Vision for Chemistry

Chemistry research communities

Round table Chemistry

2020

Vision for 2040

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Preamble

Dear reader,
Curiosity driven fundamental and applied research is essential to address the societal challenges we are facing. Curiosity driven research will provide new directions for solving these challenges by solutions we cannot yet imagine. The Netherlands has the ambition and potential to become one of the top knowledge-based, innovative countries in the world. To realise this ambition, the Netherlands must build on its strong, deep-rooted tradition of excellence in the chemical science and engineering. Dutch chemists are punching far above their weight in the global research competition. In the coming years, chemical research is essential to accomplish the missions set on the national and European agendas. The Dutch chemical research communities (werkgemeenschappen) have recorded their key role to this end in their vision for 2040, which we are proud to present here.

This vision is an open invitation to the research field to contribute to the chemical community in the Netherlands and to take part in the dialogue on the long-term vision for the chemical science and engineering in the Netherlands.

Chemistry in science and society

In terms of research excellence, the Netherlands is presently amongst the top-tier countries in chemistry and it is well positioned to make important contributions to the main interdisciplinary scientific questions that will shape the coming decades. Furthermore, society urgently demands new technologies to deal with grand societal challenges such as renewable energy, resource efficiency and scarcity, climate change, scarcity of materials, and health care. This background provides a firm base for the chemical research communities in the Netherlands.

Chemical research communities

In 2018 the NWO Round table Chemistry has, in close consultation with the research field, set up four research communities for chemistry. Through these four research communities, the research field will be able to make an effective contribution towards recommendations for research at the Dutch Research Council (NWO). The link between researchers and NWO is essential to ensure that signals in the field are picked up by NWO, and that NWO is able to keep in touch with the field. The research communities connect chemists and promote collaboration with other disciplines. Researchers from academia and industry can become member of one or more communities.

The research communities are represented by so-called advisory committees that advise the Round Table Chemistry and NWO on chemistry related matters. The committees regularly inform and consult the members of a research community with regard to relevant NWO information.

Vision 2040

To define what the scope is of the chemical research communities and what the long-term vision is for chemical science and engineering in the Netherlands, the Round table Chemistry invited the research community advisory committees to draft a vision for 2040. These visions include the scope of the research community, the state of the art and the scientific challenges ahead of us in the coming decades. They represent the vision of the research community and should be regarded as an open invitation to the field to contribute to the visions and to the chemical science and engineering in the Netherlands. They also provide a disciplinary base for interdisciplinary cooperation and a way to reach out to disciplines like physics, biology, astronomy and computer science. Furthermore, the vision 2040 will be instrumental for the Dutch Chemistry Council that was established in 2020 and will promote the interests of chemistry in the Netherlands.

It is important to emphasize here that the visions of the research communities are science driven. The visions were conceived from the point of view of science and express what science itself sees as opportunities for the long term.

Making the visions reality

Making these visions reality requires several ingredients: excellent scientists, enthusiastic students, excellent teachers, high level research infrastructure and appropriate funding. Chemistry requires a funding climate that allows both fundamental curiosity driven research and translational research. Investments in these areas have dropped far below international standards and are well below what is minimally needed*.

* Breimer 2015, Rathenau 2020, Dutch Chemistry Council 2020

Currently the Netherlands is still one of the world leaders in the various areas of chemistry, but it must, crucially, continue to invest in this area of science to maintain the leading role and grasp the many exciting opportunities offered by the rapid changes in the field.

The advisory committees of the chemical research communities and the Round table Chemistry identify four key factors that are essential for a successful realisation of the visions for 2040:

1. Focus on curiosity driven science

Significant steps towards addressing societal needs can only be realized if there is a solid basis of fundamental knowledge that is maintained and continuously expanded. Fundamental research withno strings attached is often a prerequisite for achieving breakthroughs from which applied research can benefit. Large-volume granting programs with acceptable success rates (at least 1 out of 3), indifferent with respect to whether industry is involved or not, are required for maintaining Dutch fundamental science at the level at which it has flourished for a long time already.

2. Long-term research projects

High quality research advancing the boundaries of our knowledge and the capabilities of present-day technologies takes time requiring long-term investments and long-term visions. There is currently a mismatch between the required long-term vision and the short-term scope of policies and funding instruments that favour short-term research in collaboration with commercial partners. A long-term vision needs to ensure sufficient funding for projects beyond the timespan of a single PhD student, i.e. 6-10 years, for a single or small group of researchers. In addition, attention should be paid to a fair distribution of funding, independent of career stage. Grant schemes should be developed in which PI's can spread allocated funds – which do not need to be multi-million – over an extended period.

3. Basic equipment and infrastructure to support excellent science

High impact research not only requires new and advanced equipment, it also requires the maintenance of equipment at (at least) basic levels. This holds for all research communities of Chemistry. A wide range of characterization methods and medium-scale equipment is present in Dutch university groups and NWO institutes. Such infrastructure and instrumentation may not be so eye-catching, but has over the years come to an alarming and embarrassingly low level due to lack of financing. This level needs to be brought back to levels in sync with the ambitious goals of Dutch Science. The use and output from these facilities would benefit from organisation on a national level and support in the form of personnel.

4. Access to and support for advanced large-scale facilities

Large scale infrastructure where particle beams help to elucidate structure and properties of matter are a basic need for chemists. User facilities where x-ray, pulsed laser, neutron and other beams are used enable the discovery of new phenomena, giving new insights and even paradigm shifts in science that cannot be realized by more conventional techniques. Accessibility to national high resolution (shared) infrastructures like high resolution NMRs, electron microscopy, X-ray spectroscopy, SEM, TEM, mass spectrometry, high throughput facilities and e-infrastructures are also vital base infrastructures for high quality research. Access to, staffing and support for measurements at these type of facilities is crucial for many of the communities in chemistry and requires substantial funding and organization at a national level.

The Visions papers are not static and this publication marks the starting point of an ongoing dialogue with the researchers in the field, NWO and other relevant parties. Scientific meetings, like CHAINS, will be deployed to NWO oriented follow-up on this dialogue.

On behalf of the advisory committees of the chemical research communities and the Round table Chemistry, Enjoy reading and, in a good scientific tradition, let's continue the discussion and send us your thoughts and feedback.

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Research Community

Fundamentals & Methods of Chemistry

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Vision for 2040

The Future of Chemistry is Bright and Exciting – with a proper foundation to build upon

Chemistry plays a key role in bridging basic and applied scientific disciplines at a fundamental level. As such, it is unquestionably recognized as the central enabling science that drives the major breakthroughs needed to tackle current and future challenges confronting our society, such as sustainability, energy, health, food and climate. At the same time, significant steps forward are possible only if there is a solid foundation of fundamental knowledge that is not only maintained but continuously expanded. Such a foundation is an absolute necessity for pushing the boundaries beyond what is currently considered possible. It is a sine qua non for creating the fertile breeding ground that gives rise to serendipity - the origin for so many of humanity's truly "giant leaps" forward.

The Research Community Fundamentals & Methods of Chemistry (FMC) provides a unique impetus to cross scientific boundaries. The Dutch Chemical Sciences historically have an excellent tradition in a fundamental and curiosity-driven approach to scientific challenges. The FMC Research Community in particular is a powerhouse of expertise in the disciplines necessary to advance the chemistry state-of-the-art, providing a future-proof basis for maintaining our second-to-none international reputation. Sustaining our global impact will require going beyond the traditional division of length and time scales to develop transferable, multi-scale approaches with respect to both theoretical and experimental methods. In view of the explosive growth and capabilities of the data sciences, these approaches should also be symbiotically aligned with data-driven development of novel fundamental insights and methods. This will allow us to go beyond the individual molecule to tackle complexity in multi-component systems, and control the emergent properties that arise from the collective behaviour of separate molecular entities. A multi-scale perspective will enable us to unravel the ultimate level of complexity, that which is sequestered in a cell or organism. The fundamental chemical knowledge achieved in this way will provide the sciences and society with smart molecules, smart materials, and smart technologies tailored to societal needs. Most of all, this knowledge will lead us to a smarter understanding of the fundamental principles and processes underlying the rapidly changing world around us.

The present era is one in which the Chemical Sciences are witnessing large changes in their scientific markets, both academic and applied, as they are increasingly invoked in other physical, life and engineering sciences. In order to keep up with this revolution in scientific thinking, programs targeting the establishment of fundamental yet discipline-overarching experimental and theoretical technologies need to be set up. Clearly, such programs are most optimally defined and realized by the experts in the field. The FMC Research Community therefore strongly advocates the delegation of the identification and implementation of such programs to the Research Community itself. Giving the FMC Research Community this responsibility will be the most effective way to empower us to achieve our goals, so that we will be able to say in 2040 that Chemistry has blazed new Trails into the Future.

Fundamentals & Methods of Chemistry in the Netherlands

The Holy Grail of the FMC Research Community is to discover and unravel the molecular principles of chemical reactions and networks, thereby enabling design, synthesis, analysis, and control of any type of molecule, material or process. The interdisciplinary platform that is the Research Community provides the ideal basis to pursue this ambitious objective. FMC scientists together have the knowledge and expertise to achieve the fundamental understanding and development of chemical technologies, ranging from the computation of molecular structures, their properties and behaviour, interactions and conversions, to the design of spectrometric, microscopic, and separation technologies. The Community considers it imperative to safeguard the strength and visibility of the existing chemical disciplines under our umbrella as independent players and motors of interdisciplinary research. Only in this way can we successfully identify and forge new disciplines from existing ones. We leverage fundamental research of the properties of molecules and matter as well as the analytical sciences as a prime basis for productive partnerships to both improve current technologies and develop new ones.

Detailed insight into causal relationships in combination with advanced techniques will boost the ability of chemists to achieve their ambitious targets. The Research Community enables the innovations needed for this in a wide range of disciplines, in particular the Chemical Sciences related to molecules, materials, catalysis, and life sciences. Fundamental and curiosity-driven research form the basis of our Research Community, serving as a starting point for addressing societal challenges, innovating industry, and enabling new economic activities. The translation of fundamental findings to societal and industrial applications is thus recognized as being of key importance to the FMC knowledge chain.

State-of-the-Art

The FMC Research Community combines expertise from a broad variety of experimental, theoretical and engineering disciplines that operate at scales ranging from purely molecular to macroscopic, and from materials to processes. Fields of study that are closely connected to these disciplines include - but are not restricted to - Analytical Chemistry, Spectroscopy, Physical Chemistry, Theoretical and Computational Chemistry, Functional Materials and Polymer Chemistry, Synthetic Chemistry, Supramolecular Chemistry, Catalysis, and Chemical Engineering. The expertise of Dutch researchers in all these fields is internationally recognized to be second-to-none.

This breadth of expertise that the FMC Research Community brings together is unique. As we have demonstrated repeatedly over the years, it provides the versatility that is necessary to make unexpected breakthroughs possible and follow up on them, and to seize upon novel opportunities. Collaboration between the disciplines from the very start and not just in the final stages of product manufacturing and application - be it at the level of knowledge, be it at the level of execution - is a strength of our Research Community. It is a strength that society can capitalize on when innovative solutions need to be found for societal challenges, now and in the future.

Dutch academic and industrial fundamental research has a long tradition in conceiving and constructing globally unique infrastructure from both an experimental as well as a theoretical perspective. Members of the FMC Research Community have set internationally recognized landmarks in their respective fields, and continue to do so. This is a second strength that allows the Research Community to operate successfully in a highly competitive international environment.

Research groups participating in Fundamentals & Methods of Chemistry are predominantly located at the comprehensive and technical universities as well as fundamental research institutes. Noteworthy, however, is the growing interest of scientists in medical centres and industrially- oriented laboratories to become a part of the FMC Research Community. The fundamental basis of the Research Community and its multifaceted character continues to prove essential for providing key contributions to programs associated with the Topsectors and industry. These include the Holland Chemistry program (in particular the Chemical Nanotechnology and Devices roadmap), TI COAST, Holland High Tech roadmaps, and the KIA Key technology clusters. At the same time, FMC is a natural starting point for addressing many of the routes formulated in the Dutch Research Agenda, examples of which include Measuring and Detecting, Circular Economy, Energy Transition, Materials and Personalised Medicine.

Scientific Challenges

Fundamentals & Methods of Chemistry research covers a wide range of chemistry-based science centred around transforming and controlling the chemical and physical properties of molecules and materials. Key challenges are to (i) theoretically predict and control chemical reactivity and complexity, and (ii) experimentally observe chemistry happen in real time and in situ. On the theory side novel multi-scale modelling approaches with large-scale chemical interactions need to be developed. To realize the experimental goal, it is not only necessary to design new experimental methods by combining different analysis techniques , but also to go beyond the presently available techniques and develop completely new approaches. Inputs from multi-scale modelling approaches can steer experimental in situ studies of processes on the molecular scale and beyond, providing in situ insight on how molecules, nanoparticles and surfaces interact and react. At the same time experimental findings are indispensable input for theoretical multi-scale modelling in that they will show whether the necessary ingredients are built into the theoretical models. This highlights the interplay between theoretical and experimental studies, and illustrates the potential power of such a combined effort. It will be important to (i) determine multiple physical parameters such as pH, temperature, viscosity, humidity together with molecular kinetics, reaction intermediates and spectroscopic properties at the same time, (ii) work on multiple time scales, spanning molecular vibrations as well as macroscopic movements, (iii) work on multiple length scales at the same time, from atomic resolution to the macroscopic level, and (iiii) work with multiple analysis techniques, such as confocal, IR, EM, NMR, EPR, MCD, Mössbauer, and MS. The research along the four main thrusts described below will lead to new fundamental discoveries which, through collaboration between academia and industry, will stimulate innovation.

Creating new chemistry

To control chemistry in real time, highly efficient synthesis routes and catalytic processes need to be developed that allow us to design and synthesize novel molecules, architectures, and materials with new functionalities matching specific applications. New synthetic methods must also be developed to address material scarcity and toxicity issues associated with industrial production of chemicals and materials that are relevant to society. In addition, detailed understanding of the building blocks of life concerning e.g. the regeneration of complex natural systems, their self-assembly, self-sustainability, and self-replication is sought. This understanding will ultimately allow the creation of a synthetic cell, and will provide a solid foundation for the discovery of new pharmaceuticals and vast amount of bio-inspired materials with tremendous impact on improving health, energy and food security. To realize these goals it is important and urgent that research takes place towards developing (i) advanced imaging and growth techniques to make materials atom by atom over a range of length scales, (ii) predictive synthesis using structure-property relations (for example, enabling late stage functionalisation of medicines and biomolecules), and development of scalable synthesis routes, and (iii) new catalytic processes converting biomass to useful raw materials and new smart materials to harvest sunlight and increase energy efficiency.

Mastering chemical complexity with advanced analysis techniques

Advanced analytical and spectroscopic techniques that mimic, measure, and sense chemical processes not only enable us to explore, understand, and control a vast range of complex behaviours, but are also critically important for technological breakthroughs. New spectroscopic tools combined with computer-aided design of chemical processes and catalysts for energy conversion/storage, for synthesis of sustainable materials, and for analysis of molecules in their natural environment will pave the way towards temporally and spatially resolved control over chemical processes, at length scales from single molecules to bulk products. Breakthroughs in these areas will help us to address current challenges in health and energy security. To achieve these goals research is urgently needed aimed at (i) developing hybrid/combined analytical techniques with chemical resolution, sub-nm length scale, and different time scales, (ii) developing robotics and automation of measurements, data-based analysis, and imaging methods, with the aid of artificial intelligence, and (iii) technological developments for electrochemical catalysis, time-resolved crystallography, X-ray free-electron laser, solid-state NMR, EPR, light microscopy single molecule methods, mass spectrometry, time-resolved observation of single cells with a high spatial resolution and chemical content imaging, manufacturing materials with ultimate control and precision in one, two and three dimensions, and integration of nano-materials and nano-scale devices with modified biological systems.

Modelling and designing chemical structures and processes

Recent years have seen a continuous growth of advanced hardware and software performance. State-of-the-art modelling approaches can now be used in high-throughput studies to aid in the rational design of novel molecules and materials. The hierarchy of spatio-temporal scales giving rise to properties of large systems necessitates the use of multi-scale simulation techniques. However, the vast space of model parameters on the one hand, and of chemical building blocks on the other hand necessitates the use of smart methods to deal with the huge amount of data that is input to such models and results from the models' predictions. The goal here is to connect several theoretical methods, for example, molecular simulation, machine learning, and artificial intelligence, to develop a unified methodology covering the entire simulation pipeline for the rational design of advanced large molecules and systems with customized properties matching specific applications. To realize these goals research is urgently needed in the areas of (i) integrating molecular simulation with machine learning and artificial intelligence, rationalization of the algorithms, and predictive models based on both theoretical and experimental inputs, (ii) developing efficient multi-scale simulation software with a user-friendly interface, (iii) speeding up software by integrating quantum computation into existing algorithms, (iv) computational electrochemistry and heterogeneous catalysis, regarding surface reaction dynamics and the electronic structure of molecules interacting with metal surfaces, and (v) algorithms to simulate out-of-equilibrium systems.

Infrastructure and instrumentation

Infrastructure and instrumentation is clearly at the very core of the FMC research area. The impact of this research area will be largest when (i) experimental and theoretical researchers, both from academia and industry, actively collaborate; (ii) access to large scientific facilities and instrumentation is available, and (iii) significant investments in new computational and experimental infrastructure are made. Large-scale infrastructures that come to mind in this context include (i) national supercomputing facilities, (ii) an ultrafast x-ray spectroscopy centre for in-situ characterization, (iii) an advanced characterisation centre for paramagnetic molecules (combining several 'spin-Hamiltonian' techniques, such as pulse EPR, Mössbauer spectroscopy, SQUID magnetometry and MCD) and (iv) an interdisciplinary centre for process technology, synthesis, and catalysis. At the same time, it should be kept in mind that high-impact research also requires the maintenance of equipment at a more basic level. Such infrastructure and instrumentation may not be so eye-catching, but has over the years come to an alarming and embarrassingly low level of financing. The necessary efforts should be made to bring the funding back to levels in sync with the ambitious goals of Dutch Science.

Fundamentals & Methods of Chemistry for Society

Our planet and society are dynamic and continuously face new challenges. Fundamental breakthroughs in science, engineering and technology are necessary to cope with the associated changes. Meeting the challenges calls for a solid body of knowledge to appeal on and finding innovative solutions is thus an essential corollary of the science developed by the Research Community. Because of its very nature the Fundamentals & Methods of Chemistry Research Community is active in many, often multidisciplinary, initiatives. The FMC community can make the difference in areas like Climate and Sustainability and Personalized technological devices.

The area of Climate and Sustainability calls for new technologies and methods to reduce/eliminate waste, cope with material scarcity and facilitate the energy transition, but also for a fundamental understanding of the chemical and physical processes associated with these technologies and methods. Similar observations can be made as far as a feasible implementation of the circular economy is concerned. Resources that are becoming increasingly rare are high on the list of many application-driven agendas, which most likely can only be realized if fundamental advances in the chemistry of earth-abundant elements are made.

The fundamentals of 'analytical' technologies, including technical physics, are essential for the development and construction of high-tech analytical devices, where particular attention should be paid to miniaturization end transportability, next-generation measurement techniques, and applications associated with personalized medicine and (remote) sensing. The Netherlands has a leading position in artificial intelligence, giving us an edge on the development of high-end, smart, and user-friendly technologies.

Society often asks for short-term answers and applications, but certainly also for long-lasting and 'true' solutions. In the long term this will only be possible if enough money – and much more than currently is the case – is invested in fundamental chemical research. The impact of these investments is often only seen far in the future. The future cannot be predicted. What can be predicted, however, is that without a prominent contribution of chemistry fundamentals to both research and education it will not be possible to maintain the position of The Netherlands as a leading global knowledge economy able to respond to societal needs.

Research Community

Chemical Conversion

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Vision for 2040

In the coming decades, thorough innovations are needed in the way materials, goods, and energy carriers are produced and used, especially in industrialized societies. Reduction of the environmental footprint through adaptation of the circularity principles requires thoughtful product design and more sustainable synthetic processes, taking into account not only performance and production metrics, but also life cycle analysis. Chemical products should be safe-by-design, reusable and recyclable and, if emitted to the environment, biodegradable. The use of fossil-based resources should be minimized and replaced as much as possible by sustainable and circular sources of carbon: biomass, CO_2, or waste streams. Inorganic materials should also be designed for optimal recycling. Furthermore, chemical conversion processes should become more sustainable and selective, with a clear focus on lower energy inputs, and whenever possible, driven by energy generated from CO_2-neutral processes. Here, electricity- and light-based processes using ecofriendly bio- and chemo-catalysts with superior performance for functionalization reactions are essential. Whereas globalization has flooded markets with low-cost, poorly recyclable products, awareness is increasing that this created new vulnerabilities, which calls for renewed attention for regional production in the pharma, healthcare, and food sectors, using processes that follow European environmental regulations. New energy storage- and transport technologies need to become available at costs and scales that match existing processes, allowing replacement. Improved conversion technologies are needed to help recovery of scarce or potentially harmful materials from resources and waste streams. Climate change, exhaustion of natural resources, and the increasing demand by the growing human population require drastic innovations in chemical conversion. This should lead to safer and smarter products which are synthesized in an ecofriendly manner from renewable resources, with zero-emission as the long-term perspective.

Chemical Conversion in the Netherlands

Chemical conversion and valorization of natural resources leads to numerous products that enable a convenient and healthy life in our modern society. Eye-catching examples are polymers and fibers for clothing, utensils and mechanical parts; fertilizers and protectants for the safe production and processing of food; surfactants and coatings that prevent rust and (bio)deterioration; medicines to treat infections and diseases; and numerous products for everyday household use, and transportation. Numerous chemical products are essential for value-chains in other sectors. By employing more sustainable processes and resources, innovations in chemical conversion will play a pivotal role in changing the perception that chemical industries cause more harm than good. In this regard, the last decades have seen major advances towards the sustainable synthesis of organic chemicals and materials. Such breakthrough discoveries are essential to realize the dream of fully sustainable chemistry. To achieve this, the development of novel synthetic methodologies that make use of small molecules, renewable feedstock and increase efficiency of use of fossil resources in a circular manner is essential. It requires a new generation of well-trained chemists in a range of subdisciplines including (in)organic chemistry, (bio)catalysis, photochemistry, electrochemistry, as well as theoretical- and analytical chemistry and process technology. Intensive collaborations between the academic chemical conversion community and chemical industry will stimulate rapid implementation of new technologies in industry. Industrial partners that are active in the Netherlands include BASF, Corbion, Shell, DSM, Unilever, AkzoNobel (Nouryon), OCE-Canon, MercachemSyncom, Avantium, etc.

Chemical synthesis: small molecules to products

The use of small molecules as precursors can play a vital role in reducing our environmental footprint as they can be used as an alternative to oil-based feedstock in the production of value-added chemicals and materials. For example, CO_2, CH_4, N_2, O_2 or products derived from pyrolysis or fermentation can in principle be employed for the formation of C–N and C–O bonds in complex molecules. Harnessing this potential requires understanding of the way in which unreactive and very strong bonds such as C–H or N–N bonds can be activated. Activation can be achieved under elevated thermal conditions at high pressure, but this requires a high input of energy and often leads to high CO_2 emissions. As products, materials which are intrinsically recyclable should be aimed for. A long-term challenge is to design efficient catalytic processes for synthesis of chemical building block via CO_2 capture, reduction and C–C bond formation, contributing to carbon circularity and avoiding CO_2 emission. Energy carriers such as bunker/aviation fuels, formic acid and hydrogen will continue to play an eminent role in future energy schemes. These energy carriers should be made in the most environmentally benign way.

Renewable feedstock to chemical products

With a few exceptions, chemical raw materials are currently produced from fossil resources such as natural gas, coal and petroleum. The high environmental footprint associated with the use of these feedstock calls for new and better-designed chemical products that fully integrate recyclability considerations and life cycle analysis. Furthermore, the chemical diversity from fossil sources is small and additional synthetic steps are required to generate advanced building blocks, leading to additional waste formation and energy consumption. In contrast, biomass-derived renewable starting materials often have a higher degree of functionalization and therefore can represent useful advanced building blocks for the chemical industry. In addition, some complex molecules can be obtained directly by a so-called biorefinery approach. The renewability aspect and the option to close the carbon cycle makes bio-based feedstock highly attractive, a field that is under intensive investigation in by Dutch research groups as well as internationally.

Fossil feedstock to easily recyclable chemical products

Chemical products derived from fossil resources are ubiquitous in modern society. However, the chemical and refinery industry is the largest industrial energy consumer, heavily contributing to CO_2 emissions and thus confronted with ever stricter regulations. The chemical industry still uses fossil resources for a large variety of widely used products like plastics, fertilizers, drugs, or detergents. Even before phasing them out completely, the environmental footprint associated with the use of these fossil resources can be substantially reduced by implementing efficient synthesis, with less side products, as well as by developing circular concepts. For the latter, not only separation but also chemical conversion to reusable molecules is an essential. To achieve this type of circularity, fossil-derived products should be designed to be recyclable.

Scientific challenges

To achieve the goal of fully sustainable chemistry, a better understanding of (bio)chemical conversion processes will be required. The following scientific challenges are associated with this.

Understanding small molecule activation and use of the alternative stimuli

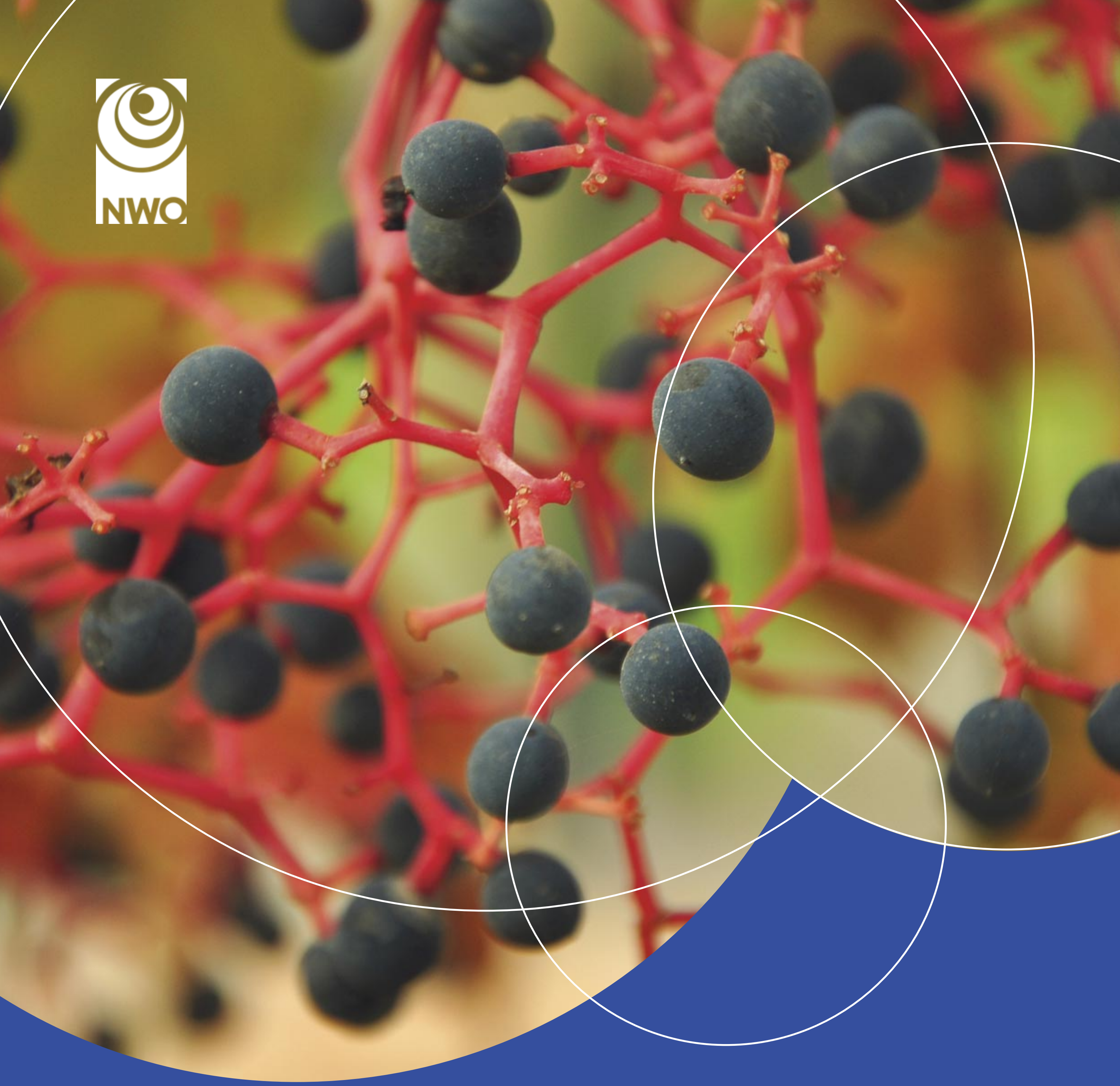
Catalytic activation of molecules offers a wide range of opportunities to promote the production of sustainable and alternative chemicals and fuels. Current challenges are the development of new (bio)catalytic processes potentially driven by the use of external alternative stimuli (electricity, light, electromagnetism, …) that permit the activation and further functionalization of small molecules under mild reaction conditions. A main challenge in this field lies in the replacement of rare-metal-based catalysts like iridium or ruthenium, by widely available elements such as iron, cobalt or nickel. In addition, understanding how stimuli such as heat, electricity and light influence activity and selectivity requires new advanced characterization techniques for studying catalyst properties and performance under reaction conditions. A better understanding of catalyst behavior and control of catalyst properties at the atomic level allows design of new processes that incorporate small molecules in synthetic schemes.

Selectivity control

The chemical industry is traditionally based on the production of value added chemicals from pristine or fossil-based feedstock. In order to switch to renewable resources or use recycle streams as feedstock, new chemical conversion processes that deal with complex mixtures need to be developed. New methodologies for selective conversion of complex feedstock to targeted products must be established. To achieve this, new separation processes as well as more regio- and enantioselective catalyst and processes are necessary. Integrated use of multi-step catalytic schemes in cascade conversions is an additional challenge, reducing formation of waste and workup costs and thus contributing to process economics. With respect to recycling, current research focuses on the development of new (bio)catalytic systems and processes for the controlled and precise depolymerisation and degradation of renewable polymers such as lignin or cellulose. Another important trend is the development of (bio)catalytic methods for the conversion of biomass-derived platform chemicals to high-value-added chemicals and materials, e.g. by incorporation of heteroatoms.

Understanding of structure-recyclability relationship to design new molecules/material

Circular chemistry is an ideal approach to reduce environmental footprint as long as fossil feedstock are still used. At the end of their lifetime, chemical products are not burned or disposed of but reused as a building block for new products. To make this type of recycling efficient, chemical products, especially polymers, have to be designed for recyclability. What such products should look like is currently an enigma. Therefore, the relations between chemical (and physical) structure and recyclability should be understood. Innovations are needed for improving the precision and efficiency of chemical recycling processes, e.g. by increasing catalyst selectivity and robustness. Catalytic processes should enable conversion of complex waste-like materials to platform chemicals for re-use, preferably without complete degradation of carbon skeletons.



Research Community

Chemistry of Life

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Vision for 2040

Chemistry of Life in the Netherlands and abroad aspires to build a molecular encyclopedia of life. We want to map all the molecules of the cell in time and space, enabling us to influence their functioning and interactions in a rational way. The fundamental understanding of life processes at the molecular level and the ability to intervene in a targeted manner will contribute to a healthy life in a sustainable society.

To achieve this, we need to invest in training new generations of chemists and molecular life scientists in state-of-the-art laboratories featuring the latest technologies. This will lead to unique economic activities in the fields of drug development, diagnostics, sustainable crops, and green production processes.

Chemistry of Life in the Netherlands

From fundamental insights to unique possibilities

Chemistry is a fundamental science that is essential for understanding the world from a molecular point of view. At the same time, it provides molecular insights that are essential for the development of new strategies and innovative solutions to address pressing societal challenges. Chemistry of Life studies the structure and function of biomolecules and their role in biological processes at the molecular, cellular, and organismal level. The field is greatly contributing to theoretical, methodological, and technological advances, including the design, synthesis, and application of novel compounds, reactions, and chemical systems. These in turn are crucial for the development of biotechnological and medical applications. Thus, Chemistry of Life explains the world around us and offers the unique possibility to even create entirely novel molecules, cells, materials, and technologies that can be used to improve health and create a sustainable society. Furthermore, these developments are based on a strong foundation of (bio)chemical disciplines, education, and innovative entrepreneurship in the Netherlands. Academia, medical centers, and other research institutes as well as biotech companies and other industries are all closely connected and contribute to this unique and thriving Chemistry of Life community.

Building on a strong foundation

The developments in Chemistry of Life are based on a foundation of strong disciplines at universities, medical centers, and research institutes. They drive technological innovations in academia and industry, and encompass fields such as health, agriculture, horticulture, biodiversity, and biomaterials and energy supply. Chemistry of Life in the Netherlands has made essential contributions to many breakthroughs: from understanding the molecular principles of life to economic development and societal wellbeing. To name a few examples these contributions range from designing molecular nanomachines (Prof. B. Feringa, Nobel prize in Chemistry, 2016), to understanding macromolecular polymers and transport within cells (Prof. A Akhmanova, Spinoza prize 2018; Prof. M. Dogterom; Spinoza prize 2018), to understanding the molecules of the immune system (Prof. P Gros, Spinoza prize 2010; Prof. Y. van Kooijk; Spinoza prize 2019, Prof. J. Neefjes; Spinoza prize 2020) and developing immunotherapeutics (Merus BV, Utrecht); from understanding gene editing and contributing to the ongoing CRISPR revolution (Prof. J. van der Oost, Spinoza prize 2018) to creating new microorganisms that enable green chemistry (Prof. J Pronk, Spinoza prize 2019). It includes developing new kinds of food, fuel and medicine (e.g. DSM, Delft); as well as creating methodologies for studying the proteins and their modifications in cells (Prof. A. Heck, Spinoza prize 2017). These examples also include the development of breakthrough drugs for the treatment of cancer and autoimmune diseases, such as Acalabrutinib, Keytruda, Filgotinib, Daratumunab and vaccines, which were discovered and developed by researchers from Acerta Pharma (Oss), Merck Sharp and Dome (Oss), Galapagos (Leiden), Genmab (Utrecht) and Crucell-Janssen (Leiden), respectively. Chemistry of Life has been a central hub for bringing together solid and innovative basic research covering different disciplines; for example, Dutch scientists have also made essential contributions to dissection of molecular mechanism of virus replication and the design of novel antiviral strategies in plants, animals and humans. In addition, Chemistry of Life offers many opportunities for addressing the grand challenges described by the Dutch Research Agenda (e.g. NWA themes Measuring and Detecting, Personalized Medicine, Origin of Life and Energy Transition), as further detailed and discussed below.

Scientific Challenges

Understanding the Chemistry of Life

Measuring the Chemistry of Life

The Chemistry of Life community develops and applies various ‘omics’ and single cell technologies, such as genomics (next-generation DNA sequencing), transcriptomics (RNA-sequencing), proteomics, lipidomics, and metabolomics (mass spectrometry and NMR). Technological breakthroughs in next generation sequencing have revolutionized the analysis of genomes and transcriptomes of organisms and cells in health and disease, and further promote the development of many future technologies. Such tools now allow powerful genetic and genomic approaches in organisms other than the classical genetic model organisms, with importance for ecology, agriculture, and pathogen transmission. The impact of these methods is widespread and growing rapidly. A genome of a new virus can now be decoded within a very short time, allowing rapid development of risk models and implementation of measures, and development of detection kits. The world-leading plant scientists of the Dutch Chemistry of Life community use the new omics technologies to determine the molecular mechanisms underlying the regulation of growth, development and immunity in plants, with effective translation to plant breeding programs. Thus, the broad societal impact of these developments cannot be overstated. All developments in next generation sequencing rely on chemical reactions and are based on innovative chemistry of nucleic acids and cellular protein assemblies, including pioneering work of Dutch scientists on chemical synthesis of nucleotides. In combination with innovative biochemical assays, advanced genetics approaches, patient-derived pluripotent stem cells, and organoids, the new ‘Omics’ analyses make it possible to rapidly identify novel biomolecules and their functions, and thereby identify potential therapeutic targets. To reap the benefits of these new technologies and connect to international initiatives (e.g. LifeTime Initiative, Human Cell Atlas) it is of utmost importance to understand the function of these biomolecules at the atomic level and to establish the druggability of these targets. The Chemistry of Life community applies methods of chemical biology, biochemistry, and structural biology to achieve this goal.

The synthesis of chemical probes that interact, correct and report on the function of biomolecules in an acute and dynamic manner provides the best opportunity to study the function and druggability of a potential drug target in a disease model. Indeed, one of the most important bottlenecks in drug discovery is the lack of validated therapeutic targets (i.e. biomolecules that can be targeted by drugs). Currently, only approximately 1-2% of the human genome (~400 proteins) are targeted by molecular therapies, and for most proteins, no chemical probes and starting points for drug discovery are available. Thus, the Chemistry of Life community focuses on the development of synthetic methodology and discovery of small molecules to study the function of proteins in their cellular network.

Integrative Structural Biology

X-ray crystallography (MX), nuclear magnetic resonance spectroscopy (NMR), and recent breakthroughs in cryo-electron microscopy (cryo-EM), together with computational modeling and simulation tools and with mass spectrometry approaches (MS), allow analyzing the three-dimensional structure and dynamics of macromolecules and their complexes at atomic resolution. The MX, NMR, cryo-EM, modeling and MS communities in the Netherlands have a long tradition and a leading role in their respective fields. NWO supports access for Dutch chemists to the European Synchrotron Radiation Facility (ESRF), and has been instrumental in establishing the NMR and MS centers in Utrecht University, the Netherlands Centre for Electron Nanoscopy (NeCEN) at Leiden University, and the Protein Facility at the Netherlands Cancer Institute (NKI): these facilities collaborate forming the Netherlands center within the Instruct-ERIC umbrella in Europe (Instruct-NL). Via the Netherlands Electron Microscopy Infrastructure (NEMI) Roadmap centers on single particle Cryo EM (Groningen), Multimodal imaging (Maastricht) and Image processing (Utrecht) national access to expertise and instruments is arranged in addition to NeCeN. Together, they provide access to the most advanced instruments that allow scientists to study molecules in atomic detail in vitro and in situ.

Combining structural information from different methodologies and integrating them into functional models for the organization of macromolecules and their complexes is a powerful research tool. It allows researchers to bridge chemical understanding into atomic detail and macromolecular and cellular function. Recent technical advances enable a broad range of structural studies, such as analyzing the networks of macromolecular complexes inside the cell by cryo-EM or soft X-ray tomography; determining the structure of complicated macromolecular complexes by cryo-EM and the dynamics and interactions of large chromatin complexes by NMR; screening for the binding of fragments or ligands to enable drug lead discovery by MX; analysis of whole proteomes even by a few droplets of blood by MS; and implementing new sampling algorithms for molecular dynamics simulations of biomolecular systems along a range of time scales

All these approaches are key for understanding the Chemistry of Life in atomic detail and for bridging scales in biology and life sciences.

Quantitative Biology

Quantitative Biology uses advanced computational approaches and technologies to accurately analyze biological systems. Such quantitative descriptions are critical to construct and model engineered life systems, and to gain a deeper understanding of the life sciences. The transforming developments in analytical sciences such as single cell analysis, DNA and RNA sequencing, proteomics, metabolomics, nanotechnology, and imaging are providing unprecedented insights into the state of each cell in the whole body over time. Chemistry of Life is playing a pivotal role in the transition to a more quantitative description of biology through the development of analytical methods, probes and analysis tools. Integrating these advances with new developments in organ-on-a-chip and organoid technologies will provide powerful opportunities to test hypotheses and improve models for physiology and targeting of cellular systems. The size of systems that can now be quantitatively studied has drastically increased, from single cells to the interplay and the molecular signals underlying the communication between microbes and a host organism.

Pathogenic microorganisms can pose a global threat to our health. Understanding the molecular machines and networks within microbes, determining how they interact with the host, and uncovering potential treatment angles are all areas of intense investigation in the Dutch Chemistry of Life community. At the same time many microorganisms are enormously beneficial for our health and wellbeing. The microbiome influences human, animal, and plant physiology in many different ways. Understanding the interplay and the molecular signals underlying the communication between host and microbiome is crucial for determining how the microbiome can be measured and targeted to improve the health of humans, animals, and plants. This field is driven by massively parallel RNA- and DNA-sequencing technologies to map the microbiome communities and deep metabolomics analyses to uncover the molecular signals and define the micro-environment.

The ongoing transition from qualitative to quantitative biology, together with new measurement techniques and the possibilities to acquire data at an ever-increasing pace leads to a rapid expansion of information and big data. As a consequence, data will no longer be interpreted by intuition but requires completely new analysis strategies. In Chemistry of Life and many other areas of science and society, there is a growing need for innovative technologies, algorithms, and artificial intelligence to interpret these huge quantities of data.

Creating new Chemistry for Life

New drugs and treatments

Small molecules and biologics (e.g. antibodies, nanobodies) have the potential to improve life span and the quality of life. The Chemistry of Life community focuses on the development of synthetic methodologies and the discovery of novel small molecules. This research is aimed at understanding the function of these compounds and how they can be used to manipulate biomolecules in a cellular context. This will in turn lead to the development of novel chemical probes, diagnostics and drugs for personalized medicine (medicinal chemistry, chemical biology, biochemistry, molecular pharmacology, molecular toxicology, pharmaceutics, computational chemistry). Additionally, the Chemistry of Life community focuses on the development of biologics to directly manipulate molecular pathways, and ultimately develop them into new drugs. Furthermore, chemistry of life is pushing the boundaries of modern-day medicine through the development of new chemical compounds that are aiding image/fluorescence-guided surgery or diagnosis.

Synthetic biology, understanding and redesigning cellular processes

Our ability to (re)design and control naturally occurring enzymatic, genetic, as well as structural molecular networks will also shed light on the minimal requirements for life. Out of all possible forms of matter, only a small fraction has been realized in nature. Chemistry of Life is learning from, and engineering beyond, nature: Chemical synthesis and bioengineering are rapidly evolving our ability to create and investigate non-natural systems. In the future, we will design and synthesize more and more sophisticated molecules with new and improved functionalities. The re-creation of complex natural systems such as synthetic living cells will provide a unique route to the fundamental understanding of how cells work. This research will thus provide novel entries into diagnostics and therapy. Advanced engineering of the molecules within the cell and state-of-the art chemical biological approaches to optimize biomolecules will offer many new opportunities. This includes innovative vaccination strategies, efficient drug delivery, image-guided surgery, smart diagnostics tools, and personalized treatment regimens for cancer, diabetes, protein misfolding diseases, and other diseases. Furthermore, the redesigning of light-harvesting structures of photosynthetic bacteria, algae and plants will allow optimization of the photosynthesis process in living organisms and development of novel artificial solar systems.

Green chemistry, Green energy and Sustainable Biomaterials

Microorganisms compose a wide array of unicellular and multicellular structures that cover viruses, archaea, eubacteria and eukaryotes. Understanding at the molecular level how bacteria defend themselves to invading DNA has led to the development of powerful and versatile genome editing tools, allowing us to break the chemical bonds of DNA within cells and thereby provide the means for editing of the genetic code at high precision. These tools, such as CRISPR-Cas, are enabling technologies that open up many new possibilities for molecular genetics as well as modifying and engineering genomes. The opportunities to take advantage of microorganisms are far reaching. The emerging power of sophisticated and precise bioengineering will create a vast amount of bio-related or bio-inspired molecules (bio-based chemicals) that will have a tremendous impact on applications in biotechnology, in academia and industry.

Synthetic biology and sophisticated genome engineering can enable more sustainable production not only of drugs and functional foods, but also facilitating synthesis of consumer products and bulk chemicals. Engineered microorganisms transforming renewable feedstock into high value-added products such as pharmaceuticals, agrochemicals, cosmetic ingredients but also polymer building blocks will become much more important in the years to come. From a green chemistry perspective this will lead to cleaner production processes (producing more efficiently and with less toxic side products) and using significantly less resources (starting material and energy). Examples of the transforming nature of the 'clean chemistry for life' are bioelectrochemical production of ammonia and synthesis of biohydrocarbons for applications ranging from the anti-Malaria drug Artemisinin to the jet fuel Farnesene and engineered enzymes enabling more selective transformations than existing chemical technologies.

Chemistry of Life for Society

Chemistry of Life offers many opportunities for addressing the pressing societal challenges described by the United Nations. The UN have set an agenda for 2030, termed the Sustainable Development Goals, for peace and prosperity for all people and the planet, now and in the future. It is an urgent call for action by all countries, including the Netherlands, to end poverty and other deprivations. This aim, together with strategies to improve health and education, reduce inequality and spur economic growth. At the same time, we need to tackle climate change and preserve our ecosystems and natural resources. Chemistry of Life, a cross-disciplinary science at the center of new innovations and technologies, offers solutions for these urgent societal problems. Chemistry of Life was, for example, the leading driving force for the discovery of antibiotics and antiviral agents, which together have saved millions of patients suffering from infectious diseases. Yet, these challenges are far from over. Antibiotic resistance is increasing rapidly and viral infections remain a serious threat, as we have seen in the recent outbreak growing into the Covid-19 lethal pandemic within a short period of time. In addition, the world is facing new challenges that are brought about both by our increasing life span and modern life style. Examples of these challenges include cancer, metabolic syndromes, neurodegenerative and cardiovascular diseases. Additional threats are neglected diseases (typically restricted to specific geographical areas, often in developing nations) and orphan diseases (whose rarity means there is a lack of commercial interest), which can be devastating for nations or individual patients. New knowledge and intervention from Chemistry of Life can be catalytic to finding solutions and will be essential to reduce the burden of all these diseases in both health and economic terms.

Other world-changing developments that rely on research from the field of Chemistry of Life are found in the areas of agriculture, horticulture, biodiversity, biomaterials and energy supply. The emerging power of sophisticated and precise bioengineering will create a vast number of biomolecules and bio-based chemicals. These will undoubtedly have a tremendous impact on applications in biotechnology, in academia and in industry for the sustainable production of food, fuel, drugs, and a large variety of other chemical building blocks. Thus, by uncovering the fundamental molecular principles that govern life from microorganisms to humans, Chemistry of Life will continue to provide solutions to improve human health, a healthy environment, and sustainable well-being.

Challenges for the future

Dutch Chemistry of Life research is among the best in the world and can lead the way in addressing todays pressing global challenge to provide food and health care for an ageing world population (treatments/diagnostics/) while preserving our planets climate, resources and biodiversity (green chemistry/energy/sustainable biomaterials). The investments needed to sustain and expand our leading role are the following: First, we need to train tomorrow’s top Dutch Chemistry of Life scientists. Fortunately, young people are very interested in the Chemistry of Life university programs, and the number of students enrolled in such programs has doubled in the past ten years. The graduates from these programs have an excellent position in the labor market in the Netherlands and beyond. To support this positive development, investments in teaching positions in biology and chemistry will remain a top priority. Second, and critically, the community needs access to equipment and infrastructure investments. In addition, it requires a funding climate that allows both fundamental curiosity driven research and translational research. Investments in these areas have dropped far below international standards and are well below what is minimally needed. Thus, the Netherlands is still one of the world leaders in Chemistry of Life, but it must, crucially, continue to invest in this area of science to maintain the leading role and grasp the many exciting opportunities offered by the rapid changes in the field.

Research Community

Chemistry of Materials

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Vision for 2040

New materials are at the basis of solutions for societal challenges, ranging from transition to sustainable energy production and sustainable chemical processes to the discovery of adaptive and responsive materials, the development of sensing systems for e.g. health care and the food industry, all the way to quantum technologies for next-generation electronics. Our societies face an ever-accelerating succession of materials eras, where applications of materials rapidly become obsolete. This rapid succession of new materials does not always take full account of issues such as recycling and disposal, energy efficiency and scarcity. Designing and developing the materials that will define our societies in the future thus requires inventing radically new approaches, and chemistry is at the core of this effort since it is the science that bridges the atomic and molecular world with the macroscopic world. While the increased attention to functional materials that started in the previous century was to a large extent based on serendipity, the next decades will show a transition towards predictive properties and controlled assembly of materials; to design and engineer highly sophisticated, energy-friendly and circular materials that also take the scarcity of resources into account, and that can drive our societies towards the next materials era.

Chemistry of Materials in the Netherlands

Materials play a key role in virtually all aspects of our lives, in low- and high-tech products and applications. Dutch chemistry has been at the forefront of research and innovation of materials and successfully continues to do so, with strong links to other disciplines and innovative companies. We envision that the chemistry of materials will become the key enabling science that we need to address the societal challenges of scarcity, sustainability and energy challenges. The increased understanding of the properties of materials ultimately allows us to predict and design materials with the required functionality for specific applications. New structures can be built up from the atomic and molecular scales, up to the macroscale with unmatched precision and efficiency. Chemistry is at the heart of these developments. It deals with the synthesis and processing of materials and the study of their properties, spanning a wide range of the core chemical disciplines, including (in)organic chemistry, macromolecular chemistry, theoretical, analytical chemistry and physical chemistry. Internationally, the chemistry of materials is contributing to tackling a wide range of societal challenges, including efficient energy conversion and storage, reduced use of feedstock and energy, solutions for switching from single-use to reuse, improved sorting and (chemical) recycling, miniaturization, multifunctional coatings, and affordable and personalized healthcare for an aging society.

Furthermore, a wide range of industrial partners are active in the Netherlands, including e.g. DSM, Unilever, Shell, AkzoNobel, Nouryon, OCE-Canon, Arkema, Perkin Elmer, BASF, Philips, ASML, Corbion etc. Direct links between industry and academia exist and are active and effective, both in bringing forward transformative ideas and in generating intellectual property leading to new industrial productivity.

Materials for sustainable energy

Supplying energy in a sustainable way and at a reasonable cost remains a key societal concern. Overcoming this challenge requires a bifurcation from current fossil fuel-based technologies to renewable sources such as wind and solar energy. This transition requires a massive push towards even more affordable and efficient devices. For example, the cost-effective conversion of energy from sunlight requires new sustainable materials that can result in cheap high-efficiency solar cells. Examples of such new materials include organic semiconductors, semiconductor nanocrystals, perovskites and novel inorganic materials. In addition to active materials themselves, also the electrode materials, (mechanically flexible) substrates and sealings, and photonic materials for light management are being developed. These alternative energy sources are accompanied by the problem of intermittency: energy supply is not always available when it is needed. Therefore, storage of energy in a suitable form is equally important as the conversion of energy itself. In the energy storage, new battery and supercapacitor materials including polyelectrolyte membranes, solid electrolytes and high-voltage cathode materials are of prime importance.

Materials for the circular economy

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 finite and not circular, and climate change should force 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. Novel materials will have in common: less non-renewable energy use and less green-house gas emission during the synthesis, construction, processing, packaging, transportation, usage, recycling and re-use and disposal of these materials.

Materials for chemical conversion

Catalysts are key components in chemical conversion processes. Many industrial processes use catalysts that are either solids or in the form of nano-porous and nanocrystalline materials, for instance metal-organic frameworks, zeolites, or supported nanoparticles and clusters such as nickel, gold or platinum. While solid catalysts are important in 'traditional' chemical processes, they are also of strong interest in the most recent developments in the electrification of industry, where conventional processes are replaced by electrochemical conversion. In addition, the direct use of light in chemical conversion requires development of new stable and efficient photocatalytic materials.

Materials for digital technology

Digital technology is the basis of our modern society. Semiconductor components are present in all modern devices in the form of microprocessors and other integrated circuits. The ongoing miniaturization of these devices puts new requirements on the materials used in the devices themselves but also in production processes where for instance extreme UV lithography is used (EUV photoresists and EUV resistant materials). In addition to miniaturization, also completely new technologies are emerging, for instance in sensor technology, photonics and flexible (wearable) electronic devices and sensors. All these developments in digital technology require a detailed understanding and development of new materials, including semiconductors (inorganic, polymers, hybrid perovskites, nanocrystal arrays) and insulator materials, but also materials for light management in photonic devices.

Materials for health, food and medicine

Early diagnosis, effective surgical and pharmacological interventions, healthy ageing and affordable healthcare all require the engineering of stimuli-responsive, adaptive, mechanically and bioactive molecular and biomolecular materials. Examples of such materials are found in nanomedicine, self-healing prosthetics, soft robotics, tissue regeneration, drug discovery and personalized medicine. Materials that mimic those found in native tissues with respect to their structural and functional dynamics serve as an inspiration in this area. Active materials that will respond to external triggers selectively and autonomously, adapt their function, and interface with biological systems are being developed with the aim of instructing cellular behavior in vitro in developmental or disease contexts, but also for in vivo applications. The combination of these new materials with advanced processing techniques (e.g. microfluidics, 3D printing) will be vital to widen their scope in the healthcare area.

Scientific Challenges

The overarching theme in the chemistry of materials is to come to a bottom-up understanding of how structure and structural dynamics translate from the atomic and the molecular scale, across increasing length scales, and eventually up to the macroscopic and functional level. A number of scientific challenges are associated with this overarching aim:

Understanding the interplay between structure and properties

Controlling the properties of materials begins with controlling their structure on the nanoscale. Such control can be achieved, for example by making use of synthetic (in)organic chemistry, through self-assembly of (macro)molecular and colloidal building blocks into functional and sometimes dynamic superstructures, by using the sophistication of supramolecular chemistry or by controlling mesoscale morphology.

Ever improving the characterization strategies

Both the unfettered research on matter and the mission-oriented and rational design of materials requires the continuous development of characterization and analytical tools with an ever-increasing resolution in time, space and energy. Advanced characterization techniques include structural, mechanical and functionality characterization methods and in situ monitoring of materials synthesis and evolution.

Predictive computational methods

Computational approaches such as electronic structure calculations and classical force field methods are widely used to gain understanding of the properties of materials. These methods have limitations in the sample dimensions and time scales that can be studied. There is a clear need for improved computational methods that can predict the properties of materials with sufficient accuracy at the appropriate length and time scales. This requires continued development of current computational methods such as density functional and wavefunction-based electronic structure approaches, classical forcefield methods and mixtures of these, but also a broadening to the use of machine learning techniques that are rapidly emerging.

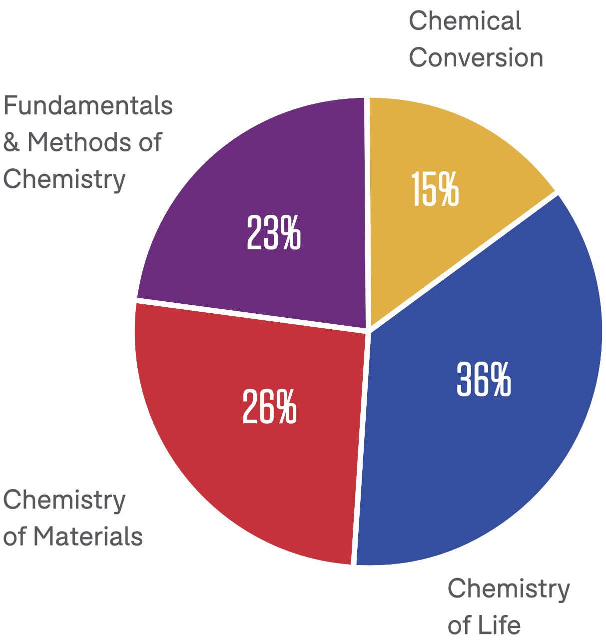
Interdisciplinarity

Addressing such diverse and complex scientific challenges in various systems and at different length scales requires exploring new fundamental frontiers at the interface between materials chemistry, physics, engineering, biology and medicine, and the research field Chemistry of Materials should play a central role in this development. This is accompanied by efficient organizational and funding resources to improve collaboration over the barrier of the different disciplines.

Facts & Figures

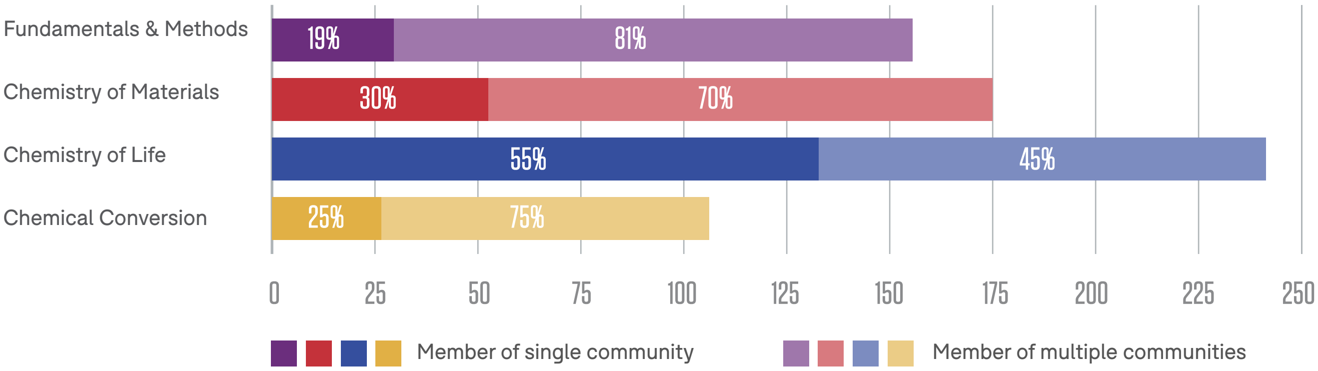
Memberships of Research Communities of Chemistry

468 researchers in Chemistry are member of one or more research communities, in total there are 682 registered memberships. Around 7% of the registered researchers are from industry or universities abroad. The largest community is Chemistry of Life with 243 members, followed by Chemistry of Materials (175), Fundamentals & Methods of Chemistry (159) and Chemical Conversion (105).



Overlap between memberships

Researchers can be members of more than one community. Most members (81%) of Fundamentals & Methods of Chemistry are also a member of another research community, whereas 55% of the members of Chemistry of Life are only a member of this community. Every single community has an overlap in memberships with all of the other communities.



Composition advisory committees Chemistry and Round table Chemistry

Chemistry of Life

Fred van Leeuwen	*chair,* gene regulation
Liesbeth Veenhoff	*vice-chair,* cellular biochemistry
Luc Brunsveld	chemical biology
Mario van der Stelt	molecular physiology
Antoinette Killian	membrane chemistry and biophysics
Ariane Briegel	cryo-electron microscopy
Jocelyne Vreede	molecular simulation of proteins and DNA
Kim Bonger	biomolecular chemistry
Anastassis Perrakis	structure and function of macromolecules
Govert Somsen	biomolecular analysis
Nadine Mascini	Secretary

Fundamentals & Methods of Chemistry

Wybren Jan Buma	*chair,* spectroscopy of photo active molecules and materials
Shirin Faraji	*vice-chair,* theoretical and computational chemistry
Marc Baldus	biophysical chemistry, NMR, (bio)materials
Bas de Bruin	homogeneous catalysis
Geert-Jan Kroes	theoretical chemistry, molecular dynamics
Evgeny Pidko	inorganic chemistry, computational chemistry, green chemistry
Anouk Rijs	physical analytical chemistry, biomolecular structures and interactions
Albert Schenning	functional (polymeric) materials & devices
Sabeth Verpoorte	analytical chemistry, microfluidics
Vera Meester	Secretary

Chemical Conversion

Tati Fernández Ibáñez	*chair,* organic chemistry
Harry Bitter	*vice-chair,* biobased chemistry
Sylvestre Bonnet	bioinorganic chemistry and photochemistry
Frank Hollmann	biocatalysis
Sascha Kersten	sustainable process technology
Pieter Bruijnincx	chemocatalysis
Dick Janssen	chemical biotechnology
Wiebe de Vos	membrane surface science
Erik Heeres	chemical reaction engineering
Maurits Boeije	Secretary

Chemistry of Materials

Ilja Voets	*chair,* self-organising soft matter
Andries Meijerink	*vice-chair,* inorganic solid state chemistry
Katja Loos	polymer science
Elias Vlieg	solid state chemistry
Jasper van der Gucht	soft matter
Roxanne Kieltyka	biomaterials
Nathalie Katsonis	bio inspired smart materials
Ferdinand Grozema	optoelectronic properties of materials
Andrea Baldi	nanomaterials for energy applications
Abeer Hossain	Secretary

Composition Round table

Patricia Dankers	*chair,* supramolecular biomaterials
Bernard Dam	*vice-chair,* materials for energy conversion and storage
Rolf van Benthem	materials science, polymers, resins, coatings, active surfaces
Matthias Bickelhaupt	theoretical chemistry
Erik Garnett	nanoscale solar cells
Heleen Goorissen	biotechnologie en fermentatie
Syuzanna Harutyunyan	synthetic organic chemistry
Joyce Lebbink	molecular mechanism and regulation of DNA repair
Johan Padding	complex fluid processing
Jana Roithova	spectroscopy and catalysis
Dirk Slotboom	membrane protein structure and function
Marcel Hoek	Secretary
Mark Schmets	Secretary

This vision for Chemistry was created by the Round table Chemistry and the advisory committees of the research communities of Chemistry with support of programme officers of the NWO Domain Science. The vision presented here does not necessarily represent the vision of NWO.