvement of efficiency of existing combustion engines. In both cases lightweight materials such as plastics are part of the solution in enabling longer range or reduced fuel consumption. Next to emissions, End-of-Life solutions are critical to meet overall LCA goals, hence the use of thermoplastics. Although these plastics have been replacing metal in cars for quite some years, cars have hardly become lighter due to increasing amounts of electronic devices for comfort and safety but also due to the limited know-how of long-term behavior of advanced structural plastics based on continuous fiber reinforcement to actually replace large metal components.

The ambition of BMC's Shared Research Program Lightweight Automotive is to contribute to sustainable (automotive) mobility by developing innovative solutions based on expertise in the field of polymeric materials such as continuous fiber reinforced thermoplastics and hybrids. To address the mentioned concerns, three sub lines are relevant: (1) Predictive material performance, (2) Recycled materials, and (3) Integrated electronics.

The main goal for (1) for 2018-2021 is to increase confidence in and use of these materials by reduction of costs needed for testing and validation by developing physics based material models. These models include effects as interface fracture, long-term behavior and impact after aging and require the development of new adhesion tests methodology for hybrids between advanced thermoplastic composites and injection molding compounds. Generated know-how will be translated into design rules for use in hybrid plastic/metal and thermoplastic composite parts. Based on gained insights materials can be improved.

The goal for (2) relates to use recycled thermoplastic composites coming from post-industrial waste streams. Main topics are development of methods and recycled materials that allow re-use in structural applications. First results in 2017 demonstrated proof-of-concept that these materials can be recycled with a performance increase versus regular long fiber compounds. For the coming program period the interaction of material behavior and processing in series processes as injection and compression molding is further studied to predict material behavior as well as to further develop recycled materials with enhanced properties.

Integrated electronics (3) combines lightweight flexible electronic technology as developed by the Holst Centre with mentioned lightweight structural plastics and adds functionalities. Identification and characterization of damage and damage

mechanisms, tracking of material state during life of parts as well as sensing and monitoring are examples of practical use. Such combination of technologies builds on the research line predictive modelling, and requires development of further adhesion tests and of interface and fracture models to determine and improve the behavior of structural material with an electric layer included.

1.4 External Connections

The program of Sustainable Chemical Industry is excellently positioned to contribute to the transition from fossil feedstocks to a sustainable renewables based circular industry. It directly connects to the following Societal Challenges:

- **Energy & CO_2**. Biorizon: use of biomass instead of fossil fuels; VoltaChem: use of renewable electricity & conversion of CO_2; BMC: efficient use of sunlight.
- **Climate & Water**. Biorizon: CO_2 reduction by means of biomass utilization; VoltaChem: CO_2 utilization; BMC: reduction of fossil fuels for heating/cooling.
- **Circular Economy**. Biorizon: valorization of municipal & industrial waste as feedstock for aromatics; VoltaChem: CO_2 utilization; BMC: new program line on recycling of plastics.

It contributes to the following Key Enabling Technologies:

- **Advanced Materials**. BMC: materials adaptive to changes in environmental conditions (dynamic response); VoltaChem: 3D-structured catalytic electrodes.
- **Photonics**. BMC: materials that interact with sunlight.
- **Electrochemical Conversion & Materials**. VoltaChem: processes & systems for electrochemical conversion of CO_2 and biobased feedstock into chemical building blocks.
- **Advanced Manufacturing & Processing Systems**. Biorizon & VoltaChem: use of nano-structured catalysts, multi-step integrated processing systems.

Finally, the program is embedded in the **Chemistry of Advanced Materials (CAM)** and **Chemical Conversion, Process Technology & Synthesis (CCPT&S)** Roadmaps of Topsector Chemie: BMC (CAM: task 1 & 2), VoltaChem (CCPT&S: task 1; CND: task 3), Biorizon (CCPT&S: task 1 & 2). In view of the NWA-routes, the program relates to “**Energy Transition**”, “**Circular Economy & Resource Efficiency**” and “**Materials**” and to “**Smart Industry**” when the exploration on digitization proves successful.

1.5 Developments

The program for the period 2018-2021 is slightly different compared to the previous program (2015-2018). The previous program contained more different elements than the new program, which is more focused. The three PPPs that are currently successful were described in the previous program, but were, when writing this program in 2014, still in its infancy. Hence, the program contained other horses to bet on. The new program is further focused on developing the three PPPs (Biorizon, VoltaChem and BMC).

Another difference is the TRL. Where in the previous program new initiatives (and technologies) were developed (low TRL), in the new program these initiatives and technologies are being scaled up, both in terms of collaboration partners, industry commitment and TRL (from 1-4 previously, now 4-6). This has especially been the case for the Biorizon activities.

For VoltaChem specific the previous period has been used to build up a large network of national and international partners from academia and industry (chemical, energy and equipment supply). We have begun building lab infrastructure and have bundled associated expertise and know-how for selective oxidation reactions from biobased feedstock. With that as a basis we have shown bench scale demonstration of one-side electrosynthesis. First generic patent applications have been filed on the basic principles of selective electro-organic synthesis.

Now we will build upon this basis to further by utilizing and expanding the high-tech electrochemical infrastructure and know-how together with research partners, collaborating with industry partners to translate this know-how into industrial development and piloting first installations in the large Dutch regional chemical clusters.

1.6 Activity Plan 2018

In 2018 the following activities will be carried out.

1. Biorizon – "Sugars-2-Aromatics"

- Further expansion of the Biorizon industrial community and of the research network.
- Optimization of Waste2Aromatics technology at TRL5.
- Process development at lab-scale for trifunctional bio-aromatics (e.g. hemi-mellitic acid).
- Development of Diels-Alder chemistry for bio-phenol and bifunctional aromatics (drop-ins such as phthalic anhydride or isophthalic acid).
- Proof-of-concept for "classical" Diels-Alder technology to produce the trifunctional bio-aromatic methylphthalic acid/anhydride.
- Production of samples (up to 1-5 kg).

2. VoltaChem

- Further expansion of the VoltaChem industrial community and research network.
- Further development of techno-economic electrosynthesis and life cycle assessment models to continuously predict business cases and direct the research work.
- Electrochemical synthesis:
  - Scouting novel liquid based electro-organic selective oxidation reactions.
  - Demonstration gas-liquid based electro synthesis using H_2O_2 as showcase.
  - Development of paired electrosynthesis technology to increase efficiency.
- Enabling technology development:
  - Further expansion of the electrosynthesis toolbox.
  - Electrochemical membrane, electrode and catalyst testing.
  - Electrolyte testing and selection.
  - Tools for electrochemical reactor and system design.
  - Downstream processing integration.

We expect to have proven at least 2 new electro-organic selective oxidation reactions at proof-of-concept level and 1 paired electrosynthesis at proof-of-principle level together with our partners.

3. Brightlands Materials Center:

- BMC – SB:
  - Development of infrared regulating window coatings that have a high transparency in the visible and autonomously switch from an IR transmissive to and IR reflective state at approx. 35°C.
  - Development of infrared regulating polymer foils that have a high transparency in the visible and autonomously switch from an IR transmissive to and IR reflective state at approx. 35°C.
  - Development of high refractive index polymer composites for light guiding.
  - Development of coatings and polymers for improving efficiency and aesthetics of photovoltaic modules.
- BMC – LWA:
  - Development of new test methods and first modeling concepts for determination of adhesion between thermoplastic composites and injection molding compounds.
  - Technology development of 2 materials from the post-industrial waste stream regarding interaction of material behavior and processing in series processes as injection and compression molding.

2 Possible extra financial input

During the preparation of this Multiannual Plan 2018-2021, there was still no clarity about a possible new research and innovation policy of the new cabinet. If there is space for additional funding for applied research within this policy, TNO sees opportunities to accelerate and intensify the knowledge development described in this report towards pilots, demo's and commercial implementation together with our partners. Also, we then foresee opportunities to increase university and SME collaboration and can enhance the exploration activities regarding digitization and plastic/composite recycling.

The TNO Strategic Plan 2018-2021 "Flywheel for Innovation in the Netherlands" describes how the chosen domains, spearheads and technological innovation connect and contribute to external challenges and agendas: "UN Sustainable Development Goals", the "Grand Societal Challenges", "Key Enabling Technologies" and "Leadership in Enabling Industrial Technologies" of the EU, the National Science Agenda, and agendas/roadmaps of Ministries and Topsectors.

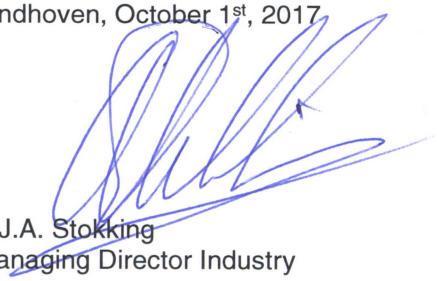
Topics of Interest for the Topsector Chemie are amongst others:

- Development of renewable raw materials
- New functional (nano)materials

These TNO spearheads support the National Science Agenda on the one hand, and on the other hand connect with the recently formulated Social Challenges and Key Technologies (MUST). The Demand-Driven Program described in this report is a concretization of these spearheads. If the new cabinet creates additional financial space for applied research in the coming years, TNO will update the program and indicate which subjects will be strengthened taking government instructions into account.

3 Signature

Eindhoven, October 1st, 2017 TNO



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