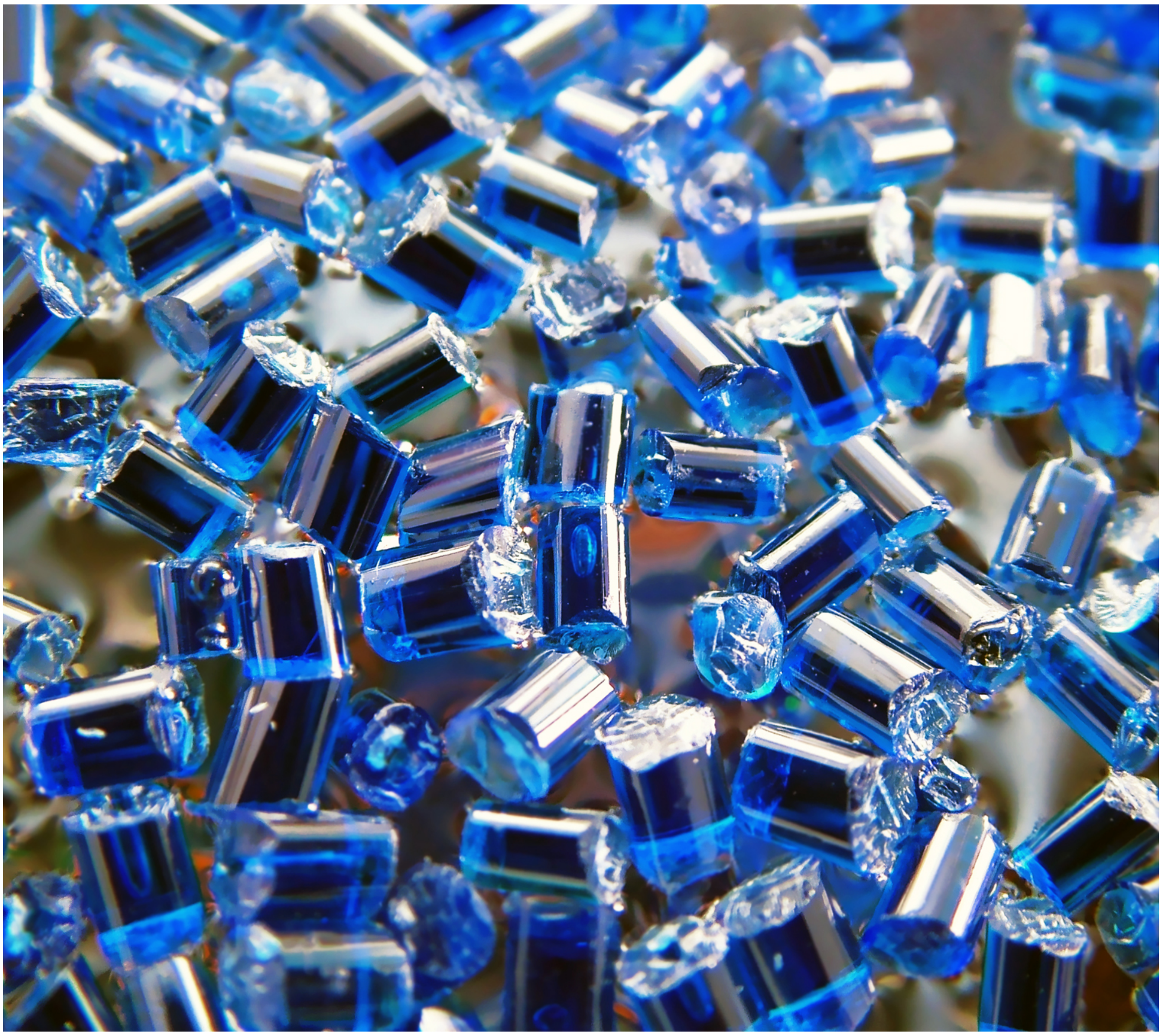
ChemistryNL

Roadmap
Chemistry of Advanced Materials



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Executive summary

Artificial materials are the cornerstone of our global society. Progress in the field of materials chemistry has enabled numerous new technologies and applications ever since the Stone Age, and will continue to do so in the coming decades. The Netherlands has a very strong position in various fields of advanced materials, and has a high ambition level for extending this position; in the period 2030-2040, The Netherlands will have settled its name globally as "rational material design" technology provider for high value-added, sustainable materials and clean energy materials. In keeping with this long-term ambition level, the emphasis of materials chemistry research on the short term should be on mechanistic insight to be obtained for each of a plethora of desired functionalities and on the medium to long term on moving from increasing insight and understanding towards rational material design capabilities and implementation of the technologies developed. For the latter, a broader scientific foundation of (multi)functionality of materials should be developed, including experimental multiscale analysis of material structure-property relations and (predictive) modelling of formulations and properties.

The roadmap Chemistry of Advanced Materials deals with the (bio)chemical synthesis or chemical modification of materials in relation to their desired functionality. This includes organic materials, inorganic materials and hybrids. Examples of organic materials are engineering plastics and resins, and examples of inorganic materials are sol-gel metal oxides or metal borides and carbides produced via chemical vapor deposition. All activities in this field should include end-of-life considerations for the materials after use. The roadmap Chemistry of Advanced Materials has focused on three tasks: **Materials with added Functionality, Thin films and Coatings, and Materials for Sustainability**. All three tasks revolve around the key word "functionality" and prepare for a future in which advanced materials exhibit new functions, new combinations of functions, or true step-change improvements in their functions. Under the first task, the functionality is defined by the continuum (or "bulk") intrinsic properties of the materials, whereas surface effects dominate those properties under the second task. Under the third task, the functionality is related to sustainability. Either directly, when the material itself is made in a sustainable way, or indirectly, when the material enables sustainable energy harvesting or energy storage, reduction of energy consumption or requiring less (scarce) resources for production. Intrinsic design of advanced materials based on, or allowing for, circular economy or replacement of advanced materials with more sustainable alternatives is bridging task 3 with tasks 1 and 2. Of course, these three tasks are not mutually exclusive. The overall ambitions of each task and the specific steps that should be taken between now and 2050 are summarized in the tables below each theme.

This roadmap on the chemistry of advanced materials is mainly sustained by the Topsector Chemistry roadmap on Making Sustainable Chemical Products and the **TKI Biobased Economy**, by providing sustainable raw materials and (catalytic) technology for control of conversion of these raw materials into advanced materials. In turn, the major beneficiaries of this roadmap are in the Topsector Chemistry roadmaps on Chemistry of Life (Biomedical Materials) and on Chemical Sensing and Enabling Technologies, as well as in the topsectors **High-Tech Systems and Materials, Energy** and **Water** for applications of these advanced materials. These applications are fully in line with the Horizon Europe themes.

	Energy Transition and Sustainability			Agriculture, water and food	Health and Healthcare	Security	Key Technologies	Societal earning capacity
ChemistryNL Roadmap	Climate and Energy (IKIA) *in particular Mission C "Industry"*	Circular Economy	Future Mobilitysystems	7 missions	4 missions	8 missions	Key technnology (ST) clusters: ChemTech, AdvMat, DigTech, EngFabTech, LifesciTech, NanoTech, PhotoTech, QanTech	3 tracks
Chemistry of Advanced Materials							AdvMat; ChemTech; NanoTech	
Materials with Added Functionality	Advanced building materials in MMIP3 Composite materials for transportation in MMIP9		Composites for ships and airplanes		Sensing materials for prevention in mission I/II	High strenght materials and sensor materials in mission 2	Sensing materials in ST3 Photonic and photovoltaic materials in ST4 Nanomaterials in ST8	
Thin Films and Coatings	Wind turbine blade coatings in MMIP1 Coatings for transportation in MMIP9		Coatings for ships and airplanes	Use of protective films for food in mission D	Biostable/resorbable and antimicrobial materials in mission III	Coatings for low detection in mission 2	Advanced materials in ST5 Biostable/resorbable materials in ST6	
Materials for Sustainability	Photovoltaic materials in MMIP2 Thermoelectric and magnetocaloric materials in MMIP4 Redesign of materials for circularity in MMIP6 Battery materials in MMIP8	Design for circularity in materials		Use of bio-based materials in mission A/B		Materials for additive manufacturing in mission 6	Materials for additive manufacturing in ST3	

1 Introduction

Mastering materials has paved the progress of mankind ever since the Stone Age. Now, thousands of years later, artificial materials are the cornerstone of our global society. Materials are present everywhere in our daily life in buildings, furniture, clothes, transportation, and electronic applications but likewise they are part of food and healthcare products, diagnostics, and biomaterials. Progress in the field of materials chemistry has enabled numerous new technologies and applications in this period. Recent examples are found in composite materials for aerospace, smart phones and tablets, energy efficient lighting, solar energy conversion, self-cleaning coatings and materials, and rechargeable batteries. Next to these examples, materials chemistry has also substantially contributed to developments in food packaging, in biobased materials, soft robotics, and in enabling regenerative medicine and making artificial skin and other tissues or even organs.

Advanced Materials in the context of the roadmap are defined as materials that offer superior levels of performance or additional features and added value compared to existing materials for a specific application. However, one can also argue that Advanced Materials are those of which the true relevance still needs to be firmly established, but that offer, at present, new exciting opportunities in terms of properties or applications. In this sense also known materials that can be processed via innovative techniques, such bottom-up self-assembly or top-down methods such as additive manufacturing, should be designated as advanced.

Advanced Materials do not exist without materials chemistry. Chemists are able to design materials and control their structure from the atomic and nanometer scale up to macroscopic dimensions. *Advanced materials chemistry* involves assembling atoms or molecules in a controlled fashion, covering microscopic, mesoscopic, and macroscopic dimensions. Whether this control is achieved by sophisticated (macro)molecular synthesis, directed crystallization or deposition or by advanced processing, understanding the interactions across all of these dimensions is key. Theory and computational methods will increasingly be used to guide materials discovery. Controlling matter and understanding its behavior over up to ten orders of length scales is a unique aspect of all modern materials: from stainless steel to specialty polymers, and from concrete to membranes for artificial kidneys. Advanced material science unites chemistry with aspects of physics, biology and engineering to understand and control materials properties and their interplay with artificial and living systems.

Advanced Materials is an internationally vibrant field of research and new developments. Novel materials with new properties, being organic, inorganic, biobased or hybrid in nature, are being discovered almost on a daily basis and are revolutionizing our society. Super strong polymer fibers, new carbon allotropes such as carbon nanotubes and graphene, gallium nitride for energy efficient lighting, and new perovskite semiconductors for solar cells and biodegradable plastics are just a few examples of materials that were unknown 25 years ago but are expected to change our world. The whole life cycle of these new and technologically advanced materials needs to be taken into account to provide solutions to the societal challenges of 21st century in areas of energy, water, health, environment, sustainability, transport, and food. New materials will improve our planet and the wellbeing of its people.

The Netherlands has a very strong position in various fields of advanced materials. Many excellent academic research groups, prominent research institutes, world leading multinationals, and innovative SMEs and start-up companies exist. The Netherlands can strengthen its position as a key player in the area of Advanced Materials, but contributing to true innovation requires focus and collaboration between all stakeholders. This roadmap provides a framework for research and innovation in Advanced Materials in The Netherlands as part of the Top Sector Chemistry in three main fields related to societal challenges:

1. **Materials with added functionality**, related to Energy, Health, Mobility, Construction, Environment and Climate
2. **Thin films and coatings**, related to Food security, Energy, Wellbeing and Health
3. **Materials for sustainability**, related to Resource efficiency, Climate, Energy, Wellbeing and Health

2. Overview of themes

In this chapter, we describe the grouping of advanced materials research in relation to the societal needs we see for the coming decades. A growing population (aspiring higher living standards) and the rapid depletion of natural resources pose future challenges. Material science is instrumental in finding solutions. In the prioritization of research areas that will be addressed within the Chemistry of Advanced Materials program of the top sector Chemistry the societal relevance is important, as well as the excellence of materials research in The Netherlands in specific areas. Both existing and future opportunities for economic activities related to these materials research areas have resulted in the selection of three main tasks:

1) **Materials with added functionality**. Our society needs materials “to do more with less”: less weight but higher strength or performance, and able to exhibit multiple functionalities too. Materials combining multiple functionalities (“smarter” materials) provide an added societal and economic value.
2) **Thin films and coatings**. In thin films and coatings, the effects of the surface on the properties, as well as the functionality that the surface properties bring in the use of the material, add to the complex needs in society for “smart surfaces”.
3) **Materials for sustainability**. Doing more with less should ultimately result in a smaller footprint of material use on our planet and less dependency on geopolitical developments. The resources of fossil fuel and raw materials are dwindling, and climate change forces society to alter the sourcing of its materials, and use materials for saving energy, sustainable production of energy and reduce, replace or recycle the use of scarce elements.

We have defined these tasks based on a ***priority analysis*** of the factors described in the following paragraphs (contribution to People, Planet and Profit, fit with Horizon Europe overarching themes, fit with the Dutch landscape, and technology gaps), with the aim of being as ***inclusive*** as possible for Dutch universities, institutes and companies, and allowing for the highest possible ***thematic overlap*** with other Topsector Chemie roadmaps (e.g. Nanotechnology and Devices, Chemical Conversion), other Top sectors (e.g. High Tech Systems and Materials, Energy, Life Sciences & Health, AgriFood) and existing vision documents.[1]

The tasks have an excellent fit excellently to with the mission driven research agenda of The Netherlands. Chemistry of advanced materials can be found as cornerstones of IKIA and KIA CE of the mission “Energietransitie en Duurzaamheid”. For instance, photovoltaic coatings and materials in MMIP2, thermolectric and magnetocaloric materials in MMIP4, redesign of materials for circularity in MMIP6, development of battery materials in MMIP8 and composite materials and coating for transportation in MMIP9 cannot be developed without strong input from the academic and industrial groups operating in the field of chemistry of advanced materials. Also many goals of the missions of “Landbouw, water, voedsel”, “Gezondheid en zorg” and “Veiligheid” cannot be achieved without strong input from this sector. The key enabling technology “Avdanced Materials” (ST5) and all related research questions resemble the three tasks outlined here and are in fact based on this roadmap. Also other key enabling technologies heavily rely on materials development such as “Chemical Technologies” –ST1, “Engineering and Fabrication Technologies” –ST3, “Photonics and Light Technologies” –ST4, “Energy Storage Materials” –ST5, “Nanotechnologies” –ST8. Long term programs defined in the scope of these key enabling technologies such as 73 MJP –“Soft Advanced Materials” and 82 MJP –“Materialen –made in Holland” will be potential drivers to develop the research agenda in this roadmap.

All three tasks revolve around the key word “functionality”. Every material has a specific purpose for its use, based on one or more implicit functions it has to fulfill. For example, a ‘simple’ coating on a metal bridge combines two essential functions: to protect (the bridge, from corrosion) and to decorate (appealing look). Or a food package that protects the food from getting dirty, but also increases shelf life. In that respect, there are no (current or future) materials that are not functional. However, a future can be envisioned in which advanced materials exhibit new functions, new combinations of functions, or true step-change improvements in their functions. For example, when the coating on the bridge can last 40 years instead of 15, can also sense and signal stresses, or be self-cleaning, it offers additional functionality. Or the food

[1] Vision Paper 2025 Chemistry and Physics (commissie Dijkgraaf)
Catalysis - Key to a Sustainable Future (Science and technology Roadmap Catalysis 2015)
Nationale Agenda Materialen-Accelerating Materials Technologies (MaterialenNL platform2021)

packaging material that also signals increased bacterial activity. We have tried to capture this under the term “added functionality”, where “added” refers to the newness introduced in comparison to the currently known uses of the materials.

Under the first task, the functionality is defined by the continuum (or “bulk”) intrinsic properties of the materials, whereas surface effects dominate those properties under the second task. Examples of the first include low-weight car parts or construction materials, biomedical implants, whereas membranes, specialty packaging, antimicrobial coatings and thin-film sensors are examples of the second. Under the third task, the functionality is related to sustainability. Either directly, when the material itself is made in a sustainable way, or indirectly, when the material enables sustainable energy harvesting or energy storage, reduction of energy consumption or requiring less (scarce) resources for production. Intrinsic design of advanced materials based on, or allowing for, circular economy or replacement of advanced materials with more sustainable alternatives is bridging task 3 with tasks 1 and 2. Of course, these three tasks are not mutually exclusive, nor meant to be. It is well possible (and well accepted) that certain innovative ideas can find connections with all three simultaneously.

Making, characterizing, understanding, and modeling new advanced materials requires multiple key enabling technologies. We are not including them as separate tasks in this roadmap, but still want to emphasize their importance. Making materials requires novel advanced synthesis techniques (e.g. new catalysts of polymerization methods), production methods like high throughput synthesis and manufacturing and processing techniques, such as for instance advanced lithographic processes or additive manufacturing. Characterizing materials with multiple added functionalities for instance requires novel techniques to measure these functionalities in situ and in a correlated fashion. To test whether intended functions are retained under realistic (in operando) conditions, we need more in-situ (realistic) characterization. To connect across length scales, we need technology for higher resolution and multi-scale characterization. Theoretical approaches and artificial intelligence will in the future play a more important role in predicting materials properties, designing de novo materials and discovering new mechanisms beyond intuitions. In addition, big data generated by modern experimental and computational techniques is becoming more readily available, data-driven or machine learning (ML) methods will open new and exciting pathways for the discovery and rational design of materials. These new enabling technologies can even drive the development of new materials themselves, such as materials that can serve as multi-modal probes (EM, light microscopy, X-ray and neutron scattering, NMR) or materials with in-built sensors such as polymers that report the local stress. Importantly, materials research requires easy access to advanced characterization facilities such as advanced HR TEM, X-ray and neutron scattering, (solid state) NMR, light microscopy and high-performance computing.

In the next chapter, we will describe in more detail what functions can be envisioned under these challenge themes, while we depict for each the Dutch profitability balance: with the available know how infrastructure and manufacturing capabilities in the Netherlands. Are we globally competitive? Can we develop the material/technology and extract the value in the Netherlands (delivering jobs in R&D as well as full scale production, a full footprint in the Dutch economy)? Or can the technology (only) be patented and valorized via worldwide licensing of Dutch technology? Which areas can be identified for which the position in The Netherlands is not strong yet but have the potential to develop if we invest?

2.1 Materials with added functionality

Introduction

For many applications, the demands on materials become higher, while at the same time the market is very competitive and global, which puts a lot of focus on reducing costs. A number of successful examples from the past have shown that the Dutch industry, together with knowledge institutes (*e.g.* Dutch Polymer Institute, Materials Innovation Institute, AMOLF, DIFFER), can pave the way in the advanced polymer, nano and hybrid (metal) materials and composites arena by using a systems approach. This implies that a strong link is needed between the chemistry of **making optimized advanced materials** and **processing with cost-efficient technologies**, so **the right application domains** can be targeted. This especially holds for materials enhancing circular economy and hydrogen mobility (e.g. aerospace and automotive). In general, it can be stated that the need for new metallic, ceramic, (bio)polymeric, and composite/hybrid light-weight materials is growing rapidly. Classic material selection approaches will no longer work. Well-known Ashby material selection charts, as shown in Figure 2.1, are an initial start, but new applications for the above-mentioned industries can only be realized when new materials become available that offer a combination of properties, e.g. they can be used as a structural load bearing component while also offering additional functionalities such as self-healing, sensing or actuation. Such new materials ideally have to be produced, processed and recycled in a sustainable manner. Value should be created according to a 'more for less' philosophy. Reduce the weight of a design but add functionality. The value will be in price per economic value added rather than producing kilograms.

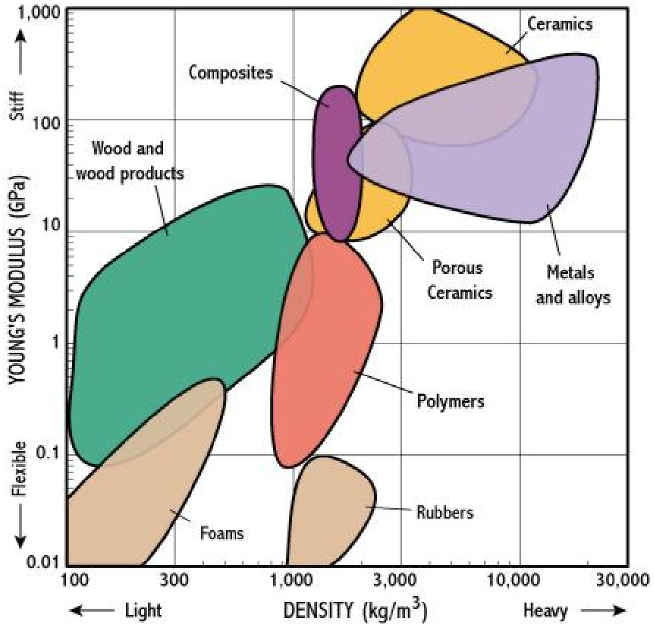

Figure 2.1 *Material selection chart as introduced by Michael Ashby. Material properties, in this case density (kg/m^3) vs. Young's modulus (GPa), are plotted in pairs on a chart, allowing the user to find the right material for the right job.* (Ashby, Michael (1999). *Materials Selection in Mechanical Design (3rd edition ed.).* Burlington, Massachusetts: Butterworth-Heinemann. ISBN 0-7506-4357-9. Cf: www-materials.eng.cam.ac.uk/mpsite/physics/str-tough_article/ of http://store.elsevier.com/Materials-Selection-in-Mechanical-Design/Michael-Ashby/isbn-9780080468648/)

Also the trend towards more personalization in products with high quality-of-life requires a different mindset toward the design and processing of new functional materials with on the one hand more automated processes, while on the other hand allowing organic materials, based on "molecules" (mainly polymers), as their design and production from raw materials (petro- or biobased) depends highly on manufacturing capabilities for which we refer to the Roadmap Making Sustainable Chemical Products.

Tasks

Description of the task and the relevance for society, industry and science

Advanced materials are characterized by their high degree of functionality. Society has always been looking for stronger, faster, and thinner, more efficient and lighter, say 'superior' materials. Solutions are therefore developed based on market-pull mechanisms and science and technology play a dominant role in the development of materials that can bridge the actuality with societal desires and needs.

Solution for this task described SMART (present-2050)

Present-2025 Starting from a strong point of NL, with excellent R&D infrastructure and a good basis for public-private partnerships in material technology development, new mechanistic insights should be obtained for each of a plethora of desired functionalities (see 2.1) in e.g. functional polymers, nanocomposites, metals, and high tech materials aimed at aiding implementation of new functionalities in products in cooperation with industrial partners. Also, more insight will be obtained on the sustainable recyclability of materials with added functionalities where the added functionality is being maintained. From a fundamental science perspective, specific functionalities should be fully understood, also in relation to each other and to other material requirements. Basic research in emerging classes of advanced materials is strengthened as a seedling for novel applications that we cannot think of yet. The entrepreneurial climate, as well as strong "designer material" knowledge base combined with the know-how how to design and manufacture with those materials, will allow the growth of start-up companies (e.g. Xilloc Medical and Chemelot InSciTe).

2025-2035 Moving from increasing insight and understanding towards rational material design capabilities, a broader scientific foundation of functionality of materials is developed, including (predictive) modelling of formulations and properties and efficient recycling. Several new technology platforms are expected that make NL an attractive manufacturing area as price per kilogram will be replaced by price per economic value added. This will be in support to typical EU industries like agricultural, car manufacturing, medical, high tech, and energy related industries and in full support of the ageing population.

2035-2050 Three decades from now, NL will have settled its name as "rational material design" technology provider for high value-added materials, and clean energy materials, based on its knowledge infrastructure and IP position, and its demonstrated infrastructure for introduction of new technologies to the market.

What <u>existing</u> competences, technologies, knowledge contribute to this task?

Traditionally, the Netherlands has a strong and internationally renowned basis in the development of sophisticated functional materials. This is due to the presence of a variety of companies in the areas of materials, and devices, as well as a well-developed R&D infrastructure (TOP institutes and technology campus models). This ranges from polymers to computer chips and from bio-medical applications to car manufacturing. The Netherlands offers state of the art Large-Scale Research Facilities (organized via the National Roadmap) for characterizing materials properties, including free-electron lasers (FELIX, Nijmegen), neutron scattering (Oyster, Delft), electron nanoscopy (NeCEN, Leiden), and nuclear magnetic resonance (Utrecht).

What <u>additional</u> competences, technologies, knowledge do we need?

Investment in the areas of bottom-up micro-meso-macro scale morphology analytics and control of (bio)polymers and/or inorganic particles (nanometer – micrometer size), nanotechnology/nanoscience and nature inspired self-assembly is crucial for the development of advanced materials. This area is highly multidisciplinary in nature and requires intimate collaboration between chemistry, physics, life sciences, and bioengineering, with a strong input from rapidly advancing analytic techniques (allowing multimodal functionality and morphology characterization on the nanoscale). In addition, integration of multiple length scales in the research is crucial to understand how functional properties on the nanoscale affect functionalities on larger length scales and can be implemented in new products. This needs to be supported by modelling and computational chemistry on all these different length scales (micro: Molecular Dynamics, meso: coarse graining, macro: finite elements); a particularly outstanding challenge is to connect models at different scales and data-driven modeling in order to achieve predictive frameworks that can guide new materials developments. In addition, knowledge on the manufacturing of materials with added functionalities needs to be built up, for instance in rapidly growing application areas such as additive manufacturing.

Designing materials with the right functionality

In many industries, e.g. automotive, aeronautics, electronics and construction, the driver for innovation is weight and cost reduction together with higher demands on the material properties in terms of thermal, mechanical and chemical properties. In said applications engineers/designers use materials that are typically optimized to fulfill one specific task or one specific function.

In this context, functionality can be defined as:

1- **Mechanical** (e.g. strength, stiffness, flexibility, fatigue or impact stability)
2- **Chemical** (e.g. chemical stability, biocompatibility, catalytic, photoconversion)
3- **Physical** (e.g. thermal and electrical conductivity, magnetic, piezoelectric, optical)
4- **Biological** (e.g. cytocompatibility, antibacterial, bioinstructive cues)

A - Traditional materials

Over the years, chemists and material scientists have designed and optimized materials for specific applications, e.g. metals for high temperature engine parts, ceramic coatings for high high-temperature turbine coatings and polymers for ductile/light-weight packing materials. Step-changes are definitely possible in extending the current property portfolio, but the limits of traditional materials have been or will be reached soon. This can be achieved by chemical structure and processing optimization, e.g. polyethylene can be processed into high modulus/high strength yarns. Optimizing the chemistry (catalysis and polymerization conditions) and processing has the potential to further improve the mechanical properties of PE-based yarns by a few percent. Aluminum, as another example, is an alloy and has now been optimized with respect to strength and ductility. In this case, alloy design and processing are expected to result in an overall improvement of a few percent at best. For steel, on the other hand, several issues need to be resolved. Understanding fatigue behavior, improve corrosion stability and how to improve polymer (coating) adhesion on steel are still issues that need to be resolved. The same is true for continuous and non-continuous fiber-reinforced composites. The design of composite structures is sufficiently understood. However, the resin-fiber interface and processing issues need to be resolved and how composite structures fatigue over time.

B - Multi-functional materials

In order to enable the design of next generation coatings, composites, packaging, sensors, actuators etc., materials are needed that combine some level of structural integrity with one or more additional functions. Self-healing polymers or ceramics with the ability to reverse crack formation have a strong advantage over traditional construction materials. Designing multi-functional materials (MFMs) requires a multidisciplinary approach and the ability to design materials at different length scales (Å to m). MFMs are often multi-component or hybrid systems. Typical building blocks include ceramics, metals and (bio)polymers. Of interest are organic/inorganic nanocomposites where the matrix offers the structural integrity and processing capability and the nanofiller introduces a second functionality, i.e. it reinforces the matrix and adds an electrical, thermal, actuating/morphing or sensing functionality. The envisioned applications could be in photovoltaics, sensors or in bulk applications such as composites. The aim is to reduce weight, add functionality, extend the life cycle and reduce maintenance costs.

C - High-Tech materials

In the high tech industry, the rapid development of new technologies often relies on research at the interface of chemistry and physics and sometimes bioengineering. An example of the latter is the leading role of the Netherlands in the area of organ-on-chip models for animal-free experiments and personalized medicine (hDMT institute). A number of startup companies are located in innovation hubs such as the Brightlands Chemelot Campus and the Leiden Bio Science Park. In addition, small scale and cheap diagnostic equipment that can be used in the home or in remote areas is a rapidly growing market. There is a strong activity in the Netherlands. Cooperation between large companies and SME's, in the biomedical field, and universities and university hospitals has been supported in several successful programs (BMM, CTMM, HTS&M). Challenges include research on the nanoscale. Bio-molecules of nm dimensions (e.g. proteins and DNA) are at the basis of diseases and (bio)chemistry now allows for the synthesis or recombinant production and the controlled self-assembly of these molecules. Future prospects in this field include:

- Control of interaction of living matter with man-made materials will allow to replace or assist dysfunctional organs beyond the traditional implants.
- Microtissue and organ-on-chip models for animal-free experiments and personalized medicine.
- Imaging using (multi-functional) nanoprobes in combination with controlled drug delivery and/or release makes a more targeted and personalized medicine possible.

Inexpensive small scale diagnostics (e.g. using lab-on-chip technology, even in combination with mobile phones) based on (nano)sensors for diagnosis at home or in remote areas is a growing area and requires a continued effort in finding new materials for more reliable and cheaper diagnosis.

Summary

Topic	Short term (-2025)	Medium term (2025-2035)	Long term (2035-2050)
Traditional materials	• Improved mechanical properties of traditional polymers (TRL6) • Understanding fatigue and improving the corrosion stability of steel (TRL3) • Insight in the resin-fiber interface for fiber reinforced composites (TRL 3) • Upscaling of self-healing polymers and ceramics (TRL 7)	• Higher strength polymers industrially produced (TRL 6) • Several insights described above (corrosion, fatigue) will lead to development of improved materials that are tested in a simulated environment (TRL 5) • Superior composites are designed based on new insights (TRL 3)	• Reinforced composites and materials with improved properties successfully introduced to market (TRL 9)
Multi-functional materials	• Development of polymers with additional functionalities (e.g. optical, magnetic, electronic, selective permeability, bioactive) (TL3) • Design of new materials for EUV lithography and for additive manufacturing (TL3) • Development of smart materials and solutions for sensors and actuators in homes and automotive (TRL 3) • Materials for higher precision positioning and improved sensitivity sensors (TRL 3) • Development of a technology platform for multiple, selective response factors (TRL 3) • Development of recycling methods for materials with added functionalities (TRL2)	• Response platform will be broadened by new concepts (TRL 3) • Sustainable recycling technologies for materials with added functionalities (TRL 5) • Sustainable recycling technologies for materials with added functionalities (TRL 5).	• New multi-functional materials successfully introduced to market (TRL 9) • Several new concepts for multi-functional materials be further developed to prototypes (TRL 7) • Sustainable recycling technologies for materials with added functionalities (TRL 7)
High-tech materials	• Design of new materials for EUV lithography and for additive manufacturing (TL3)	• Response platform will be broadened by new concepts (TRL 3) • Sustainable recycling technologies for materials with added functionalities (TRL 5).	• High tech materials proven to function in several prototypes (TRL 9) • Sustainable recycling technologies for materials with added functionalities (TRL 7)

	• Development of smart materials and solutions for sensors and actuators in homes and automotive (TRL 3) • Materials for higher precision positioning and improved sensitivity sensors (TRL 3)		
Bio-medical materials	• Control of interaction of living matter with man-made materials (TRL 3) • New platforms for theranostics (TRL 3) • Development of small scale disease diagnosis schemes (TRL 3) • Development of a technology platform for multiple, selective response factors (TRL 3)	• Selection of biomedical materials tested (TRL 5) • Sustainable recycling technologies for materials with added functionalities (TRL 5).	• Biomedical materials for diagnostics and/or controlled drug delivery in clinical trials (TRL 7) • Several new concepts for biomedical materials will be further developed to prototypes (TRL 7) • Sustainable recycling technologies for materials with added functionalities (TRL 7)

2.2 Thin films and coatings

Introduction

In addition to the challenges described for functional materials in the previous paragraph, there are specific other challenges for functional coatings and thin films , related to their surface-dominated property demands. In this task we focus on those additional functionalities, but it is clear that for a large number of applications the required thin film / coating properties also involve the continuum characteristics described earlier (mechanical, chemical, physical) as well as the dependency on the manufacturing capabilities of the (macro)”molecules” that have to constitute these functionalities.
The science in this field has made impressive progress in the past 15 years. For example, smart coatings which are switchable from IR transparent to blocking by response to external triggers such as temperature are being explored. Further development of the underlying technologies will open new opportunities.

Tasks

Description of the task and the relevance for society, industry and science
Functional coatings, thin films and membranes are of importance for a broad spectrum of applications ranging from biomedical to energy harvesting and storage. Although coatings with one or multiple passive functionalities are already known and applied, active, adaptive and even instructive systems are rare. The potential value of such systems which can adapt to their external environment or potentially even instruct biological species to perform in a certain manner, is very high. Similar considerations are valid for functional thin films and membranes. Furthermore, functional coatings, thin films and membranes should be developed to facilitate energy efficiency, harvesting and storage. This includes the development of novel, non-toxic and durable antifouling coatings for maritime applications. Additionally, membranes have the potential to become important contributors to sustainable chemical processes. Moreover, functional coatings, thin films and membranes that contribute to a circular economy should be developed, *e.g.* product related to circular packaging and reversible adhesives, and retrofit solutions to restore functionality in existing systems.

Solution for this task described SMART (present-2050)
Present-2025 The development of functional coatings, thin films and membranes should focus on following main topics: (a) the transition from coatings with one or multiple passive functionalities to active, adaptive and even instructive coatings, (b) the development of coatings, thin films and membranes tailored for energy efficiency, harvesting and storage, (c) the development of bio-instructive coatings and (d) the development of membranes for sustainable chemical processes, (e) functional coatings, thin films and membranes that contribute to a circular economy.

2025-2035 Start-up companies/SMEs in functional coatings, thin films and membranes should grow, and first demonstrators of coatings, thin films and membranes from the above mentioned categories should find their way into industry. First responsive/active biomedical systems should be industrially produced, and first bio-instructive systems should be demonstrated at TRL 5-7.

2035-2050 Three decades from now, NL will be a world leader in functional coatings, functional thin films and membrane technology and provide high value-added adaptive/active/instructive systems. Bio-instructive coatings are industrially produced, new breakthrough energy harvesting/storage concepts are developed to prototypes, and functional coatings, thin films and membranes that contribute to a circular economy should be developed, *e.g.* product related to circular packaging and reversible adhesives, are widely implemented.

What <u>existing</u> competences, technologies, knowledge contribute to this task?
Traditionally, NL has a very strong position in coatings, thin films and membrane materials, both in research institutes and industry. Advanced infrastructure allowing control down to the level of a single atomic layer, as well as characterization techniques (including large scale facilities like synchrotrons) have been established in NL (with support from programs like NanoNed and NanoNextNL) and require continued investments.

What <u>additional</u> competences, technologies, knowledge do we need?

The same needs exist here as under 2.1.1.4, but more focused on surface driven phenomena in coating, thin films and membranes. Material surface analysis and characterization on the level of such thin films has to be developed strongly (microscopy, spectroscopy, scattering, ellipsometry). Adhesion is an example of a crucial performance parameter for thin films in which fundamental understanding needs to increase substantially. Process development is required for the precision production of functional coatings, thin films and membranes, potentially involving real-time process analytical techniques. Advances in coarse grained modelling are needed to understand surface dynamics (restructuring upon different media contacts).

Designing thin films/coating materials with the right functionality

Specific surface-dominated functionalities are listed below.

1. Mechanical: adhesion of thin layers on substrates or between thin layers in multi-laminates, resistance against scratch and wear stress, switching fatigue.
2. Chemical: resistance against high-energy radiation such as UV, ozone, weather and moisture. Creation of active molecules upon absorption of high-energy radiation such as UV (photo-oxidation).
3. Physical: roughness and surface topology, optical properties of thin layers (in/outcoupling of light, matting versus gloss, reflection or antireflection), photo-active properties (photon conversion), thin layer electro-conductivity and electrical breakdown resistance. Barrier properties and perm-selectivity of thin layers and membranes.
4. Interfacial properties: solid-liquid: (super)hydrophilicity and (super)hydrophobicity, switchability. solid-solid: corrosion protection (resistance to ion migration across the buried interface), dusting. solid-cell: antimicrobial properties. solid-tissue: haemocompatibility, anti-inflammation, biostability.

A - Traditional coatings, packaging films and membranes.

Although coatings and films usually already combine different functions, we will discuss here some step changes that are still highly needed in the already known functions.

- *Anti-corrosion* is still an unsolved challenge. Advanced coatings tailored to corrosion protection of metallic substrates are of the utmost relevance to ensure reliability and long-term performance of coated parts as well as the product value of the coated materials. Durable passivation of the interface (also when damaged) remains an unmet need.
- *Barrier properties* of membranes and packaging films against most prominently oxygen, water and carbon dioxide, or even perm-selectivity are still in need of higher performance materials with tailored micro- and mesomorphology. Examples are in aluminum-free barrier packaging foils (easy to recycle, see 3.3), breathable packaging for fresh foods (water and oxygen in, carbon dioxide out), membranes for fresh water (decontamination), highly selective membranes for industrial separation processes. In addition to the above mentioned functional properties, the need for circular packaging concepts is high. This involves both the development of recycling concepts for existing commercial packaging materials, and the development of novel packaging materials according to the design-for-recycling concept.
- *Prolonged service life time* for protective and decorative coatings can result from a marked increase in UV/outdoor exposure resistance by more stable polymer design on the one hand and increased insight in stabilization mechanisms on the other. Prolonged service lifetime benefits the circular economy based on reduction of waste and less use of new materials.
- *Non-toxic and durable marine anti-fouling coatings* are highly desired in marine transport, while current technologies work only under release of heavy metals (tin, copper) or high velocities.
- *Increased use robustness of protective and decorative coatings* is a ubiquitous unmet need: car body coatings are still vulnerable to scratching, while waterborne coatings are still notoriously difficult to apply on its plastic parts without expensive pre-treatments because of loss of adhesion, membranes for energy saving separation processes have limited lifetime. Increased mechanistic insights into these mechanical properties on the micro- and mesoscale are expected to substantially increase these durability performances.

B - Active, adaptive and instructive systems The potential value of coatings which can adapt to their external environment or potentially even instruct processes that take place on their surface, is very high. Similar considerations are valid for functional thin films and membranes. Following examples illustrate potential applications of such systems:

- *Sensoring and signaling* of food packaging materials, indicating for instance heat or oxidative stress, pH change, metabolite or toxin levels, ageing or even microbial activity inside the packaging will help tremendously in prevention of food waste. But also simply monitoring the performances of thin films, coatings and membranes in situ over time without being damaged is of great desire. It will enhance the product security and safety and the response technologies will be applicable in a broad range of applications, e.g. food, water supply, construction industry, automotive, aerospace and medical equipment. A combination of responses will enhance the utility of a thin layer/coating/membrane.
- *Active ion transport* incorporated in water-permeable membranes can enable low-energy desalination devices.
- *Active scavenging or (chemo)absorption* of unwanted species (water, carbon dioxide) inside a packaging material can help to establish the ideal atmosphere for safe storage of food and medicine. All the while, packaging films become thinner, requiring less raw material to be used. This asks for a strong demand in manufacturing processes developments, e.g. multi-, micro- or even nanolayer co-extrusion processes offers enormous unexplored possibilities.
- *Coatings or films that can switch between transmission and blocking of solar infrared radiation* and *vice versa* can be applied in insulating glass units to reduce the energy consumption for heating and cooling of buildings in intermediate climates. Examples of such coatings/films are thermochromic (switch triggered by temperature), electrochromic (switch triggered by electrical stimulus) and photochromic (switch triggered by light).
- *Bio-instructive coatings* that modulate cell behaviour e.g. for engineering biofunctional surfaces of implants.

C - Coatings, thin films and membranes tailored for energy efficiency, harvesting and storage

One of the grand challenges for Europe in the coming decades will be to guarantee a sustainable supply of energy – beyond the use of fossil fuels and nuclear energy. For that purpose, efficient harvesting of renewable energy, e.g. wind or solar, and conversion into a useable form is of utmost importance. In addition, it is of vital importance to reduce the energy consumption. Both in optimizing energy harvesting/conversion en decreasing energy consumption, coatings and films play a key role. Examples include:

- *Coatings and films for photovoltaics:* light in-coupling/trapping, photon up-/down-conversion, ITO replacement, easy-to-clean, anti-dust, printable transparent conductors, passivation, improvement in life-time.
- *Coatings and films for lighting devices:* light out-coupling/extraction, photon conversion, ITO replacement, printable transparent conductors, improvement in life-time.
- *Solar control coatings for the built environment:* infrared management, switchable coatings for insulating glass units (e.g. thermochromic, electrochromic), coatings for greenhouses, aesthetic coatings for solar thermal systems.
- *Coatings for windmills:* Impingement and erosion resistant coatings are necessary to supply market demand for increasingly larger wind turbine blades. On top of that reduced materials use and recycling are of importance for the a large area applications
- *Coatings for aerospace:* anti-icing, anti-drag (micro-aerodynamics)
- Membranes for use in CCU and CCS processes. High performance coatings and membranes for energy transition. e.g. membranes for batteries

D - Coatings, thin films and membranes that contribute to a circular economy

On a planet with limited resources we have to transform linear into circular material flows. Examples of coatings, thin films and membranes that contribute to this objective are:

- Coatings and thin films that contribute to circular packaging, incl. concepts that enable the recycling of current packaging materials and novel design-for-recycling packaging concepts.
- Reversible adhesives that enable removal of materials for recycling/re-use.
- Coatings, thin films and membranes that contribute to a prolonged service lifetime of functional products.
- Membranes that are tailored for recycling processes.
- Membranes for CCU processes.
- Retrofit coatings and thin films developed to restore functionality of existing systems and as such prolong their lifetime.

ChemistryNL

Summary

Topic	Short term (-2025)	Medium term (2025-2035)	Long term (2035-2050)
Traditional coatings, packaging films and membranes	• Development of large scale high precision deposition processes for sub-micron thick functional coatings. • Growth of start-up companies in (multi-)functional coatings and films. • Advanced anti-corrosion coatings to ensure reliability and long-term performance of metallic substrates developed. • Advanced barrier coatings for membranes and packaging films developed. • Non-toxic and durable marine anti-fouling coatings developed.	• Implementation of large scale high precision deposition processes for sub-micron thick functional coatings. • Advanced anti-corrosion coatings commercially produced. • Advanced barrier coatings for membranes and packaging films commercially produced. • Non-toxic and durable marine anti-fouling coatings commercially produced.	
Active, adaptive and instructive systems	• From passive biomedical functionalities to bio-instructive coatings. • Sensoring and signaling coatings developed, e.g. for food packaging materials. • Concepts for active ion transport incorporated in water-permeable membranes developed for low energy desalination. • Concepts for active scavenging or (chemo)absorption of unwanted species developed.	• First responsive/active coatings industrially produced. • First sensoring and signaling coatings commercially applied. • Pilots with membranes for low-energy desalination established. • Pilots with coatings, thin films and membranes for active scavenging or (chemo)absorption of unwanted species.	• Responsive, active and interactive coatings, thin films and membranes industrially produced. • Bio-instructive coatings industrially produced. • Low energy desalination commercially applied.
Coatings, thin films and membranes tailored for energy efficiency, harvesting and storage	• Coatings, thin films and membranes that contribute to the energy transition, focusing on energy efficiency, energy harvesting and energy storage. • Coatings and films for photovoltaics, e.g. for increasing efficiency or prolonged lifetime. First systems commercially produced. • Coatings and films for lighting devices, e.g. for more efficient light extraction or	• Solar control coatings for the built environment: first dynamic systems for intermediate climates commercially applied. • First membranes for use in sustainable chemical processes industrially produced. • First membranes that contribute to the energy transition industrially produced.	• New breakthrough energy harvesting/storage concepts developed to prototypes.

	prolonged lifetime. First systems commercially produced. • Solar control coatings for the built environment: first dynamic systems for intermediate climates produced on lab/small pilot scale. • Concepts for circular impingement and erosion resistant coatings for windmills established. • Concepts for anti-drag and anti-icing coatings for aerospace to reduce fuel consumption developed. • Membranes that contribute to the energy transition. • Membranes for use in sustainable chemical processes such as electrochemical conversions, photochemical conversions, CCU processes.	• First pilots with innovative anti-drag and anti-icing aerospace coatings established.	
Coatings, thin films and membranes that contribute to a circular economy	• Membranes for use in recycling processes developed. • Coatings and thin films that contribute to circular packaging, incl. concepts that enable the recycling of current packaging materials and novel design-for-recycling packaging concepts, developed. • Reversible adhesives that enable removal of materials for recycling/re-use developed. • Coatings, thin films and membranes that contribute to a prolonged service lifetime of functional products developed. • Retrofit coatings and thin films developed to restore functionality of existing systems and as such prolong their lifetime.	• Membranes for use in recycling processes demonstrated in pilots. • First coatings and thin films that contribute to circular packaging commercially applied. • First reversible adhesives that enable removal of materials for recycling/re-use commercially applied. • Coatings, thin films and membranes that contribute to a prolonged service lifetime of functional products commercially applied. • First retrofit coatings/films in pilots.	• Membranes for use in recycling processes commercially applied. • Novel design-for-recycling packaging concepts commercially applied. • Coatings, thin films and membranes that contribute to a prolonged service lifetime of functional products commercially applied.

2.3 Materials for sustainability

Introduction

Materials for sustainability / sustainable materials encompass a wide spectrum of materials and includes materials that are produced in a more sustainable way, make a process/chain more sustainable and/or are used for sustainable energy production or storage" - we include materials based either on polymeric materials, or on inorganic/mineral based materials or hybrid materials.

These materials will have in common: less non-renewable energy use (NREU) and less green-house gas (GHG) emission during the synthesis, construction, processing, packaging, transportation usage, recycling and re-use of these materials. Specific subsets of such materials will even have a positive impact on NREU production e.g. solar cells.

Furthermore, the demand for raw materials increases significantly, such as for oil, rare metals etc. Whereas oil is essential for energy, chemicals and high-performance materials (plastics, fibers, etc.), minerals and metals are crucial in numerous products (electronics, catalysts, solar cells, wind turbines, fertilizers, etc.). A list of 20 critical raw materials was identified by the EU related to supply risks based and economic importance. Clearly, solutions are needed to overcome this upcoming scarcity.

Tasks

Description of the task and the relevance for society, industry and science.

Sustainability is important to accommodate the growth of the world population and its future demand of resources for water, food, energy at higher average life standard. This requires a significant change of today's practice. Changes include the minimization of the manufacturing footprint of the material, but also the sustainable gains of its use during the life cycle and clever re-use of the material or its components. Resources for energy (fossil origin) and raw materials (rare elements) are depleting and this requires a transition to sustainable energy production and reduction, replacement or recycling of rare elements and the further development of renewable or circular materials. The transition to a sustainable society will have a tremendous impact and takes place in stages. Initial efforts are aimed at reducing the footprint by making existing technologies more efficient. Via temporary solutions in intermediate stages, the final goal is a (circular) society based on truly sustainable resources for energy and materials. In this transition to a sustainable society, advanced materials will play a crucial role: a sustainable society cannot be realized without the corresponding materials that enable it.

Solution for this task described SMART (present-2050)

2020-2025 Materials for sustainability / sustainable materials are an emerging field for NL, and also worldwide and will have a tremendous (economic) impact. Our country is too small to leave a large footprint on the planet, but it can contribute to a circular economy of the coming decades, based on two competitive advantages: 1) the excellent knowledge infrastructure for generating (and selling) new technologies, and 2) the high population density and existing organization degree of our society in terms of recycling and energy distribution, enabling for example complicated recovery / separation streams for reuse of materials. We need to try and predict and design the circular material streams, stimulate IP and start-ups and test these hypotheses in small-scale demonstration projects (examples are technologies and materials for additive manufacturing developed in recent years).

2025-2035 In the next decade, regulations (national, EU and global) should be matched with the level of demonstrated circular material use and improved sustainable and clean energy concepts. Supported by this, the scale-up of the envisioned material streams should be implemented. New technologies for material replacement, reduction, reclaim and reuse will lead to large scale industrial activity. Sustainable energy production and storage systems developed in NL, IP protected and sold to areas with larger footprints. This will be supported by the growing image of NL as "designer material" technology provider (2.1.1).

2035-2050 Two decades from now, NL will have settled its name as technology provider for circular use of high value (functional) materials, and sustainable energy materials, based on its knowledge infrastructure as well as its logistic opportunities and its demonstration infrastructure for new technologies in complicated societal environments.

What existing competences, technologies, knowledge contribute to this task?
The existing competences in material (polymer, ceramic) synthesis and manufacturing can greatly contribute to the design and making of new materials / polymers to play their role in sustainability. The chemistry, as such, of these materials does probably not need to be altered completely, just adapted, improved, with enhanced control. For example, in the field of polymers using the existing principles of polycondensation or polyaddition (using renewable or circular building blocks) new polymers can be designed with more advanced functionalities than the present ones. This leaves every opportunity to use NL's leading position in this knowledge field to contribute. NL also has a strong position in research on materials for sustainable energy production, linked to nanomaterials research for harvesting solar energy (PV and more recently solar fuels). The area of clean energy and resource efficient production and reuse processes spans a wide range of chemistry and materials science where in many areas NL has relevant expertise due to the innovative role of the NL chemical industry.

What additional competences, technologies, knowledge do we need?
Raw materials: a closer backward integrating connection needs to be made with the "Making Molecules" roadmap. Also, the design principles ("assemble to disassemble") need to be rethought to enable circular material use and re-use. Research on energy storage (batteries) has declined in NL in the past decades, but offers opportunities for economic activity as the car manufacturing in EU is still strong and NL plays a key role in the supply of materials to this industry. Also, in the field of renewable or circular materials, many efforts are underway. This field, however, needs further time to implementation as cost-effective routes to existing products have to compete with optimized fossil-based assets. The focus should therefore be on truly new materials of biomass / renewable / circular origin. Molecular modelling and coarse grained modelling are expected to contribute to the understanding of the translation of novel building blocks into new materials.

Designing materials with the right functionality

A – Polymeric materials

There are several options to reduce the environmental impacts related to polymer production and use, many of which are also relevant for other bulk materials. Declining reserves of fossil feedstock and the need to mitigate CO_2 emissions enforces an increased use of biomass, other renewable (for instance carbon dioxide offers an accessible, cheap and renewable carbon feedstock for monomer production) or circular resources. In the production of polymeric materials. On the mid to longer term the importance of producing and using renewable and/or circular materials will be of imminent importance. Such materials will be based upon modified natural biopolymers (e.g. starch cellulose, proteins), but increasingly also as a result of polymerizing renewable and/or circular monomers into thermoplastic and thermosetting polymers. Bio-based polymers produced by polymerizing monomers are anticipated to grow even more in importance than the use of modified naturally occurring polymers. Initially polymers based on renewable and/or circular building blocks will have physical properties very much alike todays' petrochemically based polymers. The polymers can be structurally identical to fossil-based polymers (also known as "drop ins" e.g. bio-based polyethylene) as well as based upon unique monomers (e.g. polylactic acid).
Once having an established market share of at least 10% (envisaged for 2030), it will become increasingly important also to derive renewable and/or circular materials with novel or added properties such as improved gas barrier- fire retardancy, antimicrobial, self-cleaning and self-healing or self-assembling properties. In addition the additives used in plastic materials should be reduced to the absolute minimum to facilitate recycling processes and is still strictly required also be based on renewable and/or circular building blocks. A huge challenge is furthermore to develop "triggered degradation concepts" enabling the development of materials with a long life span but which nonetheless can be degraded under appropriate end-of-life conditions or if unintentionally released into the environment (which should of course be avoided strictly)..
In addition, improved waste management by (mechanical and chemical) recycling of materials, re-use and recovery of product components and / or compounds will become more important in the near future. Recycling of petrochemical based polymers is currently dominated by the recycling of PET. Recycling of other polymers like polyolefines should increase in importance and will require the development of novel processing and /or additive technology to be able to maintain material properties and not decrease ("downgrade") material properties while recycling.
In order to enhance the possibilities for recycling, in general materials with less complex formulations (mono-material solutions) will be desired, and the ability to recycle and recover should be regarded as one of the most important

performance characteristics of a material. For materials that are supposed to be used (virtually) as new again ("upcycling"), it is important that they can be separated, not just physically, but also chemically. This still requires a lot of basic research.
"Back to monomer recycling" of polymers will increase in importance, since recycling and use of polymers will inevitably result in material deterioration; Recycling of thermoset materials is a challenge for which dedicated technology should be developed. A promising alternative route is "design for recycling" – during the design of the material future reuse is already anticipated.

Challenges:
(a) With regard to naturally occurring biopolymers such as polysaccharides (starches and cellulose etc.), there is a need for better understanding of their physical properties in relation to their detailed structure, a need for site specific (bio)catalytic modifications strategies and a need for chemistries that allow the product to be modified while avoiding highly polar, potential hazardous solvents (e.g. NMP, DMAA). With regard to lignin as another natural occurring irregular polymer there is a higher need to develop chemo- or biocatalytic strategies to obtain well defined products at higher value. Improved biotechnological modification strategies should enable us to use these products in a broader range of applications, including e.g. water based paints, coatings, adhesives, dishwashing formulations, cosmetics etc., but also in more durable products like agrofibre reinforced materials or bio-based plastics. This will also lead to the envisioned novel or added properties.
(b) New routes to turn CO_2 into monomers and polymers will become a key driver to accelerate and facilitate the transition from existing fossil-based to future generations of renewable or circular materials. Catalysis is the key enabling technology / challenge in this respect, providing new opportunities to turn this carbon feedstock into valuable materials.
(c) With regard to identical "drop-in" chemicals (and the polymeric materials based upon them) the challenge is to develop technology to optimize biorefinery systems for generating the feedstock and optimizing biotechnological or chemo-catalytic modification methods to get to efficient ways of synthesizing the identical, drop–in chemicals. For unique molecules and materials, development of efficient synthesis routes as well as the synthesis and exploration of new unique materials based upon these monomers should go hand-in-hand.
(d) an additional challenge for renewable or circular polymers results from polymer additives (including processing aids, lubricants, heat stabilizers, antioxidants, pigments etc.) and auxiliary agents (e.g. catalyst, solvents) with reduced Health, Safety, Environment (HSE) issues. Materials for sustainability will also require polymer additives with substantially reduced HSE issues compared to many of the current ones (e.g. lead based heat stabilizers, brominated flame retardants etc.). Furthermore, polar solvent that are very important to the current and future industry like NMP, DMSO and DMAA should be replaced. It is of absolute importance to develop new classes of additives and solvents, designed and engineered for optimal functioning in new renewable or circular polymers.
(e) End-of-life solutions such as recycling and chemical/physical recovery are in their infancy in the Dutch academic and industrial landscape. A strong focus should be put on this topic to not miss this important opportunity to close the loop in the field of materials for sustainability. Life cycle analysis (LCA) should be included as much as possible when assessing materials production, use and end-of-life.

B - Sustainable synthesis and production - Increased energy efficiency and material efficiency (yields) in all processes in the value chain leading to more sustainable products
Over the years, chemical processes have continually improved in terms of their greater utilization of (secondary) raw materials, improved safety and increased productivity whilst minimizing waste and energy use. Yet, chemical industry is still facing the need to restructure and modernize by continuing to reduce energy as well as resources consumption (i.e. both raw materials and water) besides reducing waste as amounts and emissions at the same time.
Challenges:
To achieve near 100% selectivity in multi-step and complex syntheses. Exploration of new reaction pathways and conditions, reduction of the number of reaction steps, introduction of intensified separation technologies and intensification in the energy input; design of integrated processes, adapted materials (i.e. membranes for hybrid separations), solvents (i.e. ionic liquids for extraction) as well as equipment.

C - Sustainable materials for energy
As high-density energy sources like fossil fuels will take more energy to access in the future, advanced materials will be used to fulfill our energy demand. Cost-effective and energy efficient options for capturing, converting and storing

naturally available energy (solar, mechanical, thermal etc.) are highly sought after. New materials and chemical synthesis routes will provide these novel materials in the future. Photovoltaic materials like perovskites can convert light into electricity and other inorganic materials can be used to store energy in batteries.
Solar cells are already the most cost-effective option for sustainable electricity generation. However, the production of solar electricity needs to grow by about two orders of magnitude within two decades. Such enormous growth needs higher efficiency to reduce the impact that this form of electricity generation has on the environment, and ways to fabricate these solar cells at much faster rate. Foil-based solar cells and tandem geometries are ways to produce solar cells at an unprecedented speed and efficiency, and with much lower resource intensity (earth-abundant materials, low energy consumption during fabrication, fast roll-out). These solar cells require innovation in materials, interfaces and device design.
The use of materials for energy storage is expected to develop impressively in the coming decades. The need for storage of electrical energy, generated by a plethora of technologies – on large scale (the “grid”) as well as small local scale, will steeply increase. On the one hand this energy can be stored in reversible chemistry, such as in well-known in batteries (Li cells) but also in for example hydrogen cells. Recent battery developments have shown considerable progress in terms of energy density (J/Kg) but still faces challenges and limitations in terms of power density (W/Kg), while the different needs for energy storage will be requesting breakthroughs at both fronts (transport, portable devices, local solar facilities). Supercapacitators hold promise for higher power densities, but are still in their (technology) infancy. Polymer supercapacitators are in need for reliable multi-lamination technology of thin films (see also 3.2) with step-change increased electrical breakdown resistance.

Challenges:
Materials and processes are needed that can meet the energy demand. Materials composed of non-critical elements will ensure availability and reduce the cost for market introduction. Durable materials are needed that have a long lifetime or can be easily recycled. For phase-changing materials, mechanical stability is an additional issue that needs to be addressed. Processes are needed that can deliver the volumes associated with the application markets. The energy required for these processes should be kept as low as possible, since this effectively reduces the energy that can be generated with these materials.

Summary

Topic	Short term (-2025)	Medium term (2025-2035)	Long term (2035-2050)
Polymeric materials	• Develop renewable or circular building blocks • Develop sustainable polymeric materials based on “drop in” renewable or circular monomers or novel building blocks • Design of better recovery rates and more efficient mechanical recycling methods • Design of the next generation of technology for effective chemical recycling, including (bio)catalysts	• Further development of technologies for renewable or circular additives like plasticizers, flame retardants and lubricants from TRL5-6 to 9 • Establishing LCA studies for all commercial materials use • Scale up of mechanical & chemical recycling technologies	• Scaling up and usage of renewable or circular materials • Implementation of materials developed in “design for recycling” projects • Circular use of all commodity plastics established
Sustainable synthesis	• Further development of (bio)refinery technologies (especially relevant for chemical conversion roadmap) • Design of the next generation of multifunctional (bio)catalysts by integrating knowledge on hetero-, homo-, single-site and biocatalysts (see catalysis roadmap) • Development of improved (bio)catalyst technologies enabling improved control over molecular architecture of polymers and polymerizations at lower temperatures and lower energy input	• Intensified reaction and process design (including smart design of the synthetic route, micro process technologies, catalytic reactions, fluid dynamics, separation technology, particle technology, advanced process control, integration and intensification of processes combined with new catalyst concepts and increasingly sophisticated computer modelling of chemical interactions and plant simulation	• Increase energy- and resource-efficiency and reduce waste as well as emissions generation in all processes in the production chain

Sustainable materials for energy	• Understanding and modelling of the phase stability of novel materials • Understanding and modelling of the properties of novel materials • Optimizing materials for efficiency and stability (e.g. thin film perovskite solar cells with high radiative efficiency) • Stable, selective and conductive interface materials that can be processed in a roll-to-roll fashion • Develop academic and industrial research lines centered on energy storage and electrochemistry	• Prediction of phase stability of novel materials • Prediction of properties of novel materials • Understanding and modelling of mesoscopic properties • Light-management strategies for tandem solar cells • Development of fast, scalable fabrication techniques for foil-based solar cells	• Ab initio prediction of materials based on material properties • Implement designed energy production and storage solutions in industrial commercial context • Integration of, and interaction with the environment and ecosystem in solar parks of the km^2 scale