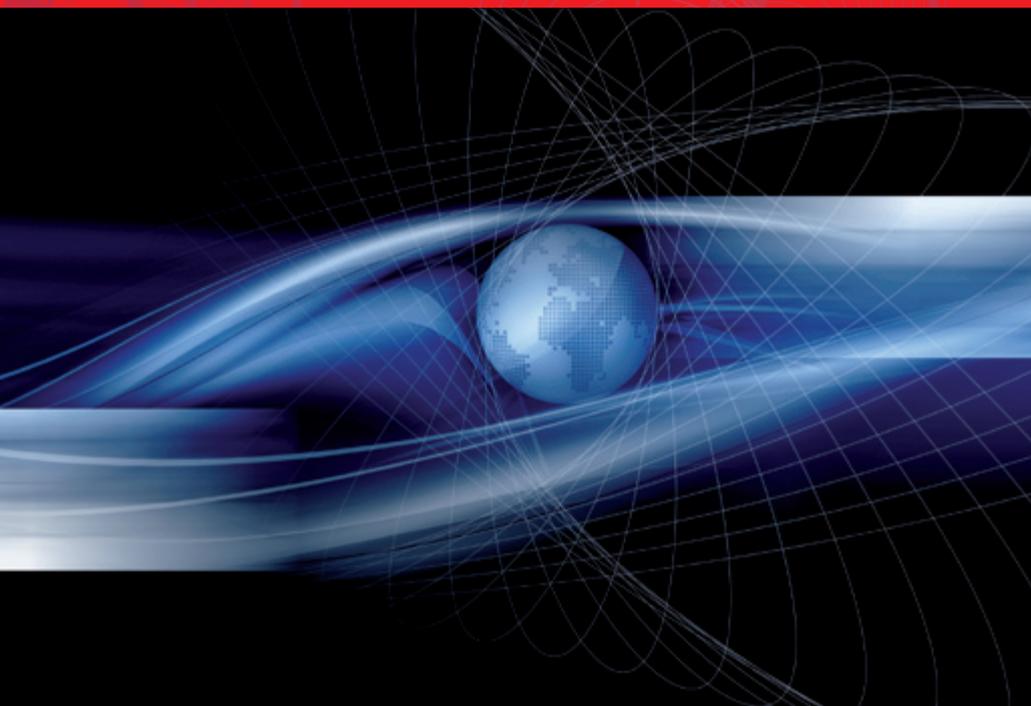




European Association for Chemical and Molecular Sciences

CHEMISTRY

Developing solutions
in a changing world





European Association for Chemical
and Molecular Sciences
EuCheMS aisbl
Nineta Majcen
General Secretary
Avenue E. van Nieuwenhuysse 4
B-1160 Brussel
www.euchems.eu

INTRODUCTION	2
EXECUTIVE SUMMARY	3
Breakthrough Science	3
Energy	3
Resource Efficiency	4
Health	4
Food	5
1.0 BREAKTHROUGH SCIENCE	6
1.1 Introduction	6
1.2. Underpinning Chemical Sciences	7
1.2.1 Synthesis	8
1.2.2 Analytical Science	8
1.2.3 Catalysis	9
1.2.4 Chemical Biology	9
1.2.5 Computational Chemistry	9
1.2.6 Electrochemistry	10
1.2.7 Materials Chemistry	10
1.2.8 Supramolecular Chemistry and Nanoscience	10
2.0 ENERGY	12
2.1 Solar Energy	12
2.1.1 Solar Electricity	12
2.1.2 Biomass Energy	13
2.1.3 Solar Fuels	14
2.2 Wind and Ocean Energies	15
2.3 Energy Conversion and Storage	15
2.3.1 Energy storage: Batteries and Supercapacitors	16
2.3.2 Energy conversion: Fuel Cells	16
2.4 Hydrogen	17
2.5 Energy Efficiency	18
2.6 Fossil Fuels	19
2.7 Nuclear Energy	20
3.0 RESOURCE EFFICIENCY	22
3.1 Reduce Quantities	23
3.2 Recycle	23
3.3 Resource Substitution	24
4.0 HEALTH	26
4.1 Ageing	26
4.2 Diagnostics	27
4.3 Hygiene and Infection	27
4.4 Materials and Prosthetics	28
4.5 Drugs and Therapies	28
4.6 Personalised Medicine	30
5.0 FOOD	31
5.1 Agricultural productivity	31
5.1.1 Pest control	31
5.1.2 Plant science	32
5.1.3 Soil science	32
5.2 Water	33
5.2.1 Water Demand	33
5.2.2 Drinking water quality	33
5.2.3 Wastewater	33
5.2.4 Contaminants	34
5.3 Livestock and Aquaculture	34
5.4 Healthy Food	35
5.5 Food Safety	35
5.6 Process Efficiency	36
5.6.1 Food Manufacturing	36
5.6.2 Food distribution and Supply Chain	36
REFERENCES	38

Introduction

Global change is creating enormous challenges relating to energy, food, health, climate change and other areas, action is both necessary and urgent. The European Association for Chemical and Molecular Sciences (EuCheMS) is fully committed to meeting these challenges head on. Working with a wide range of experts we have identified key areas where advances in chemistry will be needed in providing solutions. In each area we are in the process of identifying the critical gaps in knowledge which are limiting technological progress and where the chemical sciences have a role to play.

The EU's renewed commitment to innovation, resulting in growth and jobs, will take research from the lab to the economy. The chemical sciences will play a pivotal role in ensuring that the European Union is able to realise its vision of becoming an 'Innovation Union'. In a multi-disciplinary world chemistry is a pervasive science. In addition to be an important and highly relevant field in its own right, chemistry is central to progress in many other scientific fields from molecular biology, to the creation of advanced materials, to nanotechnology.

We have identified the following areas that should be priorities in the future framework programme. There is a strong overlap with the 'Grand Challenges' identified in the Lund Declaration¹ :

Breakthrough Science, page 6

Energy, page 12

Resource Efficiency, page 22

Health, page 26

Food, page 31

About the **European Association for Chemical and Molecular Sciences**: the European Association for Chemical and Molecular Sciences is a not-for-profit organisation and has 44 member societies which together represent more than 150,000 chemists in academia, industry, government and professional organisations in 34 countries across Europe. EuCheMS has several Divisions and Working Groups which cover all areas of chemistry and bring together world class expertise in the underpinning science and development needed for innovation.

Executive Summary

Developing Solutions in a Changing World has endeavoured to highlight the central importance of chemistry to solving a number of the challenges that we face in a changing world. The role of chemistry both as an underpinning and applied science is critical.

Breakthrough Science

The results of chemistry research are all around us: the food we eat, the way we travel, the clothes we wear and the environment we live in. All of the technological advances that surround us require breakthroughs in science and chemistry is a science that has laid the foundations for many everyday technologies. Without advances in fundamental organic chemistry for instance, we would be without our modern arsenal of drugs and therapies that allow us to fight diseases.

Eight key areas in the chemical sciences have been identified where scientific breakthrough is required to meet the global challenges:

- **Synthesis**
- **Analytical Science**
- **Catalysis**
- **Chemical Biology**
- **Computational Chemistry**
- **Electrochemistry**
- **Materials Chemistry**
- **Supramolecular Chemistry and Nanoscience**

Advances in these areas enable the breakthroughs that change the quality of our lives. Often the impact of breakthrough science is not felt until years after the initial discovery. Therefore, it is essential that fundamental chemical science research, that is not immediately aligned to an application, is given enough funding to flourish.

Energy

Europe faces vast challenges in securing a sustainable, affordable and plentiful supply of energy in the coming years. The energy ‘puzzle’ is an area that requires multidisciplinary

input from across the scientific landscape; however, the role of the chemical sciences is deftly showcased here across a variety of technologies.

- **Solar** – solar energy involves harvesting and converting the free energy of the sun to provide a clean and secure supply of electricity, heat and fuels. The chemical sciences will be central in providing the materials required for new-generation photovoltaics. The replication of photosynthesis is considered a key ‘grand challenge’ in the search for sustainable energy sources. Electrochemistry has an important role in developing systems that mimic photosynthesis and new catalysts are needed to facilitate the required processes.
- **Biomass Energy** – biomass is any plant material that can be used as a fuel. Biomass can be burned directly to generate power, or can be processed to create gas or liquids to be used as fuel to produce power, transport fuels and chemicals. Chemical scientists will be responsible for synthesising catalysts for biomass conversion, developing techniques to deploy new sources (eg. algae, animal waste) and refining the processes used for biomass conversion to ensure efficiency.
- **Wind and Ocean Energies** – new materials are needed that will withstand the harsh conditions of future offshore wind farms and ocean energy installations. Chemists will need to develop coatings, lubricants and lightweight composite materials that are appropriate to these environments. Sensor technologies to allow monitoring and maintenance are also critical to the long-term viability of such installations.
- **Energy Conversion and Storage** – this issue is vital to the challenge of exploiting intermittent sources such as wind and ocean energies and encompasses a range of research areas in which the chemical sciences is central. Electrochemistry and surface chemistry will contribute to improving the design of batteries, so that the accumu-

lated energy that they can store will be greater. Fuel cells that work at lower temperatures cannot be developed without advances in materials. Alternative energy sources such as hydrogen will not be viable without advances in materials chemistry.

- **Energy Efficiency** – chemistry is the central science that will enable us to achieve energy efficiency through a number of ways; building insulation, lightweight materials for transportation, superconductors, fuel additives, lighting materials, cool roof coatings, energy-efficient tyres, windows and appliances.
- **Fossil Fuels** – with continuing use of fossil fuels, the chemical sciences will provide solutions to help control greenhouse gas emissions, find new and sustainable methodologies for enhanced oil recovery and new fossil fuel sources (eg. shale gas) and provide more efficient solutions in the area of carbon capture and storage technologies.
- **Nuclear Energy** – this is underpinned by an understanding of the nuclear and chemical properties of the actinide and lanthanide elements. The chemical sciences will be central to providing advanced materials for the storage of waste, as well as improved methods for nuclear waste separation and post-operational clean-out.

Resource Efficiency

Resource Efficiency must support our efforts in all other areas discussed in this document. In order to tackle this challenge, significant changes need to be made by governments, industry and consumers. Our current rates of global growth and technological expansion mean that a number of metals and minerals are becoming depleted, some to critical levels. The chemical sciences have a role in assisting all of us in a drive towards using our existing resources more efficiently.

- **Reduce Quantities** – chemical scientists will carry out the rational design of catalysts to ensure that quantities of scarce metals are reduced (e.g. less platinum in new catalytic converters).

- **Recycle** – designers and chemical scientists will need to work together to ensure a ‘cradle-to-cradle’ approach in the design of new products. More consideration needs to be given to the ability to recycle items and so ensure efficient use of resources. Chemical scientists will need to develop better methodologies to recover metals with low chemical reactivity (eg. gold) and recovering metals in such a way that their unique properties are preserved (eg. magnetism of neodymium).
- **Resource Substitution** – chemical scientists will be at the forefront of delivering alternative materials that can be used in technologies to replace scarce materials. For example, the replacement of metallic components in display technologies with ‘plastic electronics’ or the development of catalysts using abundant metals instead of rare ones.

Health

There is significant inequality in provision of healthcare and the scope of health problems that humanity faces is ever-changing. Chronic disease is on the increase as average life expectancy increases, uncontrolled urbanisation has led to an increase in the transmission of communicable diseases and the number of new drugs coming to market is falling. The chemical sciences are central to many aspects of healthcare. The discovery of new drugs is only a single aspect of this; chemists will be responsible for developing better materials for prosthetics, biomarkers to allow early diagnosis, better detection techniques to allow non-invasive diagnosis and improved delivery methods for drugs.

- **Ageing** – chemical scientists will develop sensitive analytical tools to allow non-invasive diagnosis in frail patients, advances will be made in treatments for diseases such as cancer, Alzheimer’s, diabetes, dementia, obesity, arthritis, cardiovascular, Parkinson’s and osteoporosis. New technologies and materials to enable assisted living will also be developed.
- **Diagnostics** – chemical scientists will help develop analytical tools which have a greater sensitivity, require smaller samples and are non-invasive. Improvements in

biomonitoring will lead to earlier disease detection and could even be combined with advances in genetics to administer personalised treatment.

- **Hygiene and Infection** – chemical scientists will help to improve the understanding of viruses and bacteria at a molecular level and continue to lead the search for new anti-infective and anti-bacterial agents.
- **Materials and Prosthetics** – chemists will develop new biocompatible materials for surgical equipment, implants and artificial limbs, an increased understanding of the chemical sciences at the interface of synthetic and biological systems is critical to the success of new generation prosthetics.
- **Drugs and Therapies** – New methodologies in drug discovery will be driven by chemical scientists; a move from a quantitative approach (high throughput screening) to a qualitative approach (rational design aimed at a target) is essential in future research strategies. A number of other areas will also be essential; computational chemistry for modelling, analytical sciences in relation to development and safety and toxicology in the prediction of potentially harmful effects.

Food

With an increasing global population and ever limited resources (land, water), we face a global food crisis. The management of the resources that we have and development of technologies to improve agricultural productivity require the input of scientists and engineers from a range of disciplines to ensure that we can feed the world in a sustainable way.

- **Agricultural Productivity** – the role of chemical scientists is central to the development of new products and formulations in pest control and fertilisers. They will also contribute to improving the understanding of nutrient uptake in plants and nutrient transport and interaction in soils to help improve nutrient delivery by fertilisers.
- **Water** – chemical scientists will help design improved materials for water transport, analytical and decontamination techniques to monitor and purify water, as well as identifying standards for the use of wastewater in appli-

cations such as agriculture.

- **Effective Farming** – chemical scientists will develop new technologies such as biosensors to assist farmers in monitoring parameters such as nutrient availability, crop ripening, crop disease and water availability. Effective vaccines and veterinary medicines to improve livestock productivity will also be essential.
- **Healthy Food** – chemical scientists will be able to contribute to the production of foods with an improved nutritional content, whilst maintaining consumer expectations. Understanding the chemical transformations that occur during processing and cooking will help to improve the palatability of new food products. Malnutrition is still a condition that affects vast numbers of people worldwide; chemists will be essential in formulating fortified food products to help combat malnutrition and improve immune health.
- **Food Safety** – chemical scientists will contribute to new technologies to help detect food-borne diseases as well as developing precautionary techniques, such as the irradiation of food to prevent contamination.
- **Process Efficiency** – The manufacturing, processing, storage and distribution of food needs to be changed to ensure minimum wastage and maximum efficiency. Chemical scientists can contribute to improving efficiency in a number of ways. These include understanding the chemistry of food degradation and what can be done to prevent this, development of better refrigerant chemicals in the transport and storage of food and design of biodegradable or recyclable food packaging.

1.0 BREAKTHROUGH SCIENCE

1.1 Introduction

Science and technology together provide the foundation for driving innovation to continually improve our quality of life and prosperity. Major breakthroughs in chemistry are required to solve major current and future societal challenges in health, food and water, and energy. In subsequent chapters these challenges are discussed in detail, together with ways in which the chemical sciences will help to provide solutions.

A broad range of research activities will be needed to tackle societal challenges and enhance global prosperity, including curiosity-driven fundamental research. This can only be achieved by maintaining and nurturing areas of underpinning science.

Key Messages

- The chemical sciences will continue to play a central role in finding innovative solutions to major societal challenges;
- Chemistry is one of the driving forces of innovation with significant impact on many other industrial sectors.
- The solutions will require breakthroughs in science and technology originating from a rich combination of advances in understanding and new techniques, as well as major and sometimes unpredictable discoveries;
- To maximise the capacity for breakthroughs it is crucial to adequately support curiosity-driven research.

How Are Breakthroughs Made?

There is no simple “formula” that predicts how to achieve a breakthrough. Major advances often do not happen in a linear, programmable way. Historically, those scientists who have made such innovative breakthroughs often did not envisage the final application.

Breakthroughs in science and technology:

- can revolutionise the lives of citizens in positive ways;
- often are unexpected, even by the people who make them, and lead to unexpected applications;
- are made by excellent researchers usually through some combination of (i) new discoveries, (ii) creative, often brilliant, thinking, (iii) careful, collaborative hard work and (iv) access to resources and knowledge.
- frequently involve combining research from different subfields of the chemical, physical, biological and engineering sciences in a new way;
- may involve combining advances in theoretical or conceptual understanding and/or experimental laboratory-based research with novel techniques;
- can facilitate further breakthroughs in other areas of science and lead to many novel applications, the benefits of which can last and evolve for a long time;
- often happen on a time-line that is not smooth, for example there is often incremental progress for many years and work which lays the foundation for major discoveries.

Example 1: The Haber Process

One hundred million tonnes of nitrogen fertilisers are produced every year using this process, which is responsible for sustaining one third of the world’s population. In recent years this has led Vaclav Smil, Distinguished Professor at the University of Manitoba and expert in the interactions of energy, environment, food and the economy, to suggest that, ‘The expansion of the world’s population from 1.6 billion in 1900 to six billion would not have been possible without the synthesis of ammonia’.

The Haber process owes its birth to a broader parentage than its name suggests. Throughout the 19th century scientists had attempted to synthesise ammonia from its constituent elements: hydrogen and nitrogen. A major breakthrough was an understanding of reaction equilibria brought about by Le Chatelier in 1884. Le Chatelier’s principle means that changing the prevailing conditions, such as temperature and pressure, will alter the balance between the forward and the backward paths of a reaction. It was thought possible to

breakdown ammonia into its constituent elements, but not to synthesise it. Le Chatelier's principle suggested that it may be feasible to synthesise ammonia under the correct conditions. This led Le Chatelier to work on ammonia synthesis and in 1901 he was using Haber-like conditions when a major explosion in his lab led him to stop the work.

German chemist Fritz Haber saw the significance of Le Chatelier's principle and also attempted to develop favourable conditions for reacting hydrogen and nitrogen to form ammonia. After many failures he decided that it was not possible to achieve a suitable set of conditions and he abandoned the project, believing it unsolvable. The baton was taken up by Walther Nernst, who disagreed with Haber's data, and in 1907 he was the first to synthesise ammonia under pressure and at an elevated temperature. This made Haber return to the problem and led to the development, in 1908, of the now standard reaction conditions of 600 °C and 200 atmospheres with an iron catalyst². Although the process was relatively inefficient, the nitrogen and hydrogen could be reused as feedstocks for reaction after reaction until they were practically consumed.

Haber's reaction conditions could only be used on a small scale at the bench, but the potential opportunity to scale up the reaction was seized by Carl Bosch and a large plant was operational by 1913.

Example 2: Green Fluorescent Protein

Initial work in this area by Shiomura involved the isolation of the protein from the jellyfish *Aequorea victoria*. The work of Chalfie and Tsien examined the use of GFP as a tag to monitor proteins in biological environments, as well as understanding the fundamental mechanism of GFP fluorescence³.

The structure of green fluorescent protein (GFP) is such that upon folding, in the presence of oxygen, it results in the correct orientation for the protein to adopt a fluorescent form. Further studies on the structure revealed that it upon grafting GFP to other proteins, GFP retains its characteristic fluorescence and does not affect the properties of the attached protein, making it a useful biomarker.

What initially started out as a curiosity-driven quest to understand what caused this particular species to fluoresce has developed to provide researchers with a tool that can be used to monitor cellular processes in relation to conditions including Alzheimer's, diabetes and nervous disorders.

The three recipients did not directly collaborate on their work in this area and during his Nobel banquet speech, Professor Tsien referred to aspects of their work as the 'fragile results of lucky circumstances'. He also made reference to difficulties that researchers face in gaining funding for curiosity-driven research and how it is critical to the technological advances that improve our quality of life⁴.

Example 3: Coupling Chemistry

The breakthrough discovery of the Suzuki-Miyaura coupling reaction built on many years of research aiming to further understand the fundamental principles of reactivity of carbon compounds. This coupling reaction is an important tool now used by synthetic chemists in the formation of carbon-carbon bonds. Carbon-carbon bonds are fundamental to all life on earth. Without metal-coupling reactions such as this, it is very difficult to form carbon-carbon bonds. By examining the reactivity of carbon compounds in the presence of palladium, it was discovered that these compounds could be coupled *via* the formation of a carbon-carbon bond. This breakthrough led to the possibility of the synthesis of many kinds of complex molecules under relatively mild conditions.

Since its initial discovery, the Suzuki coupling reaction has become an indispensable tool for synthetic chemists to create new compounds. It also has widespread industrial applications, for example in ensuring the efficient production of pharmaceuticals, materials and agrochemicals⁵.

1.2. Underpinning Chemical Sciences

To maintain the flow of future breakthroughs and innovative ideas for our future prosperity, it is critical to advance fundamental knowledge and to support curiosity driven research. This can only be achieved by maintaining and nurturing areas of underpinning science. Modern science would not be

possible without past advances in synthesis for example, or the development of analytical and computational tools. Tools and techniques developed in one field are crucial in making progress in others. Described in this chapter are areas where scientific progress is needed for addressing global challenges. Although by no means an exhaustive list, these areas provide an indication of the critical role that chemistry plays in partnership with other disciplines.

1.2.1 Synthesis

The creation of new molecules, is at the very heart of chemistry. It is achieved by performing chemical transformations, some of which are already known and some of which must be invented⁶. Novel transformations are the tools that make it possible to create interesting and useful new substances. Chemists synthesize new substances with the aim that their properties will be scientifically important or useful for practical purposes.

Chemicals from renewable feedstocks: Today's chemical industry is built upon the elaboration and exploitation of petrochemical feedstocks. However economic and environmental drivers will force industrial end-users to seek alternative 'renewable' feedstocks for their materials⁷. To do so will require the development of new catalytic and synthetic methods to process the feedstocks found in nature (especially natural oils, fats and carbohydrates) which are in many cases chemically very different from petrochemical feedstocks and convert them to usable building blocks. Moreover, the design of new synthetic strategies will avoid, reduce or substantially minimize waste and will exploit in the best way fossil and natural resources as well.

New synthesis avoiding 'exhaustable' metals: Many chemical and pharmaceutical processes and routes are built upon the availability and use of a number of catalysts based on precious metals (see, for example, the award of the 2010 Nobel Prize in chemistry to Heck, Suzuki and Negishi for their pioneering work in organopalladium catalysis – reactions used in the synthesis of a number of blockbuster drugs). The popularity of these metal-mediated reac-

tions is because they achieve bond-forming processes and other transformations that are very difficult to do by other means. However, such metals are used in a wide variety of applications and demand is such that global supplies of many are predicted to reach critical levels or even be exhausted in the next 10-20 years⁸. The challenge for chemists is to find new methods using widely-available metal catalysts, or even metal-free alternatives, to maintain access to the key drugs and other products currently made using precious metals.

1.2.2 Analytical Science

Analytical science encompasses both the fundamental understanding of how to measure properties and amounts of chemicals, and the practical understanding of how to implement such measurements, including designing the necessary instruments. The need for analytical measurements arises in all research disciplines, industrial sectors and human activities that entail the need to know not only the identities and amounts of chemical components in a mixture, but also how they are distributed in space and time.

Developments in analytical science over many years have led to the practical techniques and tools widely used today in modern laboratories. Furthermore the accumulative data gained from some analytical procedures has significantly contributed to our understanding of the world today. For example in the field of molecular spectroscopy over the last 70 years chemical scientists have been able to characterise molecules in detail. The initial work on each molecule would not have had societal challenges in mind, but the cumulative knowledge on for example, the atmospheric chemistry of carbon dioxide, water, ozone, nitrous oxides etc. is now vital to the understanding of climate change.

Recent developments in the analytical sciences have promoted huge advances in the biosciences such as genome mapping and diagnostics. Improved diagnosis is also required, both in the developed and developing world. Many cancer cases for example remain undiagnosed at a stage when the cancer can be treated successfully. Developing

the procedure for exhaled breath analysis would lead to easy and early detection of the onset of cancer.

Analytical science can also help to meet the challenge of improving drinking water quality for the developing world⁹. There is a need to develop low cost portable technologies for analysing and treating contaminated groundwater that are effective and appropriate for use by local populations, such as for testing for arsenic contaminated groundwater.

1.2.3 Catalysis

Catalysts are commonly used in industry and research to affect the rate or outcome of a chemical reaction. They make the difference to a chemical process being commercially viable. As new reactions are developed for specific purposes, new catalysts are needed to optimise the reaction. Catalysis is a common denominator underpinning most of the chemical manufacturing sectors¹⁰. Catalysts are involved in more than 80 % of chemical manufacturing, and catalysis is a key component in manufacturing pharmaceuticals, speciality and performance chemicals, plastics and polymers, petroleum and petrochemicals, fertilisers, and agrochemicals. Its importance can only grow as the need for sustainability is recognised and with it the requirement for processes that are energy efficient and produce fewer by-products and lower emissions. Key new areas for catalysis are arising in clean energy generation *via* fuel cells and photovoltaic devices.

The challenge of converting biomass feedstocks into chemicals and fuels needs the development of novel catalysts and biocatalysts. For example, new techniques are needed for the breakdown of lignin, a naturally occurring polymer in plants and algae, and lignocellulose breakdown. Lignocellulosic biomass is the feedstock for the pulp and paper industry. This energy-intensive industry focuses on the separation of the lignin and cellulosic fractions of the biomass. Improved catalysts could greatly improve the conversion process and thereby improve efficiency, timescales and costs. Another example where research into novel catalysts is needed is improving the performance of energy storage concepts such as fuel cells which use supported catalysts. Catalysts

are fundamental to improving renewable electricity sources and the development of sustainable transport. Catalysis is central to the implementation of the bio-refinery concept, whereby biomass feedstocks in a single processing plant could be used to produce a variety of valuable chemicals.

1.2.4 Chemical Biology

This area focuses on a quantitative molecular approach to understanding the behaviour of complex biological systems and this has led both to chemical approaches to intervening in disease states and synthesising pared-down chemical analogues of cellular systems. Particular advances include understanding and manipulating processes such as enzyme-catalysed reactions, the folding of proteins and nucleic acids, the micromechanics of biological molecules and assemblies, and using biological molecules as functional elements in nano-scale devices¹¹.

Synthetic biology seeks to reduce biological systems to their component parts and to use these to build novel systems or rebuild existing ones. For example, synthetic biology will allow the development of new materials, the synthesis of novel drugs and therapies, and will provide organisms with new functions, such as the targeted breakdown of harmful chemicals in the environment.

1.2.5 Computational Chemistry

Developments in quantum mechanics in the 1920s and subsequently have led to the use of computer codes in nearly every modern chemical sciences laboratory. Such “computational chemistry” now plays a major role simulating, designing and operating systems that range from atoms and molecules to interactions of molecules in complex systems such as cells and living organisms. Collaboration between theoreticians and experimentalists covers the entire spectrum of chemistry and this area has applications in almost all industry sectors where chemistry plays a part.

Computational techniques can be used to advance medicinal chemistry by exploring the structure and function

of membrane proteins and related biomolecular systems. Computational studies can help to gain a deeper insight into enzyme reaction mechanisms related to diseases such as cancer, Alzheimers, and more. Computational modelling is invaluable in the elucidation of reaction mechanisms that are difficult to study experimentally, leading to the refinement of new reactions and processes. Another societal example of where computational chemistry is essential is in developing potential solutions to the energy challenge using solar cells. These offer an artificial means of using solar energy and have the potential to be a real alternative to the use of fossil fuels. But, if solar cells are to be developed into an efficient means of alternative energy, there is a critical need to understand the charge transport mechanisms they employ, and that is where the computational techniques are required.

1.2.6 Electrochemistry

Electrochemistry is an area of science that is critical to a variety of challenges outlined in this report, including the storage of intermittent renewable energy sources, batteries for the next generation of electric cars, the clean production of hydrogen, solar cells with greater efficiency and sensors for use in research of biological systems and healthcare. Fundamentally electrochemistry is concerned with interconverting electrical and chemical energy, but practically it can be applied as both an analytical and a synthetic tool. Currently, vast amounts of research in this area are carried out in Asia. The strategic importance of this area of science is such that Europe cannot afford to regress.

An important area for electrochemistry is in sensing. For example, for health and homeland security we will need to detect an increasing number of chemical species selectively, and ideally build this into sensing systems that can act on this information in real time. Electrochemical sensors are one means of providing this information. The challenge for complex systems is to develop multiple sensors integrated into a system able to detect and diagnose sensitively and selectively (like the multiple sensors in a nose interfaced with the brain). This requires better and more flexible sensor systems than at present.

There is much research to be done on understanding electrochemistry in living systems such as the nervous system. Nervous systems depend on the interconnections between nerve cells, which rely on a limited number of different signals transmitted between nerve cells, or to muscles and glands. The signals are produced and propagated by chemical ions that produce electrical charges that move along nerve cells. Electrochemical techniques can be applied to understand these systems and so improve therapies for neurodegenerative diseases such as Alzheimer's and Parkinson's.

1.2.7 Materials Chemistry

Materials chemistry involves the rational synthesis of novel functional materials using a large array of existing and new synthetic tools. The focus is on designing materials with specific useful properties, synthesising and modifying these materials and understanding how the composition and structure of the new materials influence or determine their physical properties to optimise the desired properties.

Materials Chemistry will play a major role in almost all sustainable energy technologies. New materials for batteries and fuel cells will be essential for storing energy from intermittent sources and for the use of hydrogen as a transport fuel respectively. Novel materials will also be required for carbon capture and storage, for the next generations of solar cells for electricity generation and for production of solar fuels on an industrial scale. Advanced light weight materials are decisive for more energy efficient mobility; materials that are durable enough to withstand long-term use in wind, wave and tidal-power will also be key.

1.2.8 Supramolecular Chemistry and Nanoscience

The integration of supramolecular chemistry and nanoscience offers huge potential in many diverse technological arenas from health to computing. Supramolecular chemistry involves the ordered structuring of discrete entities through non-bonding interactions. They can be structured in such a way as to enable information to be communicated between entities. Thus, these systems become more than the sum of

their parts. Potential applications of such technologies molecular computing, specific drug delivery, earlier detection of disease, food security, and detection of (bio)warfare agents.

Targeted Drug Delivery: Encapsulation and protection of therapeutic drugs in inert carriers that are on the length scale of biological entities offers huge opportunities for the combat of many diseases. Such entities will not only be able to recognise diseased cell types by the use of biological supramolecular interactions, reducing side-effects, but will also by virtue of their size facilitate both cellular uptake and triggered release of the drug in the diseased cell. This type of approach may lead to individual patient drug delivery if the diseased cells markers can be identified.

2.0 ENERGY

Modern life is sustained by a relentless stream of energy that is delivered to final users as fuels, heat and electricity. Currently, over 85% of the world's primary energy supply is provided by fossil fuels (81%) and uranium minerals (5.9%)¹². The current global energy demand is expected to double by 2050, mainly driven by economic growth in developing countries and by an increase of human population from the current level of 7 billion to over 9 billion people. However, by mid-century, the global fossil and fissionable mineral resources will be severely depleted, whilst global warming will have affected several regions of the planet with unpredictable economic and social consequences¹³.

Europe is the continent with the best average quality of life but is also the poorest in terms of conventional energy resources; it holds 1.0 %, 2.5 % and 3.5 % of world oil, gas and coal reserves¹⁴, respectively, and has virtually no uranium reserves¹⁵. Europe's current prosperity is based on primary energy resources coming from other continents, the populations of which are increasing their rate of consumption, inevitably limiting export capacity in the mid to long-term.

An alternative energy portfolio must be exploited, with the planet's primary energy sources of solar, geothermal and gravitational energy, featuring prominently, in this mix. Of the available options, the most abundant and versatile is solar energy, in addition to secondary sources such as wind, biomass, hydro and ocean currents¹⁶.

The energy challenge provides an extraordinary opportunity to drive the mature European industrial system towards truly innovative, sustainable energy concepts by promoting education, science and technology at all levels. However, it has to be pointed out that fossil fuels will continue to play a fundamental role in the European energy portfolio for some decades, therefore research in this area still requires support.

Chemistry is universally recognised as the "central science", since it bridges physical sciences with life and applied sciences. The energy challenge is an extraordinary multidisciplinary endeavour involving all disciplines from pure mathematics to applied engineering, passing through, physics, biology, geology, meteorology, biotechnology, computer science and many more. Indeed, energy research is the perfect setting for chemistry to fulfil its role as a central science.

2.1 Solar Energy

The sun provides the Earth with more energy in an hour than the global fossil energy consumption in a year. The sun is a source of energy many more times abundant than required by man; harnessing the free energy of the sun could therefore provide a clean and secure supply of electricity, heat and fuels. Developing scalable, efficient and low-intensity-tolerant solar energy harvesting systems represents one of the greatest scientific challenges today. The sun's heat and light provide an abundant source of energy that can be harnessed in many ways. These include photovoltaic systems, concentrating solar power systems, passive solar heating and daylighting, solar hot water, and biomass.

2.1.1 Solar Electricity

Solar photovoltaics is the fastest growing electric technology in Europe and has the potential to become a primary player in the global electricity portfolio by mid-century. Development of existing technologies to become more cost efficient and developing the next generation of solar cells is vital to accomplish key steps in the energy transition.

Solar photovoltaic (PV) systems directly convert sunlight into electricity. These systems are reliable, silent, robust and operate without moving parts; accordingly they are among the most durable energy converters. The International Energy Agency (IEA) envisions that by 2050, PV will provide 11% of global electricity production. In addition to contributing to significant greenhouse gas emission reductions, this level of PV will deliver substantial benefits in terms of the security of energy supply and socio-economic development. PV is ex-

pected to achieve competitiveness with electricity grid retail prices (grid parity), over the current decade in many regions of the world.

The current amorphous and crystalline silicon panels (80 % of the global PV market) have efficiencies between 5 and 17 % but their manufacturing is expensive and energy intensive. Thin film technologies are easier to produce but marketed products have an efficiency of 10-11%. Additionally, they pose bigger sustainability concerns since some are made with toxic (e.g. Cd) and/or rare (e.g. In, Te) elements. Current research into third generation PV systems is focussed on molecular, polymeric and nano-phase materials to make the devices significantly more efficient and stable, and suitable for continuous deposition on flexible substrates¹⁸. The cost of photovoltaic power could also be reduced with advances in developing high efficiency concentrator photovoltaics (CPV) systems and improving concentrated solar power (CSP) plants used to produce electricity in highly isolated areas¹⁹. New thermal energy storage systems using pressurised water and low cost materials will enable on-demand generation day and night *via* CSP.

Opportunities for the Chemical Sciences

- Improvements to materials used for photovoltaic cells
- Lower energy, higher yield and lower cost routes to silicon refining
- Improving the reaction yield for silane reduction to amorphous silicon films
- Base-metal solutions to replace the current domination of silver printed metallisation used in almost all of today's first-generation devices
- Development of next generation, non-Si based PV cells
- Alternative materials and environmentally sound recovery processes

2.1.2 Biomass Energy

Biomass can be utilized to generate heat, electricity and fuels but this must be done in a way that is environmentally

sustainable, economically and energetically sound, benign for greenhouse gas emissions, and not competitive with food production.

Biomass is any plant material that can be used as a fuel, such as agricultural and forest residues, other organic wastes and specifically grown crops. Biomass can be burned directly to generate power, or can be processed to create gas or liquids to be used as fuel to produce power, transport fuels and chemicals. It is therefore a versatile and important feedstock for fuel production as well as for the chemical industry²⁰. The conversion of biomass to such products is reliant on advances in the chemical sciences, such as novel catalysts and biocatalysts and improved separation techniques. The potential for increased exploitation of biomass resources is very large²¹.

The relatively low conversion efficiency of sunlight into biomass means that large areas of agricultural land would be required to produce significant quantities of biofuels. In recent years, a rising global population and volatile food prices have seen the demand for agricultural outputs increase. Concurrent development of biofuels could potentially lead to competition for land between food and fuel²², which should be avoided. However, there are significant opportunities associated with developing energy crops. For example, genetic engineering could be used to enable plants to grow on land that is unsuitable for food crops, or in other harsh environments such as oceans. Plants could be engineered to have more efficient photosynthesis and increased yields. There could also be opportunities to develop methods of producing fuel from new sources such as algae, animal or waste forms²³.

Biofuels are currently more expensive than conventional transport fuels in many regions of the world but developing improved and novel conversion technologies can broaden the range of feedstocks. The drive to increase the use of biomass and of renewable energy sources and materials, has led to the bio-refinery concept, which would use the whole of the biomass feedstock to produce a number of chemicals, in addition to biofuels. This concept could po-

tentially use a range of biomass substrates, (both primary crop and waste) to produce fuel and high value chemicals as feedstocks for commodity products from convenience plastics to life-saving pharmaceuticals.

Opportunities for the Chemical Sciences

- New tools to measure impacts of biofuels over the entire life cycle (Life Cycle Analysis, LCA)
- Improvement of bio-refinery processes
- New strategies for hydrolysing diversified biomass and lignocellulose
- Extraction of high value chemicals before energy exploitation
- New thermochemical processes with better catalysts, microbes and enzymes
- Enhanced flexibility of feedstock and output (electricity, heat, chemicals, fuel or a combination)
- Methods of producing fuel from new sources such as algae or animal and other wastes
- Design of processes for using waste products as feedstock for packaging material, for example producing novel biodegradable plastic materials made from epoxides and CO₂

2.1.3 Solar Fuels

Fuels, primarily of fossil origin, constitute about 75% of end-use energy consumption in affluent countries. It is of capital importance to establish new processes for the direct conversion of solar radiation into stable chemicals with high energy content (e.g. hydrogen and methanol), starting from cheap and abundant raw materials, particularly H₂O and CO₂²⁴.

Until now, our food and energy needs have ultimately been delivered by natural photosynthesis. One of the grand challenges of 21st century chemistry is to produce “solar” fuels by means of artificial man-made materials, systems and processes. This so-called artificial photosynthesis is aimed at producing energy rich compounds that can be stored and

transported and, after usage, are converted into the starting feedstock, establishing a potentially sustainable chemical cycle²⁵.

The key concept of artificial photosynthesis is not to reproduce natural systems, which are amazingly complex and somewhat inefficient but, rather, to learn from them and reproduce the same principles in smaller, simpler and more efficient man-made arrays. The fuels produced *via* artificial photosynthesis can be stored indefinitely (unlike electricity, that is used immediately after production) and recombined when needed with atmospheric oxygen, so as to get back the stored chemical energy. In principle, a variety of fuels may be produced by artificial photosynthesis. Carbon-rich products formed by reduction of CO₂ would be most attractive, but the multielectron catalytic chemistry involved in CO₂ reduction makes this avenue very challenging.

H₂ production from protons is a comparatively simpler two-electron process. However, this does not take into account the source of electrons. The sophisticated processes that have evolved in natural photosynthesis use H₂O as an electron source. This is difficult to reproduce using artificial catalysts²⁶.

Following the biological blueprint, an artificial photosynthetic fuel production system requires a few basic components

- a light harvesting antenna centre acting as interface toward the energy source;
- a reaction centre connected to the antenna that generates electrochemical potential upon light excitation;
- a catalyst for oxidation of water or other electron sources;
- a catalyst for reduction of precursors to hydrogen or carbon-rich fuels;
- a membrane that keeps physically separated the reducing and oxidizing processes, which is of utmost importance especially when the final products are gases like H₂ and O₂.

While encouraging progress has been made on each aspect of this complex and multidisciplinary problem, researchers

have not yet developed integrated systems. Indeed, the engineering of these diverse components in a single operating device is one of the greatest challenges in contemporary chemistry and probably in science as a whole. The production of hydrogen through light-induced water splitting would provide a versatile molecule that can be used both as fuel in internal combustion engines or fuel cell and as chemical to reduce oxidised species and produce hydrocarbons. Most importantly, it can provide solar energy storage for the dark hours, thus perfectly complementing photovoltaic systems.

Opportunities for the Chemical Sciences

- New fatigue resistant antenna systems
- New reaction centres with long-lived and highly energetic charge separated states
- Cheaper H₂ evolving catalysts
- Better (and cheaper) O₂ evolving catalysts
- Advanced photoelectrochemical cells
- Integration with photovoltaic systems, hydrogen storage systems, and fuel cells

2.2 Wind and Ocean Energies

Europe possesses vast resources of wind²⁷ and ocean energies²⁸. They must play a leading role in electricity production by mid-century due to carbon mitigation constraints and depletion of conventional resources used to feed thermal power technologies (fossil fuels and uranium).

Wind is the world's fastest growing electric technology. In 2009, wind power accounted for 39% of all new electric capacity installed in Europe²⁹. Potentials for wave, tidal and salinity-gradient energies, also called ocean energies, are smaller than wind or solar, but can be very appealing in several geographic locations such as the windy coastlines of Northern Europe. One of the biggest issues of ocean energy converters is robustness³⁰. At present, about 95% of global installations are onshore, but offshore is the next frontier and this perspective requires technological breakthroughs. Materials science will play an important role in developing coat-

ings, lubricants and lightweight durable composite materials that are necessary for constructing turbine blades and towers that can withstand the stresses – especially those that offshore installations are subjected to (corrosion, wind speeds etc). There is scope to develop embedded sensors/sensing materials which can monitor stability and damage, thus allowing instant safeguarding. The continued development of advanced long lasting protective coatings is required to reduce maintenance costs and prolong the operating life of wind energy devices.

Opportunities for the Chemical Sciences

- Lightweight durable composite materials and lubricants for wind turbines
- Long lasting protective coatings, required to reduce maintenance costs and prolong operating life of wave, wind and tidal energy devices
- Embedded sensors/sensing materials, which allow instant safeguarding of wind and ocean energy converters
- Reduce the cost or improve the efficiency of membranes to significantly improve the economics of salinity-gradient energy and electro dialysis technologies.

2.3 Energy Conversion and Storage

The use of intermittent electricity sources, such as wind and solar energy, requires high efficiency energy storage devices on the small (e.g., batteries, capacitors) and large (e.g., pumped hydro, compressed air storage) scale³¹. Substantial breakthroughs are needed in small-scale energy storage, and the chemical sciences can greatly contribute, in particular towards new devices for mobile and stationary applications, transportation, household & services, and load levelling equipments for grid stability³². Fuel cells perform the direct conversion of the combustion energy of fuels into electric energy. Their upscaling from the hundreds of kWh to the hundreds of MWh is the key for powering (electricity and heat) entire districts while reducing gas emissions.

2.3.1 Energy storage: Batteries and Supercapacitors

Excess electric energy produced by renewable sources can be easily stored in secondary batteries³³. While the wide sector of low energy tools is well covered by both non-rechargeable (e.g. hearing devices) and rechargeable (e.g. mobile phones) batteries, the availability of high efficiency rechargeable cells of medium to high energy/power is still inadequate.

The major challenge is to improve the performance of energy conversion and storage technologies (fuel cells, batteries, electrolysis and supercapacitors), by increasing the accumulated energy/power by unit mass (and/or by unit volume) and so improving capacity, lifetime, cyclability and shelf-life. Related to this is the challenge of developing energy storage devices that balance intermittent supply with variable consumer demand in applications such as household appliances and transportation³⁴.

New materials have to be developed for electrodes (cathode and anode), electrolytes (e.g. solid polymer electrolytes, ionic liquids) and structural materials to allow for demanding working conditions, as in the case of non-aqueous systems (e.g. Li batteries, supercapacitors). Developments must be coupled with advances in the fundamental science of electrochemistry and electrocatalysis, surface chemistry, and the improved modelling of thermodynamics and kinetics. One novel application in this area are redox flow batteries. A flow battery is a form of rechargeable battery in which the electrolytes flow through the electrochemical cell. Additional electrolyte is stored externally, generally in tanks, and is usually pumped through the cells of the reactor. Flow batteries can be rapidly 'recharged' by replacing the electrolyte liquid and hold great potential for large-scale applications. New materials are required to develop improved flow batteries with higher energy densities.

Opportunities for the Chemical Sciences

- New materials to achieve enhanced specific power/ power and energy/energy densities
- Longer calendar and cycle lives, recyclability and durability
- Enhanced safety of devices – i.e. problems associated with overheating
- Decrease of the cycle time of batteries – i.e. charging time to be reduced
- New materials for electrodes, electrolytes and device structures
- Replacement of strategic and expensive materials to ensure security of supply
- Lower production and material costs, including use of self-assembly methods
- Development of material recycling strategies
- Advancing the fundamental science and understanding of surface chemistry
- Modelling of thermodynamics and kinetics

2.3.2 Energy conversion: Fuel Cells

Fuel cells (FC) are usually classified according to the kind of electrolyte, that, in turn, determines the working temperature, to satisfy the requirements of conductivity, phase composition and chemical, thermal and mechanical stability. The temperature then determines the requirements of the electrocatalysts and the structural materials and influences also the choice of fuel. Current systems include high-temperature devices which operate between 600 and 800°C. The high temperature allows the use of fuels like natural gas, gasoline and coal and the use of non-precious metal electrocatalysts³⁵.

The main drawback is the stability of the structural materials and the actual goal is to reduce working temperatures below 600°C. Technologies that work at lower temperatures include proton exchange membranes (PEM)³⁶. These run at 80-90 °C, but require high purity hydrogen as fuel. Methanol, ethanol and formic acid are currently considered as alternative fuels, though problems with catalyst poisoning

and fuel crossover must be addressed. A further challenge in direct alcohol FC is the potential formation of more toxic intermediates. Further advances are needed to develop FC which will not require scarce-metal catalysts and materials that do not actively contribute to the production of undesirable side-products, such as hydrogen peroxide.

Opportunities for the Chemical Sciences

- Better oxygen reduction electrocatalysts
- Pt-free electrocatalysts for both hydrogen anodes and oxygen cathodes
- Reduced content of precious components of cathodes and anodes
- Better performances of membrane-electrode assemblies (MEA) and/or gas-diffusion layers
- Reduced anode sensitivity to CO-poisoning
- Higher conversion efficiency
- Better cell performance – i.e. increase working potentials and currents
- Improved safety of devices – i.e. problems associated with supply of fuel and air in cell stack
- Replacement of strategic and expensive materials to ensure security of supply
- Reduce production and material costs, also using self assembly methods
- Development of material recycling strategies
- Advancements in the fundamental science and understanding of surface chemistry
- Improved modelling of thermodynamics and kinetics

2.4 Hydrogen

Hydrogen will be a key energy vector of the future; however, its sustainable generation, transportation, and efficient storage have not yet been accomplished. New materials and techniques to harness hydrogen are needed in the move towards a hydrogen economy³⁷.

Hydrogen coupled with fuel cell technology offers an alternative to our current reliance on fossil fuels for transport,

electricity generation as well as for batteries in mobile applications. Despite the evident advantages, significant technical challenges still exist in developing clean, sustainable, and cost-competitive hydrogen production processes.

Hydrogen is usually obtained from fossil sources (such as methane in natural gas). The steam reforming of fossil fuels is used to produce 95% of all hydrogen used today. However, these sources are unsustainable and more energy is currently required to produce hydrogen than would be obtained from burning it. New methods of producing hydrogen using a renewable energy source would enable hydrogen based technologies to develop into more efficient and cost-effective forms of chemical energy storage. The long-term goal is hydrogen produced through renewable energy sources. The preferred renewable options include electrolysis, thermochemical water splitting, biochemical hydrogen generation and photocatalytic hydrogen extraction from water and renewable organics as well as steam reforming of renewable fuels. Significant research is required before any of these methods will become competitive with conventional processes.

Producing hydrogen from water by electrolysis using renewably generated electricity is highly attractive as the process is clean, relatively maintenance-free and is scalable. Advances are needed in the efficiency of the equipment used to perform these processes. Photocatalytic water electrolysis uses energy from sunlight to split water into hydrogen and oxygen.

Thermochemical water-splitting converts water into hydrogen and oxygen by a series of thermally driven reactions³⁸. Developing new reactors and new heat exchange materials will be necessary to achieve this. An improved understanding of fundamental high temperature kinetics and thermodynamics will be essential.

Biochemical hydrogen generation is based on the concept that certain photosynthetic microorganisms produce hydrogen as part of their natural metabolic activities using light energy³⁹. Strategies for large-scale operation and en-

gineering of the process need to be developed for efficient application. Genetically modified bacteria boosting those metabolic pathways producing biohydrogen should also be investigated.

Steam reforming of renewable fuels uses a variety of bio-derived substrates for generating hydrogen⁴⁰. A new generation of low-cost and durable, multi-reforming catalysts need to be formulated for applications such as the reforming of sugars and lignocellulosic derivatives.

Hydrogen storage is a significant challenge, specifically for the development and viability of hydrogen-powered vehicles. Hydrogen is the lightest element and occupies a larger volume in comparison to other fuels. It therefore needs to be liquefied, compressed or stored in system that ensures a vehicle has enough on board to travel a reasonable distance. Technology breakthroughs required for storing hydrogen in a safe and concentrated manner ask for alternative high-density storage options including the development of advanced materials, such as carbon nanotubes, metal hydride complexes, or metal-organic frameworks (MOFs). Storage of hydrogen in liquid fuels, like formic acid, is a credible alternative to solid containers. However utilising this methodology requires the production of catalysts that facilitate the inter-conversion of carbon dioxide and hydrogen to formic acid⁴¹.

If hydrogen production and storage can be fully integrated with the development of advanced fuel cell systems for the conversion to electricity, it can provide fuel for vehicles, energy for heating and cooling, and power.

Opportunities for the Chemical Sciences

- More efficient water splitting via electrolysis, using preferably renewable electricity
- Improvements in electrode surfaces for electrolyzers
- Higher efficiency of H₂ production from the thermochemical splitting of water
- Large-scale H₂ production processes using renewable or carbon-neutral energy sources
- New generation of durable catalysts for steam reforming of renewable fuels
- Microbial fuel cells to generate hydrogen from waste
- New efficient bio-inspired catalysts for fuel cells
- New highly porous materials for the safe and efficient storage of hydrogen
- Improvement in the efficiency of H₂ extraction from liquid fuels (formic acid, methanol, etc)
- Better materials for fuel cells and for on-board hydrogen generation and storage

2.5 Energy Efficiency

Currently, in industrialised countries, less than 50% of the primary energy input is converted into useful services to end users, the rest being lost mainly as heat due to system inefficiencies⁴². Efforts are needed to improve the efficiency of energy production, distribution and usage. Energy efficiency is the key requisite to meeting our future energy needs from sustainable sources.

The European Commission set a target of saving 20% of all energy used in the EU by 2020. Such an energy efficiency objective is a crucial part of the energy puzzle since it would save the EU around €100 billion and cut emissions by almost 800 million tonnes per year. Practically, it is one of the key ways in which CO₂ emission targets can be realised. Chemistry is the key science for accomplishing energy efficiency in many areas: building insulation, lightweight materials for transportation, superconductors, fuel additives, lighting materials, cool roof coatings, energy-efficient tires,

windows and appliances. Furthermore chemical research can lead to reduced demand for materials in manufacturing at all levels, and enhance recycling. Stabilisation of energy demand will be obtained only by breakthroughs in energy efficiency. It has to be emphasised, however, that this desirable result will be obtained only if, in parallel, efforts are made in consumer education.

Opportunities for the Chemical Sciences

- Cheaper, better insulating materials
- Improved fuel economy: high performance catalysts and next generation fuels
- Improved recycling technologies
- Use of nanotechnology to increase the strength to weight ratio of structural materials
- More efficient lighting, e.g. Organic Light Emitting Diodes (OLED) and Light Emitting Electrochemical Cells (LEC)
- Superconducting materials which operate at higher temperatures
- Novel efficient coatings, lubricants and composites
- Improvement of energy intensive processes through process optimisation
- New process routes, new catalysts, improved separation technologies

2.6 Fossil Fuels

Current fossil fuel usage is unsustainable and associated with greenhouse gas production⁴³. However, fossil fuels will play a significant part in meeting the world's energy needs for the foreseeable future. Hence more efficient use of fossil fuels is required alongside technologies that ensure minimal air, land and water pollution and carbon footprint.

Crude oil is currently being produced from increasingly hostile environments and deeper reservoirs, due to progressive depletion of "easy oil" fields⁴⁴. Enhanced oil recovery pro-

cesses and the exploitation of unconventional tar sands oil reserves require a detailed understanding of the complex physical and chemical interactions between oil, water and porous rock systems^{45,46}. One of the main challenges facing the oil refinery industry is the cost effective production of ultra-low sulfur fuels, as required by increasingly tough environmental legislations. Input from the chemical sciences is needed to overcome this issue by developing improved catalysts as well as separation and conversion processes.

The amount of primary air pollutants upon burning of natural gas is substantially smaller, compared to coal and oil, therefore potential benefits for improving air quality are significant. Technology breakthroughs in the gas industry will be required in developing cost effective gas purification technologies and developing advanced catalysts to improve combustion for a range of gas types⁴⁷. The European potential in this area is vast, but perspectives for development are uncertain due to environmental reasons^{48,49}.

Coal will play an important role in European electricity generation, provided that innovative technologies to reduce CO₂ emissions can be found, along with a better environmental performance complying with tightening environmental restrictions. Short term technical needs in coal-fired power generation relate mainly to the control of air pollutants.

Research should be focused specifically on improved materials for plant design, including corrosion resistant materials for use in flue gas desulfurisation systems, catalysts for emissions control and a better understanding of specific processes such as corrosion and ash deposition⁵⁰. Improved process monitoring, equipment design and performance prediction tools to improve power plant efficiency are also required.

Medium term challenges require development of environmentally sustainable conversion of feedstocks, such as coal and gas, into liquid and gaseous fuels. Moreover, advanced solutions to dispose of coal combustion residues (CCR) from power plants must be found, because they represent about 4% by weight of the total generation of waste and residues from all economic activities in EU.

If we continue to use fossil fuels, it is vital that some means of capturing and safely storing CO₂ on a large scale is developed so that targets for CO₂ reduction can be met. Carbon capture and storage (CCS) is an emerging combination of technologies, which could reduce emissions from fossil fuel power stations by as much as 90%. Capturing and storing CO₂ safely will rely on the skills of a range of disciplines, including the chemical sciences⁵¹. The number of technical challenges to achieve CCS on the scale required is formidable. Current technologies, such as amine scrubbing, are costly and inefficient. Further research is required into alternatives such as the use of polymers, activated carbons or fly ashes for the removal of CO₂ from dilute flue gases⁵².

Research into the storage options for CO₂ is needed together with an improved understanding of the behaviour, interactions and physical properties of CO₂ under storage conditions. It is essential that CCS technologies will be integrated with new and existing combustion and gasification plants to ensure uptake by industry.

Research into the options for CO₂ as a feedstock is also needed, for example converting CO₂ into useful chemicals⁵³.

Opportunities for the Chemical Sciences

- Better and cheaper catalysts for emissions control, particularly SO₂ and NO_x
- Corrosion resistant materials for use in flue gas desulfurisation (FGD) systems
- Improved catalysts and tailored separation/conversion for production of ultra-low sulfur fuels
- Improved understanding of corrosion and ash deposition
- Better natural gas processing and purification
- Understanding of the physical chemistry of oil, water and porous rock systems for enhanced oil recovery technologies
- Novel chemical additives to make shale gas extraction more sustainable
- Carbon capture and storage (CCS) technologies: alternatives to amine absorption, including polymers and activated carbons
- Understanding the behaviour, interactions and physical properties of CO₂ under storage conditions to grant long term sealing of wells
- Using CO₂ as a feedstock, converting it to useful chemicals
- Improved materials for supercritical and advanced gasification plants
- Environmentally safe disposal of Coal Combustion Residues (CCR)

2.7 Nuclear Energy

The problems of storage and disposal of new and legacy radioactive materials are poised to increase in the near future. Radioactive waste needs to be reduced and safely contained, while opportunities for re-use should be thoroughly assessed. These activities have to be carried out taking into account the risks of nuclear proliferation, thus requiring a great deal of political and societal action⁵⁴.

The expansion of nuclear power in Europe remains uncertain, mainly due to economic constraints and low social ac-

ceptability. The crisis at the Fukushima Daiichi Nuclear power plant in March 2011 pushed social and political concerns over nuclear power further into the public arena. Nonetheless, after almost 60 years of civilian use of nuclear energy about 300,000 tonnes of accumulated spent fuels are currently in storage and 10,000-12,000 tonnes are added each year. Accordingly, there is no doubt that nuclear clean-up will constitute a relevant field of industrial and research activity in the decades to come worldwide⁵⁵.

The storage and disposal of new and legacy radioactive waste pose a number of challenges to be coupled safe with plant decommissioning, contaminated land management, and assessment of nuclear proliferation risks. Processes for separating and reusing nuclear waste rely on reprocessing chemistry, such as recycling spent fuel into its constituent (uranium, plutonium and fission) products or using separation chemistry in nuclear waste streams, e.g. using zeolites, membranes, supercritical fluids and molten salts. Improving the understanding of solids formation and precipitation behaviour will also be relevant⁵⁶.

Using wastefrom chemistry, which includes the fundamental science of materials used in immobilising nuclear waste, could help solve a number of waste management issues. Methods of waste containment for storage in geological sites will also require further research, as each site will have differences in the geological substrata.

Opportunities for the Chemical Sciences

- Deepening the study of the nuclear and chemical properties of the actinide and lanthanide elements
- Advance the understanding of the physico-chemical effects of radiation on material fatigue, stresses and corrosion in processing and storing facilities (e.g. in cement, metals, etc.)
- Develop new and improved methods and means of storing waste in the intermediate and long term, including new materials with high radiation tolerance
- Improved processes for nuclear waste separation and reuse
- Enhance research efforts into environmental chemistry issues, i.e. hydro-geochemistry, radio-biogeochemistry and biosphere chemistry
- Develop methods for effective and safe post-operational clean-out and site remediation of nuclear facilities

3.0 RESOURCE EFFICIENCY

Human activity is depleting resources across the globe, generating environmental concerns and potential impacts on resource security. Action by industries, governments and consumers together is needed to maximise resource efficiency.

Resource efficiency relates to the use of elements within products and their successful management through the product life cycle. The periodic table contains some 80 stable, naturally occurring elements. Some of these, such as phosphorus and nitrogen are the building blocks of life, others, such as platinum and indium are in high demand due to their current rate of usage in consumable goods. It is therefore important to ensure that these elements are used wisely and are reclaimed where possible. Management of other natural reserves such as oil involve managing differing demands over a single source. Oil is both a fuel as well as a crucial feedstock for many high-value products (materials, lubricants). Chemical scientists, engineers, product designers and manufacturers can help to make management more efficient.

The use of metals and minerals within our industry is poorly managed in the majority of cases and this is resulting in metals being dispersed in the environment in such small quantities that they cannot be reclaimed. Many elements are left inside disregarded products in landfill, due to a lack of recovery and recycling.

There are imbalances between supply and demand for many natural resources. Currently, there are limits to what we can extract economically. Despite this, the demand for products is ever increasing, there has been a 45% increase in global extraction of natural resources in over the last 25 years and this is predicted to grow further in years to come⁵⁷.

Metals and other minerals are essential to almost every aspect of modern life. Phosphorus (P), in the form of phosphates, is one of the main constituents of fertiliser, and is necessary for life through incorporation into DNA and bones. Without supplies of phosphorus it would be impossible to live – it is an essential element. Metals such as lithium (Li), platinum (Pt), palladium (Pd), indium (In) and rare earth metals (a collection of 14 chemical elements) are used in a variety of applications such as batteries, catalysts to facilitate

complex chemical transformations (including the removal of pollutants from the air), components for computers, solar cells and mobile phones, and in magnets for motors such as those in wind turbines. The use of rare chemical elements in catalysts can enable industrial processes to operate efficiently at lower temperatures and with less energy.

Concern over access to mined resources is partly based on published reserves – which, in turn, are based on best estimates of the accessible deposits – together with the rate at which they are being consumed and the threat of reduced supply. The EU has identified 14 raw materials, that face potential shortages. Such shortages could have a vast economic impact⁵⁸.

Unlike fossil fuels, which are converted to CO₂ and H₂O when burned, elemental resources are not destroyed and can often be recycled and reused. However, efficient recycling depends on sound product design to enable elemental resources to be recovered at the end of a product lifecycle.

Chemical scientists can help to source, reduce, recycle and replace the use of scarce natural resources. Chemists have the potential to develop new methods to extract resources efficiently and economically from known, yet inaccessible, reserves, such as lithium from seawater. The use of nanotechnology could help to reduce our dependency on many elements, such as platinum in catalytic converters. Recycling will help to reclaim and reuse resources where possible such as phosphorus from soil, rivers and oceans. Replacing the elements will also be very effective, for example in alternative energy storage technologies that can be designed to avoid being reliant on supplies of lithium. Chemists will design new catalytic processes that do not require platinum group metals, together with new materials for appliances and solar cells that are free from indium. Alternatives to rare earth metals in a range of applications should also be considered.

A concerted global strategy to optimise the supply of scarce natural resources is urgently required in the interim, until technological alternatives can be delivered.

3.1 Reduce Quantities

Supplies of scarce natural resources are dwindling at an alarming rate and many vital, rare minerals are often obtained from politically turbulent countries. Shortages will affect the global population within a generation. Chemists can help to reduce the dependence of technology on certain resources.

Reduction in the quantities of metals incorporated into products would allow the EU to extend the lifetimes of the imported metals supplies. One example of such an approach is the smaller quantity of platinum deployed in catalytic converters developed by automotive industry, which required the input of chemists, engineers and designers⁵⁹.

Opportunities for the Chemical Sciences

- Chemical scientists will undertake the rational design and realisation of nanoscale multimetallic systems, such as alloys, with favourable properties
- Optimization of catalysts to minimize the amount of rare elements needed

3.2 Recycle

Our high level of industrial and domestic waste could be resolved with increased downstream processing and re-use. To preserve resources, product design should have greater consideration for the entire life-cycle of materials used.

The EU imports many scarce elements already incorporated within technological products such as cars, TVs, mobile phones etc. This means that once these items are discarded these scarce resources are collated on landfill sites or in some instances collated and exported abroad.

The EU would benefit from the strategic development of new recycling and extraction methods, which will require financial support of the underpinning research. Better management of waste products could produce continued supplies of metals in the longer term. Japan has suggested that 60% of their indium requirements could come from 'urban mines'. Urban Mining is the recovery of metals and other useful materials from consumer products like mobile phones, batteries, or computers and can provide an opportunity to improve resource efficiency in Europe⁶⁰. Landfill sites contain many redundant electrical equipment components and these items are important as potential sources of elements such as gold, neodymium, lithium etc. However, there are issues as to whether current sources of waste metals within the EU hold enough reclaimable metal to meet technological demand and whether recovery is cost effective⁶¹.

Currently there are no cost-effective ways to extract these metals. For example, extracting indium from even one brand of television requires several different processes since each set originates from different suppliers and is designed slightly differently. Consistent design features, with recovery processes in mind, will be a key improvement to enable sustainable and efficient metal recovery in the future.

Recycling affords the opportunity to maximise the use of available supplies within the EU. Efficient recycling depends critically on product design, and this needs to encompass design for re-use, re-manufacture as well as recycling. These demand that designers, chemists and engineers work together to ensure that all the components can be economically recovered at the end of the product life cycle. A key step to ensure recycling is adopted more widely across the manufacturing sector is that products developed from recycled components meet the same quality standards as those made from originally sourced materials. Specified design would allow for easy recycling, while appropriate standards and sufficient labelling would help to specify the quality of recycled materials. A 2010 Johnson Matthey review of global statistics for platinum supply and demand suggests that future supplies of platinum (and other metals such as ruthenium, rhodium, iridium and palladium) recovered from automotive catalysts,

jewellery and electronics are likely to increase. However, to ensure that this is the case, improved recovery and recycling processes must be developed. Currently, it can be challenging to recover metals with low reactivity (eg. gold)⁶³ or in such a way that their unique properties remain undiminished (eg. the magnetic properties of neodymium).

Technological breakthroughs to guarantee supplies of phosphorus for the survival of future generations are needed. There is currently no practical method of ensuring a supply of phosphorus without a steady supply of phosphate minerals. Phosphorus is present in soil, rivers and oceans, often originating from fertiliser run-offs. There is potential to extract it from these sources; however, there are physical and energetic barriers limiting the development of such processes. Fundamental research is urgently required to develop sustainable solutions.

Opportunities for the Chemical Sciences

- Working with designers and engineers to develop products that are easily recycled and contain features that enable scarce resources to be reclaimed at the end of use
- Research to create more cost efficient processes to recycle products at the end of their life cycle
- Encourage more companies to work with chemical scientists and designers to review the life cycle of their products and to take back products at the end of their purpose
- Chemical scientists will conceive and develop new materials that are able to selectively bind to and remove phosphorus-containing species such as phosphate from water and soil using host-guest and metal coordination chemistry
- Chemists, engineers, and biotechnologists will develop and optimise membrane technologies to selectively concentrate phosphate from water
- Develop methods for effective and safe post-operational clean-out and site remediation of nuclear facilities

3.3 Resource Substitution

In modern technologies, many of the elements are used in small amounts and as a result become dispersed into the environment. To sustain the quality of life of the modern developed world and its extension to the entire global population, new technologies either may have to use elements more efficiently or to use substitutes in place of those used in contemporary technologies.

For example, indium gallium arsenide is crucial for a new generation of more efficient solar cells but sourcing alternatives for indium is a high priority. Fundamental materials research could deliver viable alternatives to the use of indium in the next five to ten years^{64,65,66,67,68}.

Lithium (Li) is the most commonly used metal in batteries, and will continue to form part of future energy storage technologies in the short- to medium-term. Lithium also has important pharmaceutical applications. New technologies to reduce and replace the use of lithium are required. Lithium batteries could be replaced by other types of batteries, based on more abundant materials such as disodium sulfide.

There is a variety of chemical research addressing the substitution of metals in various technologies. The use of graphene (a sheet form of carbon that is one-atom thick) may potentially be used to replace platinum in solar technologies.

Even though chlorine remains an iconic molecule for industrial chemical production, its production by the electrolysis of sodium chloride is very energy intensive. The environmental and health constraints and the growing need for efficient energy usage will compel researchers to develop a new chemical strategy and to make ready a chemistry *beyond* chlorine.

Opportunities for the Chemical Sciences

- Chemical scientists will research and develop cheaper, more stable supplies of materials for solar cells, organic light-emitting diodes, and for better and cheaper display technologies
- Chemical scientists will design and perfect new light- and heat-stable transparent, electrically conducting materials with favourable properties for multiple applications
- Chemical scientists will investigate the potential replacement of lithium batteries with other types of batteries, based on sodium sulfide, magnesium, nitrogen-doped graphene or other materials
- Chemical scientists will enhance the efficiency and lifetimes of batteries for longer use
- Chemists will investigate technologies and improve on processes to extract lithium from oceans using main group metal co-ordination chemistry.
- Chemists will explore and develop alternatives to platinum in fuel cells which are based on more abundant elements, based on nanomaterials including nitrogen-doped graphene.
- Chemical scientists will enhance our capabilities in the area of rare earth metal magnetic properties, to improve magnet performance and to reduce the rare earth content
- Chemical scientists will enhance our capabilities in the area of rare earth coordination chemistry, to facilitate the design of improved capture methods.

4.0 HEALTH

On the whole, people are healthier, wealthier and live longer today than 30 years ago⁶⁹. If children were still dying at 1978 rates, there would have been 16.2 million deaths globally in 2006. There were only 9.5 million such deaths. This difference of 6.7 million is equivalent to 18,329 children's lives being saved every day⁷⁰. However, the substantial progress in health over recent decades has been deeply unequal.

Improved levels of health in many parts of the world are coupled with the existence of considerable and growing health inequalities in others. The nature of health problems is also changing; ageing and the effects of ill-managed urbanisation and globalisation accelerate worldwide transmission of communicable diseases, and increase the burden of chronic and non-communicable disorders. The challenge is to improve and maintain accessible human health in a changing world. The healthcare sector will benefit greatly from new products and technologies. The chemical sciences have a central role to play in the fundamental research that will lead to new technologies. This section covers the challenges that exist relating to ageing, diagnostics, hygiene and infection, materials and prosthetics, drugs and therapies, and personalised medicine.

4.1 Ageing

In 2007, almost 500 million people worldwide were 65 and over. Increased longevity and falling fertility rates mean that by 2025 that total is projected to increase to 835 million. Moreover, the largest number of older people will live in the transitional and developing regions. 62 % of the world's older people live in less developed countries. By 2050 this will increase to 78 %⁷¹. In an era of global population it will become essential to enable individuals to stay in good health longer, with less disability and therefore less dependence on others.

The main challenge is to enhance the life-long contribution of ageing individuals to society, while improving their quality of life. The chemical sciences have a role to play in preventing, detecting and treating age related illnesses. Prevention will require an improved understanding of the impact of nutrition and lifestyle on future health and quality of life. This will

be coupled with a shift in focus to developing the next generation of preventative intervention treatments, for example progressing beyond statins and the flu jab. Advances will need to be made in treating and controlling chronic diseases such as cancer, Alzheimer's, diabetes, dementia, obesity, arthritis, cardiovascular, Parkinson's and osteoporosis. This must be linked with improved understanding of the role of genetic predisposition in the development of these diseases and improving detection and treatment technologies.

Technological breakthroughs will be required to identify relevant biomarkers and sensitive analytical tools for early diagnosis of disease, which will allow the development of practical, non-invasive bio-monitoring tools, such as from breath, urine, saliva and sweat, which will be particularly valuable to frailer patients. There will also be a need to develop new materials for cost effective, high performance prosthetics, for example artificial organs, tissues and eye lenses. To meet the demand for independent living from those suffering from long-term adverse health conditions, significant advances will also be needed in technologies and materials for assisted living. Developments will be required in areas such as drug delivery, packaging, incontinence, physical balance, recreation and in designing living space and communities.

Opportunities for the Chemical Sciences

- Prevent, treat and control chronic diseases – e.g. cancer, Alzheimer's, diabetes, dementia, obesity, arthritis, cardiovascular, Parkinson's, osteoporosis
- Focus on preventative intervention – e.g. statins, flu jab
- Improve the understanding of the impact of nutrition and lifestyle – e.g. nutraceuticals – on future health and quality of life
- Develop practical non-invasive bio-monitoring tools – e.g. breath, urine, saliva, sweat
- Identify relevant biomarkers and sensitive analytical tools for early diagnosis
- Assisted living: design devices for drug delivery, packaging, incontinence, compliance, physical balance and recreation
- Develop new materials for cost effective, high performance prosthetics – e.g. artificial organs, tissues, eye lenses etc

4.2 Diagnostics

Improved diagnosis is required in the developed and developing world. Quick and accurate diagnosis benefits individual patients by improving their treatment, in addition to ensuring the efficient use of resources and limiting the spread of infectious diseases⁷². Technology breakthroughs in detection include identifying relevant biomarkers and developing sensitive analytical tools for early diagnostics, which require smaller samples and will deliver more complete and accurate data from a single, non-invasive measurement. Further advances could ultimately lead to information-rich, point-of-care diagnostics resulting in a reduction in the need for diagnosis and subsequent treatment in hospital, with the associated costs.

Improved biomonitoring techniques could also allow the identification of disease risks. This could result in personalised treatment and medication tailored to the specific needs of the individual. In combination with basing treatment on targeted genotype rather than mass phenotype, an increased focus on chemical genetics could prevail.

The chemical sciences have a role to play in monitoring the effectiveness and safety of therapies and medication. An understanding of the chemistry of disease progression is required to achieve this and research should be done to enable the continuity of drug treatment over the disease life cycle. Point-of-care diagnostics can be used to monitor disease progression and treatment efficacy enabling responsive treatment, such as changes of drug dose, thus reducing hospital hours. It is possible that technological breakthroughs in diagnostic techniques and therapeutic devices could lead to combined devices that detect infection and respond to attack.

Opportunities for the Chemical Sciences

- Develop sensitive detection techniques for non-invasive diagnosis
- Develop cost effective information-rich point-of-care diagnostic devices
- Develop cost effective diagnostics for regular health checks and predicting susceptibility
- Identify relevant biomarkers and sensitive analytical tools for early diagnostics
- Understand the chemistry of disease onset and progression
- Research to enable the continuity of drug treatment over disease life cycles
- Focus treatment on targeted genotype rather than mass phenotype
- Increase the focus on chemical genetics
- Produce combined diagnostic and therapeutic devices – smart, responsive devices that detect infection and respond to attack

4.3 Hygiene and Infection

Infectious diseases account for over a fifth of human deaths and a quarter of ill-health worldwide⁷³. In addition to the appearance of new infectious diseases, such as SARS (severe acute respiratory syndrome), and the worsening of current dis-

eases through climate change, we also face the challenge of antibiotic resistance. The main challenge is to prevent and minimise acquired infections by improving techniques, technologies and practices of the anti-infective portfolio. To do this there will need to be an improved understanding of viruses and bacteria at a molecular level, and of the transition of disease across species. Delivery methodologies also require improvement; this will encompass improved materials for drug capsules and coatings. This must be coupled with breakthroughs in detection strategies, for example:

- developing fast, cheap and effective sensors for bacterial infection;
- developing new generation materials for clinical environments, such as coatings for drugs;
- developing advanced materials that detect and reduce airborne pathogens, for example materials for air filters and sensors.

The increased incidence of new genetic and resistant strains requires an improved ability to control and deal with them quickly. There is a need for the rapid development of novel synthetic vaccines and the accelerated discovery of anti-infective and antibacterial agents.

Opportunities for the Chemical Sciences

- Improve understanding of viruses and bacteria at a molecular level
- Accelerate discovery of anti-infective and anti-bacterial agents
- Develop fast, cheap and effective sensors for bacterial infection
- Develop new generation materials for clinical environments – e.g. paint, coatings
- Detect and reduce airborne pathogens – e.g. material for air filters and sensors
- Improve ability to control and deal quickly with new genetic/resistant strains
- Produce novel synthetic vaccines more rapidly
- Improve understanding of the translation of disease across species

4.4 Materials and Prosthetics

It is estimated that demand for donor organs exceeds current availability by 50 %⁷⁴. There is a need to develop new materials for cost effective, high functional prosthetics, for example, artificial organs, tissues and eye lenses, in addition to the continued demand for developing advanced materials to use in orthopaedic implants. The challenge is to exploit replacement organs to enhance sustained function fully.

Materials breakthroughs will be required in polymer and bio-compatible materials chemistry for surgical equipment, implants and artificial limbs. Smarter and/or bio-responsive drug delivery devices are required for diabetes, chronic pain relief, cardiovascular disease and asthma, and research into biological macromolecule materials as templates and building blocks for fabricating new (nano)materials and devices. This must be supported by an increased understanding of the chemistry at the interface of synthetic and biological systems. Repairing, replacing or regenerating cells, tissues, or organs will require further research into soluble molecules, gene therapy, stem cell transplantation, tissue engineering and the reprogramming of cell and tissue types. Improvement is required in the ability to modulate neural activity, for example, by modifying neuron conduction, allowing the treatment of brain degeneration in diseases such as Alzheimer's.

Opportunities for the Chemical Sciences

- Research polymer and biocompatible material chemistry for surgical equipment, implants and artificial limbs
- Research biological macromolecule materials as templates and building blocks for fabricating new (nano) materials/devices
- Develop smarter and/or bio-responsive drug delivery devices – e.g. for diabetes, chronic pain relief, cardiovascular, asthma
- Use synthetic biology for targeted tissue regeneration Develop tissue engineering and stem cell research for regenerative medicine
- Modulate neural activity, for example, by modifying neuron conduction, to allow the treatment of brain degeneration in diseases such as Alzheimer's

4.5 Drugs and Therapies

Chronic diseases, including cardiovascular, cancer, chronic respiratory, diabetes, neurodegenerative diseases (e.g. Alzheimer's, Parkinson's, etc) and others (brain disorders and joint problems) caused 35 million deaths globally in 2005⁷⁵. These diseases affect both the developed and developing world.

Chronic diseases cause more than twice the number of deaths per year than infectious diseases, maternal and perinatal conditions and nutritional deficiencies combined. The prediction is that unless the causes of chronic diseases are addressed, deaths will increase by 17 % between 2005 and 2015.

Developing drugs and therapies that can target chronic diseases have the potential to save a huge number of lives worldwide. Major problem seem to include a poor target validation process and at least partial failure by new technologies to give the expected results⁷⁶. Thus, the tendency in drug discovery has to move from a "quantity process" (combinatorial chemistry, high throughput screening) to a "qualitative approach" using rational design, synthesis and evaluation/characterisation of new compounds aimed at a target. The chemical sciences have a vital role in harnessing and enhancing basic sciences to help transform the entire drug discovery, development and healthcare landscape so new molecular entities and therapies can be identified and delivered. To achieve this, a number of breakthroughs are required in:

- identifying new biological targets;
- improving the knowledge of the chemistry of living organisms, including structural biology;
- identifying small molecules to characterize new biological targets;
- exploiting new targets to identify innovative therapies
- designing and synthesising small molecules that attenuate large molecule interactions, for example protein-protein and protein-DNA interactions;
- integrating chemistry with biological entities for improved drug delivery and targeting (next generation biologics);

- developing advanced chemical tools to enhance clinical studies, for example non-invasive monitoring, *in vivo* biomarkers and contrast agents.

Systems biology enables a holistic analysis of individual systems and processes as well as investigations of how different processes interact in complex living systems. The different sub-disciplines of the chemical sciences will all play a role. For example, computational chemistry will contribute to better systems biology approaches and process chemistry modelling. Better understanding at the molecular and cellular level will be supported by physical organic chemistry. The analytical sciences will play a key role in every aspect of the drug discovery and development process.

Assessing the effectiveness and safety of drugs is an essential component of the complex, costly and lengthy drug discovery and development process. There is a need to understand communication within and between cells and the effects of external factors to combat disease progression. Improved targeting to particular diseased cells, through understanding of drug absorption parameters within the body, such as the blood brain barrier, will improve efficacy and safety. Increased understanding of the chemical basis of toxicology and the derivation of new guidelines for toxicology will improve the prediction of potentially harmful effects. In addition to this, developing toxicogenomics will allow drugs to be tested at a cellular and molecular level, and better understanding of the interaction between components of drug cocktails will increase the ability to avoid adverse side effects.

Monitoring the effectiveness of a therapy could improve compliance and the treatment regime, and in turn improve efficacy. These advances must be linked to the development of improved drug delivery systems through smart devices and/or targeted and non-invasive solutions

Opportunities for the Chemical Sciences

- Chemical tools for enhancing clinical studies – e.g. non-invasive monitoring in vivo, biomarkers, contrast agents etc
- Design and synthesise small molecules that interact with innovative biological targets
- Understand the chemical basis of toxicology and hence derive improved guidelines for toxicology
- Integrate chemistry with biological entities for improved drug delivery and targeting (next generation biologics)
- Apply systems biology understanding for identifying new biological targets
- Understand communication within and between cells and the effects of external factors in vivo to combat disease progression
- Improve drug delivery systems through smart devices and/or targeted and non-invasive solutions
- Target particular disease cells through understanding drug absorption parameters within the body – e.g. blood brain barrier
- Avoid adverse side effects through better understanding of the interaction between components of cocktails of drugs
- Develop model systems to improve understanding of extremely complex biological systems and of how interventions work in living systems over time
- Improve knowledge of the chemistry of living organisms including structural biology to ensure drug safety and effectiveness
- Develop toxicogenomics to test drugs at a cellular and molecular level

4.6 Personalised Medicine

Technological advances in the past 10 years have reduced the cost of sequencing the whole human genome by a staggering 1000-fold or more⁷⁷. The speed and cost of the sequencing process brings personalised medicine one step closer. The combination of improving our understanding of

the human genome and disease genes, with the ability to rapidly and cheaply sequence an individual's genome, will allow identification of disease risks and predisposition for an individual⁷⁸.

Genomic technology should allow better prediction of how individuals will respond to a given drug and improve the safety and efficacy of treatments by providing the data required to tailor them to individual needs. To be able to deliver specific, differentiated prevention and treatment on an individual basis, breakthroughs will be required in applying advanced pharmacogenetics to personalised treatment regimes, developing 'lab-on-a-chip' technologies for rapid personal diagnosis and treatment, and developing practical non-invasive bio-monitoring tools and sensitive molecular detectors that provide information on how physical interventions work in living systems over time.

These advances have preventative applications, as well as curative. Nutrient requirements depend on factors including genetics – the availability of rapid methods in genomics, proteomics and metabolomics is allowing the impact of gene expression in individuals, and individuals' genetic sensitivity to food intake, to be studied.

Opportunities for the Chemical Sciences

- Apply advanced pharmacogenetics to personalised treatment regimes
- Identify new patient-tailored biological targets
- Discovery and develop new molecular entities as personalized drugs
- Develop sensitive molecular detectors, which can inform how physical interventions work in living systems over time
- Develop 'lab-on-a-chip' rapid personal diagnosis and treatment. Translate research advances into robust, low cost techniques
- Develop practical non-invasive biomonitoring tools

5.0 FOOD

The world faces a food crisis relating to the sustainability of global food supply and its security. The strain on food supply comes primarily from population growth and rising prosperity, which also bring competing land and energy demands. By 2030 the world's population will have increased to over eight billion⁷⁹. Climate volatility and the declining availability of water for agriculture will greatly increase the challenges facing farmers.

To match energy and food demand with limited natural resources, such as water, without permanently damaging the environment, is the greatest technological challenge humanity faces. Chemistry and engineering are a key part of the solution. Many opportunities exist for the chemical sciences to supply healthy, safe and affordable food for all. The main challenges concern agricultural productivity, water, healthy food, food safety, process efficiency and supply chain waste.

5.1 Agricultural productivity

A rapidly expanding world population, increasing affluence in the developing world, climate volatility and limited land and water availability mean we have no alternative but to significantly and sustainably increase agricultural productivity to provide food, feed, fibre and fuel.

A doubling of global food production will be required by 2050, to meet the Millennium Development goals on hunger⁸⁰. This demand for increased food production is exacerbated by economic growth in the emerging economies. As these countries become more affluent, this will translate directly into increased food consumption, particularly for high value-added food such as meat and dairy products⁸¹. The World Bank estimates that by 2025 one hectare of land will need to feed five people; in 1960 one hectare was required to feed only two people⁸². This needs to be achieved in a world where suitable agricultural land is limited and climate change is predicted to have an adverse impact on food production due to the effects of changing weather patterns on primary agriculture and shifting pests.

Increasing productivity from existing agricultural land represents a significant opportunity because current technologies

can be applied to areas where yields are still below average. Historically, increases have come from higher yields as a consequence of improved varieties, better farming practices and applying new technologies such as agrochemicals and more recently agricultural biotechnology. To meet growing demand for food in the future, existing and new technologies, provided by the chemical sciences, must be applied across the entire food supply chain.

By sharing best practice in agricultural science and technology, farmers can minimise inputs and maximise outputs to increase productivity. Increased precision in the field will have a positive impact on agricultural efficiency. New technologies will allow farmers to pinpoint nutrient deficiencies, target agrochemical applications and improve the quality and yield of crops.

5.1.1 Pest control

Up to 40 % of current agricultural outputs would be lost without effective use of crop protection chemicals⁸³. Agriculture is facing emerging and resistant strains of pests. It is therefore essential that new crop protection strategies, chemical and non-chemical, are developed.

As new farming practices are adopted, such as hydroponics (the growth of plants using nutrient solutions, rather than soils), newly developed agrochemicals should be tailored to more diverse growing conditions. Formulation science will be essential for developing novel mixtures of existing agrochemicals, ensuring a consistent and effective dose is delivered to the insect, fungus or weed at the right time and in the right quantity.

Opportunities for the Chemical Sciences

- Development of new high-potency, targeted agrochemicals with new modes of action that are safe to use, overcome resistant pests and are environmentally benign.
- Computational and predictive tools, developed and in use for drug design, could be applied directly in designing agrochemicals.
- Development of pest control strategies that use pheromones and other messenger chemicals as a starting point.
- Development of crops that are resistant to attack by pests and to environmental stresses, including drought and salinity.

5.1.2 Plant science

Improving the efficiency of nutrient uptake and utilisation in plants is a major challenge in agricultural productivity. By understanding the metabolic pathways by which nutrients are absorbed and used, biotechnologists can work with chemists to develop crops that deliver higher yields. This could be by generating crops with improved efficiency in utilising nitrogen or water.

The use of fertilisers has been pivotal to securing long-term food supplies in the midst of a growing global population. However, in the future chemists will need to develop smarter formulations that ensure efficient delivery of nutrients (nitrogen, phosphorus and potassium) and minimise loss of such key elements to the surrounding environment. These new formulations will need to be produced using processes that are more energy efficient. Refinement of the Haber process (see section 1.1) means it now uses 6 times less energy than it did in 1903.

Opportunities for the Chemical Sciences

- Improving our understanding of the roles of macro- and micronutrients together with carbon, nitrogen, phosphorus and sulphur cycling to help optimise nutrient uptake
- Improving our understanding of the roles plant growth regulators can play in modulating plant water and nitrogen use
- Improving our understanding of plant biochemical signalling to facilitate the development of new crop defence technologies, with positive implications for crop yields.

5.1.3 Soil science

Maintaining good soil structure and fertility are important to ensure high productivity. It is therefore necessary to understand the complex macro- and micro-structural, chemical and microbiological composition of soil and its interactions with plant roots and the environment. Research to improve the understanding of the biochemistry of soil systems and how this connects to related areas such as mechanical properties of soil is crucial.

There is also scope for optimising how fertilisers are used. Fertilisers should be formulated to improve soil nitrogen retention and uptake by plants.

Opportunities for the Chemical Sciences

- Improving our understanding of the chemistry of nitrous oxide emissions from soil and the mobility of chemicals within soil
- Development of methane-fixing technologies through improved understanding of methane oxidation by soil bacteria
- Development of low energy methods to synthesise nitrogen- and phosphorus-containing fertilisers would increase the sustainability of agricultural production by reducing indirect input costs and resource requirements.
- Development of in situ biosensor systems to monitor soil quality and nutrient content.

5.2 Water

Maintaining an adequate, quality water supply is essential for agricultural productivity. In addition, clean drinking water is a basic human right alongside sufficient access to food. Strategies for conserving water supplies include using 'grey water' (of sufficient quality) and more targeted water irrigation systems such as through drip delivery (more 'crop per drop').

71 % of the Earth's surface is covered in water so there is no physical shortage, but most of the resource is saline (97 %) and therefore non-potable (not fit to drink). The remaining 3 % is freshwater of which 90 % is locked away in glaciers, the polar ice caps and inaccessible groundwater. Humanity's growing needs must therefore be met with only 0.3 % of the Earth's total water. With this in mind water research must include the whole of the water cycle together with the impact on the ecosystem and the consequences that this has for economic growth and social justice.

5.2.1 Water Demand

With household, agricultural and industrial demands in competition, chemical scientists, alongside engineers, have an important role to play in making clean water, of an appropriate quality, economically accessible for all. To achieve this, products must be designed to minimise water and energy use during their production and use⁸⁴.

Opportunities for the Chemical Sciences

- Development of efficient, safe and low maintenance systems for domestic and industrial water recycling
- Development of efficient water supply systems and anti-corrosion technologies for pipework, including materials for preventing leakage and for water quality maintenance.

5.2.2 Drinking water quality

Access to safe drinking water and adequate sanitation varies dramatically with geography and many regions already face severe scarcity. The World Health Organization esti-

mates that safe water could prevent 1.4 million child deaths from diarrhoea each year⁸⁵. Clean, accessible drinking water for all is a priority. Water treatment is energy intensive and global energy requirements will increase as nations are forced to exploit water resources of poorer quality. Water scarcity will lead to energy intensive desalination and water reuse and recycling. The chemical sciences therefore have a dual role to play in treating water, by both making it potable and also by removing contaminants from wastewater and industrial waste streams.

Opportunities for the Chemical Sciences

- Development of energy efficient desalination processes.
- Development of energy efficient point of use and centralised purification, for example disinfection processes and novel membrane technologies.
- Development of low cost portable technologies for analysing and treating contaminated groundwater that are effective and appropriate for use by local populations in the developing world.
- Development of rapid and biochemical detection methods for pathogenic organisms in drinking water.

5.2.3 Wastewater

With the future threat of water scarcity there will be an increased interest in the recycling and re-use of water from agricultural sources. The removal of the wide range of contaminants contained in many sources of waste water is energy intensive. The challenge is to make waste water treatment energy-wise optimal and to enable the beneficial re-use of its by-products. Advanced, energy efficient industrial wastewater treatment technologies are needed.

In addition to developing treatment technologies, chemical science is key in developing processes for localised treatment and re-use of wastewater to ensure that appropriate quality of water is easily accessible. Specifically, it is important to identify standards for rainwater and grey water so that, coupled to appropriate localised treatment, rain/grey water can be harvested and used for secondary purposes.

Opportunities for the Chemical Sciences

- Development of novel membrane, catalytic and photochemical processes for the removal of a range of contaminants from wastewater
- Development of improved methods for treating domestic wastewater, to void the high energy input and sludge generation associated with using biological processes
- Design of robust, simple and inexpensive processes for localised treatment and re-use of wastewater in the developing world⁸⁶.
- Identification of standards for rainwater and grey water so that, coupled to appropriate localised treatment, these water sources can be harvested and used for secondary purposes.

5.2.4 Contaminants

More research is required into the measurement, fate and impact of existing and emerging water contaminants.

Human activity has resulted in the emergence of chemical contaminants in the environment, typically mobilised by water. Further research will help determine and control the risks of contaminants to the environment and human health, and will help the European Union to implement the objectives of environmental treaties, such as the Stockholm Convention on Persistent Organic Pollutants⁸⁷.

Our understanding of the major fate processes for many contaminants is well developed. Experimental and computational modelling approaches are available to determine how a substance could behave in the environment and to establish the level of exposure. However, knowledge gaps include the environmental fate of nanoparticles and pharmaceuticals, and identification and risk analysis of how contaminants may change in the environment.

Opportunities for the Chemical Sciences

- Improved methods for assessing the risks of mixtures of chemicals at low concentrations to the environment and human health.
- Improving our understanding the impact of contaminants on and their interaction with biological systems.
- Improved understanding of the effect of temperature and precipitation changes (due to global warming) on the input of chemicals into the environment, and their fate and transport in aquatic systems.

5.3. Livestock and Aquaculture

In addition to crops, global livestock production faces enormous short-term challenges. Total global meat consumption rose from 139 million tonnes in 1983 to 229 million tonnes in 1999/2001 and is predicted to rise to 303 million tonnes by 2020⁸⁸. Technologies are needed to counter the significant environmental impact and waste associated with rearing livestock. Livestock production currently accounts for one-fifth of greenhouse gas emissions worldwide.

Most wild fisheries are at or near their maximum sustainable exploitation level⁸⁹. In 2004, 43 % of the global fish supply already came from farmed sources⁹⁰. The inevitable growth of aquaculture will involve further intensification. Few effective drugs are available for treating diseases in fish because of environmental concerns and a relative lack of knowledge about many fish diseases.

Opportunities for the Chemical Sciences

- Development of next generation veterinary medicines, including new vaccines, to tackle disease in farmed animal
- Improving our knowledge of the effects of foods and food constituents on gene expression (nutrigenomics) to understand and guide improvements in feed conversion.
- Use of modern biotechnology to improve disease resistance, feed conversion and carcass composition.

5.4 Healthy Food

Nutrition is a major, modifiable and powerful factor in promoting health, preventing and treating disease and improving quality of life. Today about one in seven people do not get enough food to be healthy and lead an active life, making hunger and malnutrition the number one risk to health worldwide – greater than AIDS, malaria and tuberculosis combined.

In stark comparison, the developed world sees issues arising that relate more to excess production and consumption. Over-nutrition and reduced physical activity have contributed to the growth of diseases such as obesity⁹². Understanding the interaction of food intake with human health and providing food that is better matched to personal nutrition requirements is therefore essential. A greater knowledge of the nutritional content of foods will be required to understand fully the food/health interactions, which could facilitate more efficient production of foods tailored to promote human and animal health.

The chemical sciences are key to identifying alternative supplies of 'healthier foods' with an improved nutritional profile. One of the main challenges is to produce food with less of the fat, salt and sugar components that can be detrimental to health, while maintaining consumer perception and satisfaction from the products. Many foods can be reformulated, but the sensory quality during eating must be maintained. A greater appreciation of the chemical transformations which take place during processing, cooking and fermentation will help to maintain and improve the palatability and acceptability of food products. Another challenge is developing improved food sources and fortifying foodstuffs to combat malnutrition and to target immune health. Even a diet that contains more energy than required can be deficient in micronutrients.

Opportunities for the Chemical Sciences

- Develop a better understanding of formulation science for controlled release of macro- and micro-nutrients and removing unhealthy content in food;
- Identification of novel satiety (feeling full) signals, for example, safe fat-replacements that produce the taste and texture of fat;
- Production of sugar replacements and natural low calorie sweeteners to improve nutrition and combat obesity;
- Use of the glycaemic load of food in understanding nutrition, and the role of glucose in health and the onset of type II diabetes;
- Developing and understanding fortified and functional food with specific health benefits, including minor nutrients.

5.5 Food Safety

Foodborne pathogens are a significant cause of global health problems. In the EU, campylobacteriosis remained the most frequently reported animal-transmitted (zoonotic) disease in humans, with 175,561 confirmed cases in 2006⁹³. Physical, chemical and radiological contaminants can also pose risks to consumers. The chemical sciences can support the European Food Safety Authority in securing Europe's food safety⁹⁴.

Vast improvements can be made in both the detection and control of hygiene issues and food safety. Microbial contamination of food is the most common cause of health problems for consumers (either by spoilage or by adulteration) and therefore remains a critical food hygiene and safety issue. While significant emphasis is placed on detection, there is a role for the chemical sciences in developing and using intelligent packaging to improve the control of food spoilage, hygiene and food safety.

Opportunities for the Chemical Sciences

- Application of irradiation methods to remove bacterial pathogens and prevent food spoilage
- Technology breakthroughs in real-time screening and sensors are necessary to support rapid diagnostics that can detect contaminants and ensure food authenticity and traceability
- Developing processes for the detection of industrial chemicals, allergens, toxins, veterinary medicines, growth hormones and microbial contamination of food products and on food contact surfaces.
- Technologies to address domestic food hygiene through visible hygiene indicators.
- More effective methods for safety testing and designing new food additives, such as 'natural preservatives' and 'antioxidants' is required.
- Further research into naturally occurring carcinogens in food such as acrylamide and mutagenic compounds formed in cooking, with similar studies to encompass the effects of prolonged exposure to food ingredients.
- Development of microsensors to measure food quality, safety, ripeness and authenticity, and to indicate when the 'best before' or 'use-by' date has been reached.

5.6 Process Efficiency

The manufacture, processing, distribution and storage of food have significant and variable resource requirements. We need to find and use technologies to make this whole process much more efficient with respect to energy and other inputs.

The challenge in this area is to develop and use technologies that make the entire process significantly more efficient with regard to managing water and waste, improving the use of energy and developing extraction technologies for recovering and using by-products.

5.6.1 Food Manufacturing

Sustainable small scale manufacturing operations are needed with a focus on improving process efficiencies. This will

require improvements in operational efficiency throughout the entire manufacturing process as materials are received, stored and transferred.

The development of new methods for the efficient use, purification and cost effective recovery of water in food processing would reduce water wastage, with the aim being to develop water-neutral factories.

Opportunities for the Chemical Sciences

- Intensification of food production by scaling down and combining process steps;
- New routes for by-product and co-product processing to reduce waste and recover valuable materials;
- Development of milder extraction and separation technologies with lower energy requirements;
- New technologies to minimise energy input at all stages of production, such as high pressure processing and pulsed electric fields;
- Optimisation of the forces needed to clean food preparation surfaces together with development of new anti-fouling surface coating technologies to minimise energy requirements for cleaning;
- New methods for synthesising food additives and processing aids;
- Improved understanding of how the chemistry of food degradation is inhibited;
- New chemical stabilisation technologies for produce to improve formulation and delivery.

5.6.2 Food distribution and Supply Chain

The transport of food in various stages of a product lifecycle can increase its carbon footprint and therefore have a negative impact on the environment. While shorter supply chains through local sourcing can cut CO₂ emissions this must be balanced against possible increases across the product lifecycle. It is therefore necessary to adopt lifecycle analysis which takes into account an assessment of the overall carbon footprint of products.

The biggest opportunity for the chemical sciences in addressing food distribution challenges lies in sustainable and efficient transport. However, optimising food distribution will also require analytical techniques to ensure quality measurement and control of foodstuffs in transit. The chemical sciences can deliver advanced food storage technologies and optimised methods to distribute foods with minimal energy requirements and environmental impact.

The food industry is a major user of packaging, which protects products from damage, deterioration and contamination. The chemical sciences have a role to play in developing sustainable packaging, which is biodegradable or recyclable and compatible with anaerobic digesters.

Opportunities for the Chemical Sciences

- Development of new, more efficient refrigerant chemicals that will help avoid environmental damage and will save energy;
- Increased efficiency of refrigeration technology at all stages in the supply-chain, such as super-chilling as an alternative to freezing;
- Development of ambient storage technologies for fresh produce;
- Design of improved food preservation methods for liquids and solids, including rapid chilling, heating and salting;
- Design of flexible thin films made from corn starch, polyacetic acid or cellulosic materials which can withstand the chill-chain, handling and storage;
- Development of food packaging that is compatible with anaerobic digesters.

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