Roadmap
Chemistry of Advanced Materials

Note to reader: This is a dynamic document. In Q1 2021 we expect some last finetuning of the roadmaps, and potentially some additions of topics. If in doubt whether your proposed research fits in to one (or more) of our roadmaps, always contact the office of ChemistryNL via tkichemie@tkichemie.nl.

To guide you through the landscape of roadmaps and KIA's we will shortly also publish a quick guide to the connection between the mains tasks of each roadmap with the national mission and key technology KIAs.

ROADMAP CHEMISTRY OF ADVANCED MATERIALS

0. 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 on 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 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. For the latter, a broader scientific foundation of functionality of materials should be developed, including (predictive) modelling of formulations and properties.

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 exert 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 2040 are summarized in the table below.

This roadmap on the chemistry of advanced materials is mainly sustained by the Topsector Chemistry roadmap on Making Sustainable Chemical Products and the Topsector Biobased Economy, by providing sustainable raw materials and (catalytic) technology for control of conversion of these raw materials into advanced materials. This connects to the EU Horizon 2020 theme of Resource Efficiency. In turn, the major beneficiaries of this roadmap are in the Topsector Chemistry roadmaps on Chemistry of Life (Biomedical Materials) and on Nanotechnology and Devices, 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 EU Horizon 2020 themes Health, Energy, Transport, and Nutrition Security.

	Short Term Now – 2020	Medium Term 2020-2030	Long Term 2030 - 2040	Program Line Ambition
Materials with Added Functionality	• Improved performance of existing materials. • Development self-healing polymers and ceramics. • Mechanistic insight for functional polymers, nanocomposites, metals, high tech materials.	• Higher strength polymers industrially produced • Rational material design capabilities. • Knowledge base for start-ups future materials, e.g. biomedical and self-healing.	• Reinforced composites and multi-functional materials successful in market. • High tech materials proven in prototypes for automotive and home. • Biomedical materials in clinical trials.	*NL will have settled its name as "rational material design" technology provider for high value-added functional materials and clean energy materials.*

Thin Films and Coatings	• New corrosion protection technologies for automotive, construction and Hi-Tech • Coatings with antimicrobial properties. • Sensoring response coatings Self-healing technologies for thin films and membranes.	• First responsive and active coatings industrially produced • Development of nanolayer production technologies. • Growth of start-up companies in areas like specialty coatings, ion/molecule sensing and air/water purification	• Bio-interactive coatings industrially produced. • Implementation of nanolayer production technologies. • New energy creation concepts developed to prototypes.	*NL will be a world leader in thin film technology and provide high value-added functional coatings, protective coatings and membranes combining sensory functions with separation technology.*
Materials for Sustainability	• Predict and design circular material streams, start-ups. • Improved control molecular architecture of polymerisations with lower energy input • Design of novel materials for energy harvesting and storage	• New technologies for material replacement, reduction, reclaim and reuse. • Dedicated polymer additives for biobased polymers	• Implement energy production and storage solutions in industrial commercial context. • Multifunctional (bio)catalysts for effective recycling. • Use of green solvent	*NL will be leading as technology provider for circular use of high value (functional) materials, bio-based materials, and sustainable energy materials.*
Enabling Science/ Technology	• Electrochemistry and research on energy storage (batteries) • Basic research in emerging classes of advanced materials. • Initiatives like NanoNextNL Large scale infrastructure	• Modelling and computational chemistry on different length scales. • Material surface analysis and characterization of thin films (microscopy, spectroscopy, scattering, ellipsometry).	• Integration of multiple length scales. Understanding of how functional properties on the nanoscale translate to functionalities on larger length scales, leading to implementation in new products.	

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, rechargeable batteries. Next to these examples, materials chemistry has also substantially contributed to developments in food packaging, in biobased materials and in enabling regenerative medicine and making artificial skin and 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 as 3D-printing, self-assembly, or 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 in these dimensions is key. Theory and computational methods will increasingly be used in 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 a vibrant field of research and new developments. Novel materials, being organic, inorganic or hybrid in nature, with unprecedented properties 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. Several 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, Transport
2. Thin films and coatings, related to Food security, Energy, Wellbeing
3. Materials for sustainability, related to Resource efficiency, Energy, Health

2. Overview of Tasks

2.1. What tasks can be defined and how does the programme council prioritize these?

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 "do" more things too. Materials combining multiple functionalities ("smarter" materials) provide an added societal and economic value.
2) **Thin films and coatings**. Besides the intrinsic properties of materials, in thin films and coatings the effects of the surface on its properties, as well as the functionality that the surface properties brings 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 2020 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]

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, the vision documents mentioned all display a future in which advanced materials exert 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 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.

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

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[1] Vision Paper 2025 Chemistry and Physics (commissie Dijkgraaf)
Catalysis - Key to a Sustainable Future (Science and technology Roadmap Catalysis 2015)
Dutch Materials, Challenges for Materials Science in the Netherlands (FOM, 2015)

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?

2.1.1. Materials with added functionality

2.1.1.1. 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, 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.

2.1.1.2. Solution for this task described SMART (present-2040)

- 2015-2020 Starting from a strong point of NL, with excellent R&D infrastructure and a good basis for public-private partnerships in material technology development, a mechanistic insight should be obtained for each of a plethora of desired functionalities (see 3.1) in e.g. functional polymers, nanocomposites, metals, high tech materials aimed at aiding implementation of new functionalities in products in cooperation with industrial partners. From a fundamental science perspective, specific functionalities should be fully understood, also in relation to each other and 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.
- 2020-2030 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. 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. The entrepreneurial climate, as well as strong "designer material" knowledge base will allow the growth of start-up companies (e.g. example for future materials like biomedical and self-healing materials) and expand the materials field in an area without cheap resources. This will be in support to typical EU industries like agricultural, car manufacturing, medical, high tech, and energy related industry and in full support of the ageing population.
- 2030-2040 Two 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.

2.1.1.3. 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. Large scale infrastructure (synchrotron radiation, free-electron lasers, neutron scattering, electron microscopy, nuclear magnetic resonance, etc.) are increasingly used to investigate and characterize materials properties. The Netherlands has access to and strong expertise with materials research using these large scale facilities.

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

Investment in the area of bottom-up micro-meso-macro scale morphology analytics and control of 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 and bio-medicine, with a strong input from rapidly advancing analytic techniques (allowing 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: MD, meso: coarse graining, macro: finite elements).

2.1.1.5. How do the tasks connect to grand challenges in H2020?

This task can be connected to many of the overarching Horizon 2020 themes, but most prominently with:

- Smart, Green and Integrated Transport. For example energy saving by reducing weight of vehicles (based on new designs, enabled by new functions and self-healing capabilities), or developing new materials for use in (manufacture of) new high-tech devices.

- Health, Demographic Change and Wellbeing. For example biomedical materials, new materials enabling life style (sports, clothing, ICT) and quality of life (ageing population, health care, diagnostics).

2.1.2 Thin films and coatings

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

Thin films and coatings are everywhere as they form important barriers to selectively protect or selectively allow permeation. For many applications the desired properties are not met, as is exemplified by the still unsolved problem of metal corrosion. .

2.1.2.2 Solution for this task described SMART (present-2040)

- 2015-2020 Similarly to the first task, NL has the luxury of strong starting position due to the active presence of coating companies (AKZO, DSM, DOW, SME's), water treatment companies and TOP institutes (Wetsus, DPI, MESA+, DIFFER, etc.). Building on this strength, connections should be made between the different actors in pre-competitive cooperation consortia, with the aim to obtain mechanistic insight into desired functionalities of thin layers (see 3.2) with emphasis on surface effects. Recent advances give an unprecedented control over layer thickness and composition, down to the atomic level, and allows for tunable physical properties. However, more is needed. The strong position of NL in this field requires further investments in expensive infrastructure both for short term and long term advanced materials development.
- 2020-2030 Moving from increasing insight and understanding towards rational material design capabilities, a broader scientific foundation of functionality of thin films and coatings is to be developed, including (predictive) modelling of properties. Several new technology platforms are expected that make NL an attractive manufacturing area as price per kilogram will be replaced by price per square meter surface value added, yielding high profit margins for coatings with added functionalities (e.g. sensing capabilities) and/or better protective capabilities with applications ranging from 'smart' food packaging to coatings for the aeronautics industry. The entrepreneurial climate, as well as strong "designer film" knowledge base will allow the growth of start-up companies in areas like specialty coatings, medical diagnostics, ion/molecular sensing and air/water purification based on thin film and membrane technology.
- 2030-2040 Two decades from now, NL will be a world leader in thin film technology and provide high value-added functional coatings for a wide range of applications where NL presently already has a strong position (protective coatings, (food) packaging). A strong industrial activity based on functional coatings and membranes combining sensory functions with thin film separation technology is established in areas like medical diagnostics and clean air/water industry.

2.1.2.3 What existing competences, technologies, knowledge contribute to this task?

Traditionally, NL has a very strong position in coatings and packaging 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) has been established in NL (with support from programs like NanoNed and NanoNextNL) and requires continued investments.

2.1.2.4 What additional 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 thin films. 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. Continued support for initiatives like NanoNextNL is crucial to keep the (expensive) infrastructure competitive. Advances in coarse grained modelling are needed to understand surface dynamics (restructuring upon different media contacts).

2.1.2.5 How do the tasks connect to grand challenges in H2020?

With the specific focus on surface-dominated material properties, this task can be connected most prominently with:

- Food Security, Sustainable Agriculture and Forestry, Marine, Maritime and Inland Water Research and the Bioeconomy. For example new packaging materials that allow the optimal storage atmosphere inside (breathing), sense and signal deterioration, prevent waste of foods and nutritional value.
- Health, Demographic Change and Wellbeing. For example self-cleaning coatings, antimicrobial coatings, new membrane materials enabling low-energy water desalination, or new thin-(multi)layer materials for use in photovoltaics, sensors or EUV lithography. This will be in support to typical EU industries like architectural, domestic and life style, health, manufacturing and energy related industry and in full support of the ageing population.

2.1.3 Materials for sustainability

2.1.3.1 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 bio-based materials. The transition to a sustainable society will have a tremendous impact and take 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.

2.1.3.2 Solution for this task described SMART (present-2040)

- 2015-2020. Materials for sustainability 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.
- 2020-2030. 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).
- 2030-2040. Two decades from now, NL will have settled its name as technology provider for circular use of high value (functional) materials, bio-based 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.

2.1.3.3 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, using the existing principles of polycondensation, polyaddition or polyolefin chemistry, new polymers can be designed with higher functionality than the present ones, based on bio-based building blocks. This leaves every opportunity to use NL's leading positions 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 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.

2.1.3.4 What additional competences, technologies, knowledge do we need?

Raw materials: a closer backward integrating connects 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. 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 bio-based 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 origin. Molecular modelling and coarse grained modelling are expected to contribute to the understanding of the translation of biomass building blocks into new materials.

2.1.3.5 How do the tasks connect to grand challenges in H2020?

This task has a direct or indirect impact on the Climate action and Resource Efficiency theme, for example by renewable materials (via biobased building blocks), low-carbon footprint manufacturing of materials, recovery and reuse of materials, circular economy, materials enabling conservation, generation and storage of energy. But also finding alternatives for rare element based materials are in scope, as well as resource efficient material manufacturing such as 3D printing, enabling both Health and Life-style.

3. Principal activities of tasks

3.1 Task 1 Materials with added functionality

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, NanoNextNL, Materials Innovation Institute), 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 the energy (e.g. oil&gas, wind energy and solar energy), health (e.g. in-vivo health monitoring), high tech (e.g. opto-electronics) and transport (e.g. aerospace and automotive) domains. In general, it can be stated that the need for new metallic, ceramic, polymeric, 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 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 and in addition offer functionality, e.g. they can sense, actuate and/or self repair. In addition to adding functionality such new materials 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.

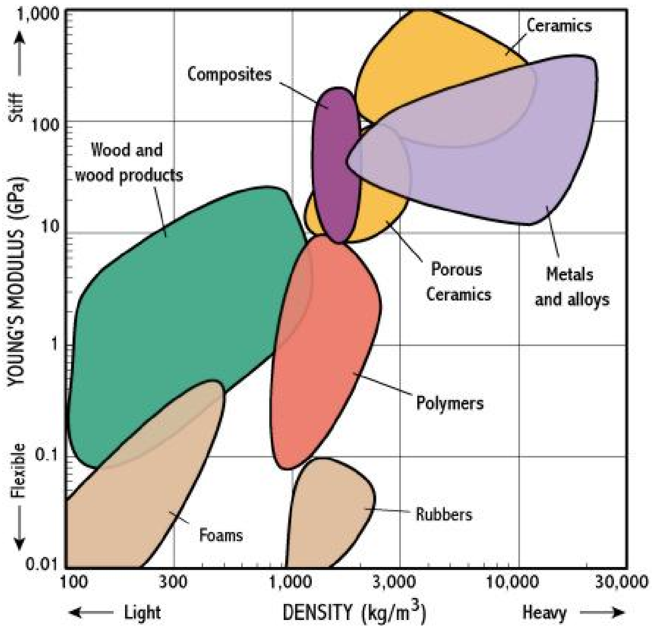

Figure 3.1 *Material selection chart as introduced by Michael Ashby. Material properties, in this case density (kg/m³) vs. Young's modulus (GPa), are plotted in pairs on a chart, allowing the user to find the right material for the right job.* (Ashby, Michael (1999). *Materials Selection in Mechanical 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 allow for the use of additive manufacturing technologies (3D printing). In that sense, multi-functionality and design go hand in hand, and design encompasses both technical and use or "human interface" aspects. The creative industry can help the design of materials in the specification of the different functionalities (existing and new ones) to be combined.

Although this task encompasses different classes of materials (see also Figure 3.1), a special mention should be made for 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.

3.1.1 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)
3- **Physical** (e.g. thermal and electrical conductivity, magnetic, piezoelectric, optical)

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, with a strong contribution from the field of nanoscience. The size-dependent physical and chemical properties of nanomaterials allow the design of functional materials with unique properties, e.g. optical, magnetic, photonic, sensory or electronic functionalities that revolutionize rising markets like telecommunication, information technology and semiconductors. Also more traditional markets like lighting, displays, automotive and aerospace increasingly benefit from high tech materials. Well-being, also for the ageing population, is improved by incorporating high tech solutions in consumer products and homes where due to unique functionalities substantial added value can be created. The Netherlands has a strong position in research on high tech materials and nanomaterials. The high tech industry around Eindhoven, including the high tech campus, is at the forefront worldwide and provides many examples of successful interaction between academia and industry.

- In the semiconductor industry high tech materials are needed to push the boundary close to the physical limits in processor power.
- Transparent conductors with high stability and superior conductivity are required for a variety of application, including solar cells and displays.
- Advanced integrated systems for (remote) control and security of and in homes and businesses rely on high tech solutions incorporating a.o. sensory function, telecommunication, smart windows and lighting.

- The automotive industry benefits from high tech materials in the development of the car of the future (energy efficient, improved safety by smart lighting solutions and sensors).
- High resolution imaging systems for science and industry, including electron microscopy and scanning probe techniques, are dependent on new materials for more sensitive detectors for a.o. charge, force and light and materials allowing higher precision and reproducibility in positioning.

D - Bio-Medical materials

The field of biomedical has made impressive progress in the past decades. Where the discovery of new medicines is slowing down, biomedical materials are increasingly applied in the medical field. Two types of biomedical materials can be distinguished: materials that are used to restore functions in the human body and materials for medical diagnostics, possibly linked to targeted therapeutic action (theranostics). The line between artificial materials and living matter is blurring as interdisciplinary research between the bio-medical field and chemistry now allows for the artificial creation of living matter. 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, university hospitals has been supported in several successful programs (BMM, NANONED, CTMM, HTS&M). Challenges include research on the nanoscale. Bio-molecules of nm dimensions (proteins, DNA) are at the basis of diseases and (bio)chemistry now allows for the controlled synthesis and 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.
- 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 and requires a continued effort in finding new materials for more reliable and cheaper diagnosis.

  - {solution} A strong integration between developing chemistry for advanced materials with added multi-functionalities, i.e. combine a structural component with a functional component, e.g. a sensing, morphing and/or self-healing functionality. The molecular and physical interactions need to be understood and optimized in order to introduce these functionalities.
    Specific steps required present-2040:
    - Optimizing protocols for physical/chemical interaction between different material classes as used in hybrid materials/composites,
    - Understanding/controlling dispersion methods of nanofillers,
    - Control and tune physical properties (optical, magnetic, electronic) on the nanoscale and translate these to superior high-tech materials
    - To meet these goals, smart solutions and a focused multidisciplinary approach are needed, integrating chemistry with physics, bio-medical and engineering. This requires developing new catalyst systems, the design and synthesis of new building blocks, nanoscience giving control over physical properties, optimized reactor technology, mixing protocols, materials processing techniques and optimized design of products taking into account the specific material properties, which might be highly anisotropic.

- O {milestones} **A**- 10 years, **B**-20 years until 2020:
  - Improved mechanical properties traditional polymers (TRL6)
  - Understanding fatigue and improve corrosion stability steel (TRL3)
  - Insight resin-fiber interface for fiber reinforced composites (TRL 3)
  - Development self-healing polymers and ceramics (TRL 3)
  - Development of polymers with additional functionalities (optical, magnetic, electronic) (TL3)
  - Design of new materials for EUV lithography (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)
  - 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).

- 2020-2030:
  - 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)
  - Prototypes of several products successfully tested (TRL 7)
  - Self-healing properties for polymers and ceramics demonstrated (TRL 4)
  - Selection of biomedical materials tested (TRL 5)
  - Response platform will be broadened by new concepts (TRL 3)

- 2030-2040
  - Reinforced composites and multi-functional materials successfully introduced to market (TRL 9)
  - High tech materials proven to function in several prototypes for automotive and home (TRL 9).
  - Biomedical materials for diagnostics and/or controlled drug delivery in clinical trials (TRL 7)
  - Several new concepts for multi-functional materials and biomedical materials will be further developed to prototypes (TRL 7)
  - Response platform will be broaden by new concepts (TRL 3)

o Expected result present- 2040 {position in innovation chain};
o *Scientific/technological goal:* Understand the design rules, synthesis and processing conditions of new multi-functional materials and their performance.
o Industrial end goal: Utilize new advanced multi-functional materials and processes using cost-efficient and sustainable technologies with the aim to design new enabling material-based technologies.
o Societal goal: Weight, fuel and cost reduction. Sustainable materials for a sustainable future.
o *Suitable funding frameworks*: M2i and DPI 2.0.

3.2 Task 2 Thin films and coatings

In addition to the challenges described for functional materials in the previous paragraph, there are specific other challenges for functional thin films and coatings, 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, surfaces which are self-healing or self-replenishing, possess specific barrier properties, are switchable from hydrophobic to hydrophilic by response to external triggers such as temperature have been explored. Other response triggers known today are for example light, heat and scratching. Further development of the underlying technologies, however, will open new opportunities.

3.2.1 Designing thin film / coating materials with the right functionality

Specific surface-dominated functionalities are listed below.

o {solution}

1. **Mechanical:** adhesion of thin layers on substrates or between thin layers in multi-laminates, resistance against scratch and wear stress.
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 semiconductor manufacturing use is made of photoresists for nanolithography that should be transparent to extreme-UV. Also block-copolymer self-assembled layers are used for that purpose. Challenge is to create smaller but more powerful processors by even higher resolutions in nanolithography.
- 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.
- Non-toxic 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 - Multifunctional and responsive coatings and thin films

Apart from many applications that actually require a combination of the functionalities mentioned under A (new combinations of surface dominated functionalities), the following examples illustrate the needs for combinations of new surface functionalities:

- Self-healing capabilities can be incorporated into coatings to repair damages, for instance as a result of insufficient scratch resistance or in order to further increase on anti-corrosion properties or prolonged service lifetime, by transporting material from "reservoirs" to the damage area. Self-healing materials have become a very active field of research since several years, but self-healing technologies of materials which also heals the (surface) functionality are scarcely known.
- Self-cleaning coatings can remove (with an external trigger like rainfall or sunlight) liquid or dust autonomously by virtue of their (super)hydrophilic / hydrophobic or photo-active surfaces), while anti-soiling coatings can prevent dusty solids from settling and adhering on their surface. Switchability between lyophilicity even enhances on these effects and creates extra external triggering.
- 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.
- 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. In one aspect one response factor might trigger another response factor (cascading response).

C - Bio-(inter)active sensors, coatings and films

More specific examples of the latter inside the body (in-vivo), as part of biomedical devices or implants are mentioned here because of the expected strong growth of this research area in response to the global need for health care and the ageing population in the West:

- Coatings and surfaces that have a positive material-biology interaction, such as sustained release of drugs and other actives, cell growth stimulation and tissue integration will greatly enhance the ability of man-designed technology to become a functional part of the damaged / imperfected human body.
- Antimicrobial surfaces. Hygienic conditions and sterile procedures are particularly important in hospitals, kitchens and sanitary facilities, air conditioning and ventilation systems, in food preparation and in the manufacture of packaging material. In these areas, bacteria and fungi compromise the health of both consumers and patients. In these areas there is a strong need for antimicrobial (wet and dry, log-kill rates varying from 3 to 7!), mechanically and chemically robust coatings.
- Bio-resorbable membranes can temporarily prevent post-operative organ adhesions, or act as a scaffold to grow new skin from stem cells after severe burns. In 3D (printed), layer-on-layer deposition of material-cell combinations in principle holds promise to grow artificial organs from a patient's own cells without immunogenic response. Rate of bio-degradation and resorption of the material residues by the body need to be carefully designed.

D - Coatings for energy creation / saving

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.

- Coatings and films for photovoltaics: light in-coupling/trapping, photon up-/down-conversion, ITO replacement, easy-to-clean, anti-dust, printable transparent conductors, passivation, barrier → reduction in costs per Watt-peak, improvement in life-time.
- Coatings and films for lighting devices: light out-coupling/extraction, photon conversion, ITO replacement, printable transparent conductors, barrier → reduction in costs per lumen, improvement in life-time.
- Solar control coatings for the built environment: infrared management, switchable coatings (e.g. thermochromic, electrochromic), coatings for greenhouses, aesthetic coatings for solar thermal systems
- Coatings for windmills: Impingement 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)
- Coatings for fridge doors/freezers: anti-fogging, IR reflection, heat diffusion barriers.

  - Similar to Task 1, a strong integration between developing chemistry for advanced thin film materials with added multi-functionalities, i.e. combine a protective / decorative component with a functional component, e.g. a sensing, transporting, electron-hole pair creation, surface self-replenishing and/or self-healing functionality. The molecular and physical interactions in said systems need to be understood and optimized in order to support and design these functionalities.

  - Specific steps required present-2040:
    Development of technology platforms for functional coatings, thin films and membranes with a strong focus on development of new concepts for chemical and physical related properties such as (but not limited to) antimicrobial, corrosion protection and permeation controlled properties and the development of enhanced response technologies and new self-healing technologies which enhances and/or creates new performances with improved product life time (incl predictability) and product security.

- until 2020:
  - first multi-functional coating industrially produced and applied
  - Development of new corrosion protection technologies for automotive, construction and Hi-Tech applications. (TRL 3)

  - Development of coatings, thin films and membranes with durable antimicrobial properties for domestic hygiene and hospital environments (TRL 3)
  - Sensoring response: Development of nanosensors and films for e.g. oxygen detection, temperature, UV light (TRL 3)
  - Development of self-healing and self-replenishing technologies for functional coatings/thin films and membranes (TL3)
  - Development of a technology platform for multiple, selective response factors (TRL 3).

- 2020-2030:
  - first responsive and active coatings industrially produced and applied
  - A couple of selected technologies described above (corrosion, antimicrobial) will be demonstrated in operations environment (TRL 7). In-depth knowledge will be obtained for understanding and application of newly developed technologies. Development of nanolayer production technologies.
  - Sensoring response technologies will be further broadened (TRL 3)
  - Selected sensoring response technologies will be demonstrated in operations environment (TRL 7)
  - Self-healing platform for functional coatings will be broadened
  - Selected self-healing platform for functional coatings will be demonstrated in operations environment (TRL 7)
  - Response platform will be broadened by new concepts (TRL 3)
- 2030-2040
  - first bio-interactive coatings industrially produced and applied
  - A couple of prototypes will be fully proven in operational environment (TRL 9). Implementation of nanolayer production technologies.
  - A couple of new energy creation concepts will be further developed to prototypes (TRL 7)
  - Response platform will be broaden by new concepts (TRL 3)

o Expected result present- 2040: from selling coatings per kg material towards selling functionalities (in € per m□, or € per piece); forward integration of Dutch companies in the value chain (not only producing polymers, but also applying coating materials and films).

o *Scientific/technological goal*:
A: understanding that enables step-change improvement in performance of coatings and thin films of known functionality, B: combining known and/or new functionalities in thin films and coatings, C: understand biology-material interactions leading to bio(inter)active coatings and D: design of thin films that enable new energy applications.

o *Industrial end goal*:
  - (1) Optimization of the primary functionality, addition of new functionalities in the same coating (towards multi-functional coating systems), improvement of life time/durability (towards the full lifetime of devices such as photovoltaics or windmills), reduction in costs (parallel to device cost reduction). It will also create leading positions in existing markets, education of talented people, cutting edge research and co-creation platforms, innovation driven high tech material development.
  - (2) From passive functionalities via responsive and active systems towards interactive ones. These products will open new market opportunities, like for instance for medical devices, improved and "smart" coatings for advanced applications, novel active and sensing packaging materials. Ultimately: coatings that adapt towards their environment. E.g. blocking of light upon interaction with specific wavelengths.

o *Societal goal*:
The new responsive properties will improved the well-being, safety and food security. The reliability of the performance of a coating will be enhanced. The new response technologies will lead to less (food) waste, improved safety of corrosion damageable constructions, lower carbon footprint an improved quality of life (air, water).
Societal goal: reduce energy consumption and improve harvesting of sustainable energy

o *Suitable funding frameworks*:
Additional funding will be sought from both private and public sources (regional, national and international). Examples of public funding opportunities are Brightlands Materials Center, Cornet, DPI, Interreg, NMP.

3.3 Task 3 Materials for sustainability

Materials for sustainability 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 recently identified by the EU related to supply risks based and economic importance. Clearly, solutions are needed to overcome this upcoming scarcity.

3.3.1 Replacement of petrochemical feedstocks by bio-based feedstocks

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 feedstocks and the need to mitigate CO_2 emissions enforces an increased use of biomass in the production of polymeric materials. On the mid to longer term the importance of producing and using biobased materials will be of imminent importance. Such biobased materials will be based upon modified natural biopolymers (e.g. starch cellulose, proteins), but increasingly also as a result of polymerizing biobased monomers into thermoplastic and thermosetting polymers. Biobased polymers produced by polymerizing biobased monomers are anticipated to grow even more in importance than the use of modified naturally occurring polymers. Initially biobased polymers will have physical properties very much alike todays' petrochemically based polymers. Such biobased polymers can be structurally identical to fossil based polymers (also known as "drop ins" e.g. biobased 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 biobased materials with novel or added properties such as improved gas barrier- fire retardancy, antimicrobial, self-cleaning and self-healing or self-assembling properties. 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 once, unintentionally released into the environment e.g. in the form of "plastic soup".

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. (b) 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 feedstocks, 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. (c) an additional challenge for biobased 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, designed and engineered for optimal functioning in new (biobased) polymers.

Improved (bio)catalytic 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 biobased plastics. This will also lead to the envisioned novel or added properties.

B - Sustainable synthesis - 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.

3.3.2 Improved waste management by recycling of materials, re-use and recovery of product components and / or compounds

A – Polymeric materials
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 will be desired, and the ability to recycle, recover or (bio)degrade in the environment 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. Improved thermolysis/ depolymerisation technology, enabling to recover the constituting monomers is highly desired. A promising alternative route is "design for recycling" – during the design of the material future reuse is already anticipated.

Challenges: Recycling and chemical/physical recovery is in its 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.

Specific steps required present-2040: (a) design of better recovery rates and more efficient recycling processes (2015-2030); (b) design of the next generation of multifunctional (bio)catalysts for effective recycling (2020-2035);

B - Challenge in relation to replacement of scarce metals.
The world-market for rare elements is faced with a supply risk for some elements as well as a demand that is rapidly outpacing supply. In 2010 the European commission recognized that raw materials are fundamental to Europe's economy, and they are essential for maintaining and improving our quality of life. Since the identification of critical raw materials and the publication of the list of 13 critical raw materials in 2011 by the European Commission, the list has been updated and it contains now 20 critical raw materials.

The challenge is to develop economic feasible extraction of (some) metals together with the valorization of the mineral fraction into high added value. Electrolysis and leaching are besides physical processes key processes both in mineral processing as for reuse or regaining critical elements / materials. Chemical interactions can be used for material recovery from (waste) materials to bring back the original element suitable for new applications. This step requires knowledge and processes that enable coupling of material properties and chemistry.

In many cases, harvesting these elements from the earth is even too energy consuming since many tons of materials need to be processed to extract a few ppms of the desired metal. This creates a clear need to replace scarce metals by more easily available alternatives, while maintaining the same functionality (i.e. drop-in solutions). Examples of this include the replacement of noble metals by transition metals in Catalysis (Roadmap Catalysis - Key to a Sustainable Future) and the recent development of Al-based batteries that could replace Li-batteries that are critical to the development of electrical transportation/sustainable energy. Another challenging problem is to find alternatives for the use of rare earth elements like Neodymium (for $Nd_2Fe_{14}B$ alloys in super magnets). Some alternatives have already been developed, but in many applications the search for conservation of functionality based on alternative raw materials still faces challenges.

In order to replace scare raw materials, functionality of materials needs to be understood fundamentally better and descriptors for predictive modeling have to be developed to support the quest for alternatives. In the field of catalysis, this has already resulted in examples where new formulations were predicted and validated in the experimental domain. Further development of the toolbox for this is a pre-requisite in this domain. Investment in electrochemical processes towards total resource efficiency. Most material synthesis processes are now thermochemical driven. With the change in the Energy landscape and the switch to more renewable electricity a surplus of electricity will occur giving a stimulus for electrochemical material synthesis processes.

3.3.3 Sustainable materials for energy

CO_2-related global warming as well as the limited amount of accessible fossil fuel brings the world facing a complete change in energy policy. A shift from fossil to non-polluting, renewable energy sources is demanded to realize the perspective of a greener and sustainable energy future. Cost-effective and efficient options for capturing, converting and storing naturally available energy (solar, mechanical etc.) are highly sought. New materials and chemical synthesis routes will have provide these novel materials in the future.

Solar cells will be instrumental in the transition towards a sustainable energy supply. The development of more efficient solar cells and realizing a lower price per Wp is an important challenge. Thin film materials plays a crucial role and in section 3.2 important future directions for solar cell research are addressed. For smaller scale solutions, implementation of functionalities into the structural materials such as conductivity, piezoelectricity, magnetic features etc. will render the overall material smart and therefore independent of, for instance, external electricity sources.

For now and the foreseeable future, batteries, in particular lithium-ion batteries (LIBs), remain the most promising electrical energy storage system. Thereby, a key factor for population-wide purpose lies in the enforcement of electric (EVs) and hybrid electric vehicles (HEVs). Despite the fact that LIBs already entered the sustainable electric vehicle market, it is well known, that the performance of state-of-the-art systems is still limited. In order to improve the energy and power density of these systems new (nanostructured) electrodes, separators, electrolytes have to be developed.

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.

Specific steps required up to 2040: (a) further development of (bio)refinery technologies (especially relevant for chemical conversion roadmap) (2015-2025); (b) development of improved (bio)catalyst technologies enabling improved control over molecular architecture of polymers and polymerizations at lower temperatures and lower energy input (2015-2030); (c) further development of technologies for biobased additives like plasticizers and lubricants from TRL5-6 to 9 (2015-2025); (d) basic research on alternatives that are equally effective as brominated flame retardants (2015-2025); to higher TRL levels beyond 2025; (e) development of dedicated polymer additives for biobased polymers (2020-2040); (f) development of alternative solvents to NMP,DMAA (2015-2030); (g) development of biobased polymers with new unprecedented properties (2030-2040)

The Dutch academic and industrial landscape is one of the global front-runner in the field of biobased materials. Examples include: (a) in the Biobased Performance Materials (BPM) programme in which knowledge institutions and industry are working together on new biopolymers (feedstock for bioplastics) and on applied research to improve the properties of bioplastics.

Specific steps required present-2040: (a) design of the next generation of multifunctional (bio)catalysts by integrating knowledge on hetero-, homo-, single-site and biocatalysts (see catalysis roadmap) (2015-2030); (b) 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 (2020-2035); (c) increase energy- and resource-efficiency and reduce waste as well as emissions generation in all processes in the production chain (2030-2014); (d) use of green solvent (2030-2040)

*Specific steps required present-2040: (*a) design of novel materials for harvesting of solar, mechanical etc. energy (2015-2030); (b) develop academic and industrial research lines centered on energy storage and electrochemistry (2015-2020); (c) using simulations and multi-scale modeling to gain more insight into the behavior of materials from the atomic level to macroscopic scales (2015-2025); (c) implement designed energy production and storage solutions in industrial commercial context (2025-2040)

Suitable funding frameworks: Biobased Performance Materials (BPM) programme, regional programs like Op-Zuid, Bio Economy Region Northern Netherlands (BERNN), NWO-, EU programmes, Centers for open chemical innovation

3.4 Connections

- Current initiatives
- Organizations/companies in the field

In the past 15-20 years two large consortia of public and private parties in materials research have evolved; the Dutch Polymer Institute (DPI) and the Materials Innovation Institute (M2i). DPI unites 38 companies and 51 (international) academic partners, while M2i spans 45 companies and 21 academic partners. Companies are assembled in industry associations like NRK (rubber and plastics), VVVF (paints/coatings), VNCI (chemicals), FME (metals), and VA (waste). A non-exhaustive list of companies in the field of (advanced) materials that have ties with the Dutch research community is given below.

Sabic. Dow Benelux, Evonik, Bayer, Synbra, Huntsman, Lanxess, Arkema, Tata Steel, Apollo Vredestein, Philips, ten Cate, Fokker, Airborne, DutchSpace, SKF, VDL, Momentive, Oerlemans Plastics, Magnetochemie, AkzoNobel, Solvay, ICL, Eastman, Tejin Aramid, Fuji film, ASML, NXP, ASMI, Océ, Krehalon, PPG, Van Wijhe, Nuplex, Pervatech, Avery Dennison, Elopak, Unilever, FrieslandCampina, Heinz, Danone, DSM, Shell, Braskem, Cargill, Arizona Chemicals, Avantium, Croda, Avebé, VDL, Solliance, Corbion Purac, and BASF,

Given the transition DPI and M2i are currently undergoing as part of the ‘topsector’ policy of the Dutch government, it is likely that the budget for public-private partnership programs in the chemistry of advanced materials requested from other regional (provinces), national (NWO) and international (EU) funding organization will increase. A prudent scenario for 2016-2017 is presented in the overall *Kennis en Innovatie Agenda, part C.*

- Other Top Sectors/program councils

The three priority research lines for the TKI Chemie Roadmap Chemistry of Advanced Materials outlined above connect to the research agendas of many of the TKI’s and topsectors. The main connections are pointed out below, grouped per topsector.

- Topsector/TKI Chemistry
  - Roadmap Chemistry of Life: biomedical materials
  - Roadmap Conversion Chemistry: synthesis of materials, synthesis of new catalyst materials, catalysts for recycling
  - Roadmap Nanotechnology & Devices: nano-composites, materials for sensors
- Topsector Energy
  - materials for (sustainable) energy use and savings
- Topsectors Agri&Food, Tuinbouw&Uitgangsmaterialen
  - biobased materials
- Topsector HTSM
  - throughout most of the HTSM Roadmaps; where HTSM focusses on the use of (advanced) materials, our Roadmap is more directed towards the design and synthesis of the (advanced) materials concerned
- Topsector Water; TKI Watertechnology
  - water purification (membrane technology, sensors)
  - CO_2 separation
- Topsector Life Sciences & Health
  - biomedical materials
  - materials for controlled release of drugs