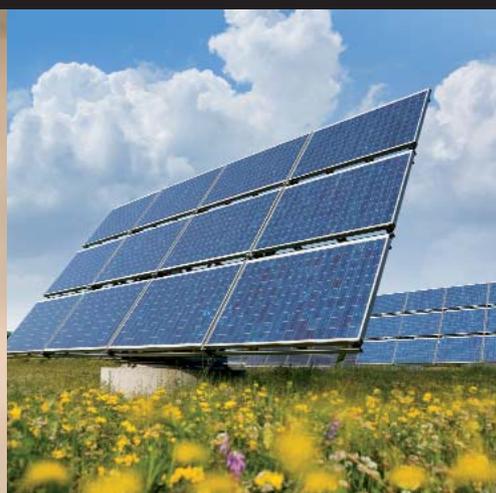
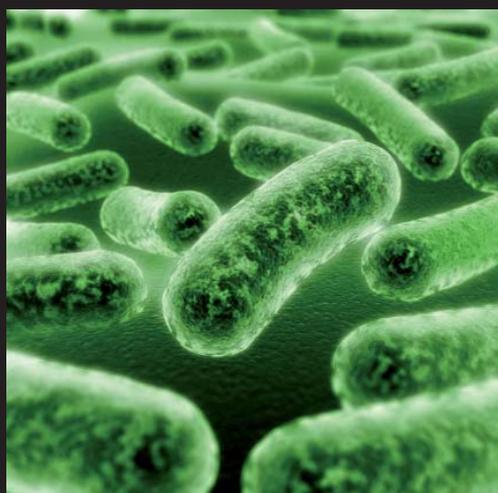


# Chemistry for Tomorrow's World

A roadmap for the chemical sciences  
July 2009



## About this Publication

The world is undergoing unprecedented change. With rising populations, and the realities of climate change, our fragile environment and resources are being stretched beyond their limits. Over the past year, the Royal Society of Chemistry (RSC) has gathered expertise and views from its members and the wider community from around the world. Through a series of workshops and online consultation we have identified priority areas and opportunities for the chemical sciences. This document presents the outcome of the consultations and identifies the key challenges of immediate concern. These should drive the UK and international science agendas for the next 5–10 years.

## About the RSC

Since 1841, the RSC has been the leading society and professional body for chemical scientists and we are committed to ensuring that an enthusiastic, innovative and thriving scientific community is in place to face the future. The RSC has a global membership of over 46,000 and is actively involved in the spheres of education, qualifications and professional conduct. It runs conferences and meetings for chemical scientists, industrialists and policy makers at both national and local level. It is a major publisher of scientific books and journals, the majority of which are held in the Library and Information Centre. In all its work, the RSC is objective and impartial, and it is recognised throughout the world as an authoritative voice of chemistry and chemists.



## Foreword

Having identified the vital role that the chemical sciences will play over the coming decades in addressing the global challenges faced by society, the publication of this report represents the beginning of an exciting time for the Royal Society of Chemistry (RSC).

This is the distillation of a huge amount of information and views that have been collected over the past year from a series of workshops and online consultations with members, non-members and a range of stakeholders worldwide.

The RSC is extremely grateful for the breadth of valuable contributions it received. Special thanks must go to all the enthusiastic people who have supported and taken part in this project so far. A special mention should also be given to Alison Eldridge who managed this project at the RSC.

As we move into the implementation phase, we hope that as many individuals and organisations as possible will grasp the opportunity to work with us to promote and develop the chemical sciences for the benefit of society, and ensure that action is taken to solve the challenges we face.

### **David Prest CChem FRSC**

Chemistry for Tomorrow's World Steering Group Chairman

Royal Society of Chemistry Member of Council

Managing Director, European Region, Emission Control Technologies, Johnson Matthey plc

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## EXECUTIVE SUMMARY

With global change creating enormous challenges relating to energy, food and climate change, action is both necessary and urgent. The Royal Society of Chemistry is committed to meeting these challenges head on and has identified where the chemical sciences can provide technological and sustainable solutions.

The RSC is in the ideal position to enable solutions to the world's problems by working in partnership with governments, professional bodies, non-governmental organisations, academics and industry, across the world. We will help decision makers to generate policy which is based on the best available evidence, and we will support the science needed to tackle complex challenges.

Addressing global challenges means advancing fundamental scientific knowledge, supporting excellence in chemical science research and maximising the number of future breakthroughs. It will require an interdisciplinary approach and the RSC will build bridges between chemistry's sub-disciplines, and with other sciences and engineering. The RSC's internationally active networks will be instrumental in implementing this approach.

This report presents the first stage of this initiative, which started in January 2008, to address how the chemical sciences can support society in a changing world. We brought together over 150 internationally-renowned scientific experts in seven workshops to discuss issues facing today's society, identifying seven priority areas (see below). Within these seven areas, 41 challenges were defined and the role that chemistry will play in providing solutions was examined. In addition, the expertise, attitudes and opinions of the wider community were incorporated via a web based consultation. (A glossary of terms defining the terminology used in this initiative can be found in Appendix A9.)

Throughout this exercise, we have attempted to align the RSC with existing strategies and priorities from a range of partners, who were involved in the consultation process, strengthening our relationships and the capacity for this work to have real impact.

These seven priority areas have many areas of overlap, with strong links between associated challenges. The themes of sustainable development and climate change underpin the majority of the challenges.

**The seven priority areas are summarised as follows and the key opportunities for the chemical sciences in each priority area are highlighted in the subsequent tables. Full details of the priority areas are outlined later in this report.**

**Energy** Creating and securing environmentally sustainable energy supplies, and improving efficiency of power generation, transmission and use

**Food** Creating and securing a safe, environmentally friendly, diverse and affordable food supply

**Future cities** Developing and adapting cities to meet the emerging needs of citizens

**Human health** Improving and maintaining accessible health, including disease prevention

**Lifestyle & recreation** Providing a sustainable route for people to live richer and more varied lives

**Raw materials & feedstocks** Creating and sustaining a supply of sustainable feedstocks, by designing processes and products that preserve resources

**Water & air** Ensuring the sustainable management of water and air quality, and addressing societal impact on water resources (quality and availability)

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 1:

# ENERGY

Creating and securing environmentally sustainable energy supplies, and improving efficiency of power generation, transmission and use

## 5 Years

### Biofuels and biopower

- Better ways of hydrolysing diversified bio-mass and lignocellulose

### Energy efficiency

- Increased strength-to-weight ratio for structural materials, such as those used in transport, including use of nanotechnology

### Nuclear

- Better understanding of the physicochemical effects of radiation on material fatigue, stresses and corrosion in nuclear power stations

## 10 Years

### Nuclear

- New and improved methods and means of storing waste in the intermediate and long term including new materials and radiation tolerance

### Hydrogen

- More efficient water electrolysis

### Fossil fuels

- Develop better coal gasification technology

### Solar energy

- Develop third-generation photovoltaic materials

### Wind and water

- Develop lightweight durable composite materials, coatings and lubricants

## 15 Years

### Energy efficiency

- Superconducting materials at higher temperatures

### Energy conversion and storage

- Improve energy density of storage technologies
- Advance the fundamental science and understanding of surface chemistry
- Develop next generation fuel cells, batteries, electrolyzers and superconductors

### Fossil fuels

- Carbon capture and storage
  - Enhance oil recovery (EOR)
  - Saline aquifers
  - Amine scrubbing
  - Alternatives to amine absorption, including polymers, activated carbons or fly ashes
  - Understand corrosion and long term sealing of wells
  - Understand the behaviour, interactions and physical properties of CO<sub>2</sub> under storage conditions
  - Maximise storage potential
  - Conversion of CO<sub>2</sub> to chemicals
  - Integrate with combustion and gasification plants

### Hydrogen

- Storage of hydrogen

### Solar energy

- Mimic photosynthesis

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 2:

# FOOD

Creating and securing a safe, environmentally friendly, diverse and affordable food supply

## 5 Years

### Food safety

- Visible indicators to improve domestic hygiene
- Irradiation for removing bacterial pathogens preventing food spoilage

### Packaging

- Develop biodegradable or recyclable, flexible films for food packaging – *eg* corn starch, polylactic acid or cellulose feedstock, able to withstand the chill-chain, consumer handling, storage and final use – *eg* microwave or conventional oven
- Develop functional – *ie* antimicrobial, and intelligent packaging films providing specific protection from moisture, bacteria and lipids improving texture and acting as carriers for various components – *eg* nanotechnologies
- Recycle mixed plastics used in food packaging

### Pest control

- Formulation technology for new mixtures of existing actives, and to ensure a consistent effective dose is delivered at the right time and in the right quantity
- Reduce chemicals in crop protection strategies through wider use of GM crops

### Natural resources

- Better yields of components for biofuels and feedstocks through the use of modern biotechnology
- Nitrogen and water usage efficiency – *eg* drought resistant crops for better water management

# 10 Years

## Fertiliser synthesis

- Low energy synthesis of nitrogen and phosphorus-containing fertilisers – alternatives to Haber-Bosch

## Supply chain sensors

- Harness analytical chemistry to design rapid, real-time screening methods, microanalytical techniques and other advanced detection systems to screen for chemicals, allergens, toxins, veterinary medicines, growth hormones and microbial contamination of food products and on food contact surfaces
- Quality measurement and control: analytical techniques to detect pesticide residues, adulteration and confirm traceability
- Sensors to monitor food stuffs in transport
- Develop microsensors in food packaging to measure food quality, safety, ripeness and authenticity and to indicate when the 'best before' or 'use-by' date has been reached

## On farm sensors

- Develop rapid *in situ* biosensor systems and other chemical sensing technologies that can monitor soil quality and nutrients, crop ripening, crop diseases and water availability to pinpoint nutrient deficiencies, target applications and improve the quality and yield of crops

## Raw material processing

- Extract and apply valuable ingredients from food waste – eg enzymes, hormones, phytochemicals, probiotics cellulose and chitin
- Develop milder extraction and separation technologies with lower energy requirements
- Secondary metabolites for food and industrial use

# 15 Years

## Vaccines and veterinary medicines

- Develop new vaccines and veterinary medicines to treat the diseases (old/new/emerging) of livestock and farmed fish – ie zoonoses

## Pest control

- New high-potency, more targeted agrochemicals with new modes of action that are safe to use, overcome resistant pests and are environmentally benign
- Pesticides tailored to the challenges of specific plant growth conditions – eg hydroponics

## Formulation

- Better understand formulation technology for controlling the release of macro and micro nutrients and removing unhealthy content in food
- Formulate for sensory benefit

## Nutrition and food quality

- Formulation science to increase nutritional content of food
- More nutritious crops through GM technologies

## Food chemistry

- Understand the biochemical processes involved in produce ripening and food ageing, enabling shelf-life prediction and extension
- Understand the chemical transformations taking place during processing, cooking and fermentation processes, that will help to maintain and improve palatability and acceptance of food products by consumers

## Soil science

- Optimise farming practices by understanding the biochemistry of soil ecosystems, for example, the chemistry of nitrous oxide emissions from soil, the mobility of chemicals within soil, and partition between soil, water, vapour, roots and other soil components

## Nutrients

- Understand feed in animals: feed conversion *via* nutrigenomics of animals; bioavailability of nutrients
- Improve the understanding of carbon, nitrogen, phosphorus and sulfur cycling to help optimise carbon and nitrogen sequestration and benefit plant nutrition

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 3:

# FUTURE CITIES

Developing and adapting cities to meet the emerging needs of citizens

## 5 Years

### Monitoring and improving air quality

- Catalysts for efficient conversion of greenhouse gases with high global warming potential (in particular  $N_2O$ ,  $CH_4$  and  $O_3$ )
- Develop low cost, localised sensor networks for monitoring atmospheric pollutants, which can be dispersed throughout developed and developing urban environments
- Improve catalysts for destroying pollutants, in particular  $CO$ ,  $NO_x$ , hydrocarbons, VOC, particulate matter
- Advance end of pipe treatment, including separation methods, catalysis and using plasma surface etching *etc*
- Healthy buildings: air quality management and functionalised surfaces for decomposing VOCs in homes

### Use of alternative energy sources

- More flexible low cost photovoltaics based on 'first generation' silicon materials

### Resources

- Increase the proportion of city waste to be recycled – *eg* improved processes for recycling plastics

### Mobility

- Develop new recyclable materials for the lightweight construction of vehicles
- Eco-efficient hybrid vehicles will require new energy storage systems (enhanced lithium batteries and supercapacitors)
- Improve the internal combustion engine
- New tyre technologies to reduce fuel consumption and noise
- Improve sensor technologies for engine management and pollution detection
- Reduce  $CO_2$  emissions from transport

### Construction materials

- Develop functionalised building materials – *ie* self-healing and self cleaning nanocoatings
- Develop new high performance insulating materials – *eg* aerogel nanofoams
- Develop self-cleaning materials

### Public safety and security

- Early detection of potential pandemic diseases through developing effective, rapid analytical techniques

## 10 Years

### Use of alternative energy sources

- New solar panel production approaches, hybrid materials, new electrodes, photovoltaic paints

### ICT – Miniaturisation for device size and speed

- Integrate nanostructures in device materials
- Self-assemble biological and non-biological components to produce complex devices such as biosensors, memory devices, switchable devices that respond to the environment, enzyme responsive materials, nanowires, hybrid devices, self-assembly of computing devices, smart polymers
- Polymers for high density fabrication: identify suitable materials meeting resolution, throughput and other processing requirements
- Printed electronics
- High density, low electrical resistance, interconnect materials to enable ultra high speed, low power communication: metallic nanowires; metallic carbon nanotubes

### Mobility

- Alternative catalyst technologies compatible with jet engines
- Catalysts for fuel quality and emissions control for ships

## 15 Years

### Use of alternative energy sources

- Biogas fuel cells
- Harness thermal energy – eg excess heat from car engines
- Harvest geothermal energy through improved heat transfer and anti-corrosion materials

### Public safety and security

- Chemical and biological sensors: remote, rapid and reactive sensors: sensor networks; chemical analogue of CCTV; home security networks

### Resources

- Reduce, recycle and re-use of materials used in information and communication technology

### Construction materials

- Develop intrinsically low energy/low CO<sub>2</sub> emission construction materials
- Recyclability and reduced dependence of strategic construction materials

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 4:

# HUMAN HEALTH

Improving and  
maintaining accessible  
health, including  
disease prevention\*

\* Health priority areas for the chemical sciences will include cancer, cardiovascular disease, stroke, mental health and well-being, infectious disease, respiratory disease, obesity and diabetes, the ageing population as taken from *MRC strategic plan 2004–2007*

## 5 Years

### Hygiene and infection

- Detect and reduce airborne pathogens – eg material for air filters and sensors

### Diagnostics

- Develop sensitive detection techniques for non-invasive diagnosis
- Identify relevant biomarkers and sensitive analytical tools for early diagnostics

### Materials and prosthetics

- Research polymer and bio-compatible material chemistry for surgical equipment, implants and artificial limbs
- Develop smarter and/or bio-responsive drug delivery devices

## 10 Years

### Ageing

- Improve understanding of the impact of nutrition and lifestyle on future health and quality of life

### Hygiene and infection

- Develop fast, cheap effective sensors for bacterial infection
- Improve the ability to control and deal quickly with new antibiotic resistant strains
- Accelerate the discovery of anti-infective and anti-bacterial agents: therapeutics and safe and effective cleaning/antiseptic agents

### Drugs and therapies

- Chemical tools for enhancing clinical studies – eg non-invasive monitoring *in vivo*, biomarkers, contrast agents

### Drugs and therapies: Effectiveness and safety

- Monitor the effectiveness of a therapy to improve compliance
- 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 – eg the blood-brain barrier
- Develop toxicogenomics to test drugs at a cellular and molecular level

### Materials and prosthetics

- Develop tissue engineering and stem cell research for regenerative medicine

### Diagnostics

- Develop cost effective, information-rich point-of-care diagnostic devices

## 15 Years

### Drugs and therapies

- Design and synthesise small molecules that attenuate large molecule interactions – eg protein-DNA interactions
- Understand the chemical basis of toxicology and hence derive 'Lipinski-like' 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

### Diagnostics

- Develop cost effective diagnostics for regular health checks and predicting susceptibility
- Produce combined diagnostic and therapeutic devices (smart, responsive devices, detect infection and respond to attack)

### Personalised medicine

- Develop lab-on-a-chip and rapid personal diagnosis and treatment
- Apply advanced pharmacogenetics to personalised treatment regimes

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 5:

# LIFESTYLE AND RECREATION

Providing a sustainable route for people to live richer and more varied lives

## 5 Years

### Creative industries

- Sustainable and renewable packaging coupled with emerging active and intelligent materials – eg developing time, temperature, spoilage and pathogen indicator technologies

### Household

- Continue to move formulation of household and personal care products from 'black art' to a more scientific basis

### Advanced and sustainable electronics

- Advances in display technology – eg flat lightweight and rollable displays for a variety of applications

## 10 Years

### Advanced and sustainable electronics

- Develop design concepts and new materials for microsized batteries and fuel cells for mobile and portable electronic devices
- The ability to exploit the interface between molecular electronics and the human nervous system – *eg* using the brain to switch on a light

### Sporting technology

- Keeping sport and recreation accessible to the wider population, especially the ageing population through advances in healthcare, notably develop an array of new technologies for managing chronic illness and promoting active lifestyles
- Use of active (non-invasive) diagnostic and monitoring to assist personal performance – *eg* hormone levels

### Creative industries

- Develop new materials for use in architecture, in designing new buildings and structures

### Household

- Develop self-cleaning materials for homes
- Controllable surface adhesion at a molecular level – *ie* switchable adhesion – *eg* self-hanging wall paper
- Improve the understanding of the chemical basis of toxicology in new/novel household products and their breakdown in the environment, to a level where good predictive models can be developed and used, such as computational chemistry (safety assessment without the use of animals) for human and eco-toxicology

## 15 Years

### Advanced and sustainable electronics

- Further enhance information storage technology – *eg* molecular switches with the potential to act as a molecular binary code
- Develop biological and/or molecular computing
- Understand biomimicking self-assembling systems. Printable (allowing dynamic re-configuration) electronics based on new molecular technologies

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 6:

# RAW MATERIALS AND FEEDSTOCKS

Creating and sustaining a supply of sustainable feedstocks, by designing processes and products that preserve resources

## 5 Years

### Conservation of scarce natural resources

- Recover metals from 'e-waste', contaminated land/landfills
- Reduce material intensity through thrifting, substitution and applying new technologies – eg nanotechnology for improved battery design

### Conversion of biomass feedstocks

- Develop bioprocessing science for producing chemicals
- New separation/purification technologies involving membranes and sorbent technology, and pre-treatment methods
- Develop novel catalysts & biocatalysts for processing biomass
- Converting platform chemicals to value products will require oxygen and poison tolerant catalysts and enzymes, and new synthetic approaches to adapt to oxygen-rich, functional starting feedstocks

### Recovered feedstocks

- Process waste as a feedstock through novel separation and purification technologies, and develop genuine, innovative recycling technologies

## 10 Years

### Sustainable product design

- Wider role of chemical science in design of products for 4Rs (reduction, remanufacture, reuse, recycle)
- Manufacturing process intensification and optimisation through atom efficiency, green chemistry and chemical engineering, process modelling, analytics and control
- Improved life-cycle assessment tools and metrics will require clear standards, methods to assess recycled materials and tools to aid substitution of toxic substances
- Improve the understanding of ecotoxicity

## 15 Years

### Recovered feedstocks

- Activate small molecules to use as feedstocks: CO<sub>2</sub>; biomimetic conversion of CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub> to chemicals and artificial photosynthesis/solar energy conversion

# OPPORTUNITIES FOR THE CHEMICAL SCIENCES

## PRIORITY AREA 7:

# WATER AND AIR

Ensuring the sustainable management of water and air quality, and addressing societal impact on water resources (quality and availability)

## 5 Years

### Air quality and climate

- Develop low-cost sensors for atmospheric pollutants (ozone, nitrogen oxides, particulates *etc*), which can be dispersed throughout developed and developing urban areas for fine-scale measuring of air quality
- Develop novel analytical techniques for detecting complex reactive molecules, which affect air quality and are harmful to health

### Drinking water quality

- Development low cost portable technologies for analysing and treating contaminated groundwater that are effective and appropriate for use by local populations in the developing world – *ie* for testing of arsenic contaminated groundwater

### Water demand

- Household products and appliances designed to work effectively with minimal water and energy demands and include better water re-cycle systems
- Efficient water supply systems and anti-corrosion technologies for pipework needed including the development of materials for leakage prevention and water quality maintenance (in the developed world)

## 10 Years

### Air quality and climate

- Develop space-borne techniques for measuring major pollutants, including particulate aerosol, with sub-20 km horizontal resolution and able to resolve vertically within the lower troposphere. Use geostationary satellites to provide continuous coverage

### Contaminants

- Studies into the breakdown of and transport of substances in the aquatic environment, including emerging contaminants such as pharmaceuticals and nanoparticles
- Research into understanding the impact of contaminants on and their interaction with biological systems

### Waste water

- Develop processes for localising treatment and re-using waste water to ensure that appropriate quality of water is easily accessible. Standards for rainwater and grey water identified so that coupled to appropriate localised treatment rain/grey water can be harvested and used for secondary purposes such as toilet flushing or irrigating crops

### Water demand

- Better strategies for using water and re-using for agriculture systems

## 15 Years

### Air quality and climate

- Geo-engineering solutions to climate change, such as ocean fertilisation to draw down carbon dioxide, or increasing the Earth's albedo\* by enhancing stratospheric aerosols

### Drinking water quality

- Energy efficient point of use purification such as using disinfection processes and novel membrane technologies
- Energy efficient desalination processes developed

\* The proportion of incident light reflected by the Earth

## Next steps for the RSC

This document identifies seven global issues of high societal relevance with 41 associated challenges and highlights where the chemical sciences, in conjunction with other disciplines, are capable of playing an important role in delivering solutions. To make a significant contribution and secure progress, the RSC

must work with the scientific community and policy makers to focus on a finite number of challenges.

The RSC has identified 10 of the 41 challenges as priorities for the next 5-10 years. These were chosen following consultation with the RSC membership. The challenges, listed in alphabetical order, are as follows.

### ● **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.

### ● **Conservation of scarce natural resources**

Raw material and feedstock resources for both existing industries and future applications are increasingly scarce. We need to develop a range of alternative materials and associated new processes for recovering valuable components.

### ● **Conversion of biomass feedstocks**

Biomass feedstocks (whether they are agricultural, marine or food waste) for producing chemicals and fuels are becoming more commercially viable. In the future, integrated bio-refineries using more than one biofeedstock will yield energy, fuel and a range of chemicals with no waste being produced.

### ● **Diagnostics for human health**

Recognising disease symptoms and progress of how a disease develops is vital for effective treatment. We need to advance to earlier diagnosis and improved methods of monitoring disease.

### ● **Drinking water quality**

Poor quality drinking water damages human health. Clean, accessible drinking water for all is a priority.

### ● **Drugs & therapies**

Basic sciences need to be harnessed and enhanced to help transform the entire drug discovery, development and healthcare landscape, so new therapies can be delivered more efficiently and effectively worldwide.

### ● **Energy conversion and storage**

The performance of energy conversion and storage technologies (fuel cells, batteries, electrolysis and supercapacitors) needs to be improved to enable better use of intermittent renewable electricity sources and the development/deployment of sustainable transport.

### ● **Nuclear energy**

Nuclear energy generation is a critical medium term solution to our energy challenges. The technical challenge is for the safe and efficient harnessing of nuclear energy, exploring both fission and fusion technologies.

### ● **Solar energy**

Harnessing the free energy of the sun can provide a clean and secure supply of electricity, heat and fuels. Developing existing technologies to become more cost efficient and developing the next generation of solar cells is vital to realise the potential of solar energy.

### ● **Sustainable product design**

Our high level of industrial and domestic waste could be resolved with increased downstream processing and re-use. To preserve resources, our initial design decisions should take more account of the entire life cycle of a product.

This process has highlighted a number of exciting and important opportunities and will drive the scientific agenda for the RSC and wider community over the coming years.

For each one of the challenges listed, we will develop an associated project, and for areas where the RSC has already done major pieces of work – *eg* energy, food and water – a process of careful review will take place.

In the short term, we will open a dialogue with a number of key existing and potential partners, along with RSC member networks, to produce a comprehensive implementation plan. This process will include a series of workshops to define critical gaps in knowledge, which are limiting the technological progress within the fields of the 10 key challenges.

Over the next five years, we will manage a comprehensive programme of initiatives aligned with these challenges and their associated opportunities for the chemical sciences.

This work provides a great opportunity to build on the RSC's global networks and we must collaborate with scientists around the world to take this work forward. The RSC has international cooperation agreements with seven other chemical societies. We are also supporting links across Africa as part of the Pan Africa Chemistry Network, and facilitating connections with India through the Chemistry Leadership Network. Building on this, we will establish a new electronic network for chemists in industry and academia, which will enhance global connections, and increase our potential to influence policy makers around the world.

In order for this initiative to have real impact, and to drive the science and education agendas in the future, the chemistry community must act together. Support, advice and expertise from chemists are needed in order to continue to move forward with this programme.

There are many ways to get involved to help us inform key stakeholders, disseminate and exploit new and existing knowledge, as well as help to facilitate the discussions that need to be had around the world.

## CONTACTING US

For more on this important RSC initiative, and for updates as these projects evolve, please visit our website. [www.rsc.org/roadmap](http://www.rsc.org/roadmap)

To work with us and to find out about the latest events and projects in your region – please contact us at [roadmap@rsc.org](mailto:roadmap@rsc.org) or at our Cambridge office on 01223 420066.

Alternatively, contact one of our specialists at the RSC.

### RSC Science Policy

[sciencepolicy@rsc.org](mailto:sciencepolicy@rsc.org)

### Industry and Business

[industry@rsc.org](mailto:industry@rsc.org)

### Interest Groups

[interestgroups@rsc.org](mailto:interestgroups@rsc.org)

### RSC Events and conferences

[conferences@rsc.org](mailto:conferences@rsc.org)

### Education

[education@rsc.org](mailto:education@rsc.org)

### International Development

[rscinternational@rsc.org](mailto:rscinternational@rsc.org)

## 1. INTRODUCTION

Global change is creating enormous challenges for humanity. By 2030 the world's population is expected to have increased by 1.7 billion to over eight billion,<sup>1</sup> with the majority of those people living in cities. Global energy requirements will continue to increase as will the pressure on the Earth's natural resources to provide this rapidly expanding population with enough food, water and shelter. The newly industrialised countries of Asia and Latin America are experiencing very rapid economic growth that is bringing modern society's environmental problems, including air and water pollution and waste problems, to wider areas of the globe.

The ecological problems caused by human activity such as climate change are worsening. At the same time, it is estimated that more than one billion people now live in poverty without sufficient food, water or adequate sanitation and healthcare provision.<sup>2</sup>

Mitigation of these challenges will rely on adopting sustainable development; the ability to meet the needs of the present without compromising the ability of future generations to meet their own needs. This requires, increasingly, the eco-efficient processes and products that the chemical sciences can provide.

The chemical sciences help to make our lives healthier, safer and easier to live. They provide us with food, potable water, clothing, shelter, energy, transport and communication, while at the same time helping us in conserving scarce resources and protecting the natural environment in which we live.

Progress made in the chemical sciences will clearly be critical to: future advances in environmentally benign and more sustainable energy production, storage and supply; increased food production with less demand on arable land; advanced diagnostics and novel disease prevention therapies based on exploitation of the human genome; designing processes and products that preserve resources; and the provision of clean accessible drinking water for all. Advances in chemistry will also be needed to develop functional materials to construct our homes and buildings, and to develop lightweight vehicles to make them more energy efficient and thus reduce greenhouse gas emissions.

The chemical sciences, therefore, have a clear role in pursuing sustainable development and in providing technological solutions to the challenges facing society today and in the future. The technologies that the chemical sciences engender will improve the quality of daily life, underpin prosperity and will increase our readiness to face the challenges of the future.

## 2. CREATING A SUPPORTIVE ENVIRONMENT

Progress in the chemical sciences is required to provide the technological solutions needed by society, in order to solve the global challenges in energy, food, health, water and sustainability. Achieving this does not depend solely on major research and technological advances in the areas defined by this report. It requires developing a supportive environment.

The supportive environment requires the supply of an appropriately skilled and diverse scientific workforce, investing in research, and a business and regulatory framework that protects society and promotes enterprise. This will also require engagement with key stakeholders, ranging from industrialists, academics and educationalists to governments, funding organisations and non-governmental organisations. There is also a need to invest in innovation – the translation of findings into usable developments. Society and its leaders need to be clearly aware of these issues and, in seeking to achieve this, the role of education is critical.

The issues in this chapter are based on UK and European data received for this report. Future activity of the RSC in this area should look at these issues from a global perspective.

### 2.1 Engagement and trust

Developing a supportive environment will require engaging with key stakeholders and with the general public to ensure the successful introduction of new and emerging technologies. This is a complex process that often requires a sustained effort over a long period. It often depends on effective stakeholder dialogue on the costs, benefits and risks to consumers and/or the environment of the technology concerned. However, perceptions of risk differ widely within society and with low public confidence in some parts of the chemicals sector. There is often a perception of high-risk and an excessive focus on the potential negative impacts of new technologies.

The public is often unaware of the contribution the chemical sciences already make to today's society. The benefits of the chemical sciences to essential products are hidden and often inadequately communicated. There is a need to understand where the common ground is and how consensus can be developed.<sup>3</sup> To progress science and technology and ultimately facilitate the uptake by society of new products and processes it is therefore necessary to create an open dialogue between stakeholders. This must be based on

knowledge and a common understanding of the health, safety, environmental, social and ethical concerns. To build trust amongst all stakeholders there must be a clear understanding of the benefits and burdens of new technologies, as well as the risks posed by failure to adopt new technologies.

### 2.2 Appreciation of chemistry

To create a supportive environment, it is important to take long-term action to foster an appreciation of the chemical sciences and stimulate an interest in studying chemistry and careers in science. Chemistry underpins our understanding of all aspects of the world around and as a result the subject has a role to play in everyone's general education. Our young people are the future of society. They will live in a world that is influenced strongly by the present contributions of research and development based on the chemical sciences.

This means that chemistry has an important role in the school curriculum not only in providing future scientists, but also in developing a future society where the place of chemistry is grasped in terms of its underpinning role in tackling key global challenges. The early years of secondary education are known to be critical and teaching must focus on what is accessible at these ages. Research has shown that this approach generates an increase in demand amongst young people to study chemistry. It also secures an excellent basis for enabling everyone to see the role of chemistry in the way it can contribute in taking society forward in addressing major challenges.

The majority of those who study the chemical sciences at undergraduate or postgraduate level do so to pursue an interest in the subject. It is therefore important that children in primary and the early years of secondary schooling are given the opportunity to see the real excitement of chemistry either within their schools or through other intervention programmes, where they can access facilities that schools cannot provide. The earlier these interventions take place the better. Early impressions of science will stay with children longer. However, it is equally important that those early messages are reinforced throughout young people's schooling with other intervention programmes.

When students are approaching the point of making the subject choices that will determine what they can study later it is important that they are provided with information about careers that they can follow by studying subjects like chemistry.

## 2.3 Education, skills and capacity building

To ensure the long-term viability and innovative capacity of the chemicals and other chemistry-using industries, an adequate supply of appropriately trained scientists and a broader technically-literate society with the relevant knowledge and skills will be required.

The UK government has recognised the vital importance of increasing the numbers of young people studying science, technology, engineering and mathematics (STEM) subjects and raising the level of STEM literacy among those entering adult life.<sup>4</sup> The supply of STEM talent directly impacts on all areas of research and development, innovation and hence the ability of the science and engineering-based industries to play their part in the economy. Despite the number of chemical science entrants to UK university courses showing significant signs of improvement (a 31 per cent increase in the past five years), this only brings it back to the level it was in 1997.

To overcome the global challenges facing society, long-term and long-lasting input needs to be made in the areas of education, skills and capacity building. All levels of education have a crucial role to play in creating a supportive environment. Primary and secondary education's role is to build the base for scientific understanding and literacy, to raise young people's interest and curiosity in the sciences and to stimulate interest in the further study of the chemical sciences and careers resulting from science. There is a need to identify and develop effective curriculum material to support teachers. These teachers must be trained and qualified in their subject and must be supported in a school environment with modern facilities for inspirational practical learning. In addition, there must be a sufficient provision of university places to educate the next generation of scientifically literate graduates and researchers for a wide range of careers or further study.

In line with the findings of educational research, primary schools should focus on the tangible and descriptive aspects of the sciences. Secondary schools should steadily move away from this towards the goal of enabling students to begin to understand the world around them in terms of the insights and understandings that have been offered by chemistry. Research in science education now offers clear guidelines about the kinds of curriculum structures and

teaching and learning approaches that can match these goals. Research has shown consistently that two of the key factors are the actual curriculum approach along with the quality and commitment of teachers. It is vital that new curricula are designed in line with the clear findings from research and that steps are taken to ensure the supply of adequate numbers of teachers fully qualified in chemistry.

Education and training institutions have an important role in ensuring that there is a flow of people with the skills required by the technology based industries of tomorrow, but industry is crucial to further developing these skills and competencies. Investment in in-service training and life-long learning is needed to develop skills at all levels to ensure the sector and individual companies remain competitive. With the introduction of new technologies, it will also be of commercial interest for whole sections of the work force to keep their skills and knowledge up to date and to ensure that new technologies are mastered. With an ageing workforce this will become particularly important in the future.

## 2.4 Opportunities for all

The majority of the graduate population in the UK and in most of Europe is now female. More women than men have graduated from UK higher education institutions for well over ten years. 57 per cent of those who graduated in 2008 were female.

In the UK, women are under-represented in the majority of STEM subjects, the biological sciences being the exception. Women are less likely than men to choose to read chemistry in the UK, where women make up around 47 per cent of those graduating at undergraduate level but 58 per cent of those graduating from all disciplines. Recent increases in the overall number of chemistry graduates may also be counteracted by the relatively low retention rate of women in comparison to men.

The attrition of women from chemistry is particularly bad in comparison to most other STEM subjects and it is therefore important to create an environment that supports the career aspirations of both men and women in academia and in industry. Looking to the future, many businesses have already identified improving their workforce diversity as a way of accessing a new labour pool. For the chemical sciences, improving the culture to attract more women to make their long-term careers in research is equally important.

## 2.5 Encouraging innovation

The pace of technological development required necessitates urgent investment in research and support for innovation. This is especially true for the UK and Europe. In general, European innovation performance has been weak compared to competing regions in the world.<sup>5</sup>

The UK government has started to address this by establishing a business-led Technology Strategy Board in 2004 and subsequently by establishing the Knowledge Transfer Networks (KTNs). Chemistry Innovation KTN has provided a focus for improved innovation in UK businesses, increasing their ability to turn knowledge and expertise into new technologies and products.

However, there are extensive structural, social and political factors that significantly impact on the ability to innovate successfully. Overall there is a need to ensure increased and long-term commitment to innovation by the leaders in key companies. These leaders are ultimately responsible for generating the motivation and employee behaviour that cultivates an environment conducive to successful innovation. There are other well documented challenges such as ensuring people in addition to those working in R&D are actively involved in the complete innovation process and offering direct and visible support for new or different business models such as those that rely on open innovation and external collaboration.

In the higher technology areas of innovation, improving the trust of chemical and biotechnology industries will help towards the goal of achieving a better balance for risk-benefit sharing amongst stakeholders. Industry's commitment to increased transparency will also help in this process. However, this will need concrete, coherent and continued public support via key governmental institutions.

More effective interaction between companies and their supply chains will also be essential for improving innovation. Ultimately this will require using the existing national, local and regional initiatives more effectively as it is these that provide the most direct access to the SMEs and future downstream customers. In general, better cooperation along the supply chain should lead to increasing the probability of successful innovation.

## 2.6 Regulatory environment

To create a supportive environment for innovation and to meet the challenges facing society it is necessary to monitor developments in UK and EU Environment, Health and Safety (EH&S) policy and related legislation. A proactive approach needs to be taken in influencing and informing policy makers so that chemicals control legislation is scientifically sound, risk-based, proportionate, workable and sustainable.

While it is imperative to protect health and the environment, it is not possible to design-out all risks over the life cycle of chemical substances and products. Legislation needs to strike a balance between reducing risk as far as is possible and the benefits to society of chemicals. For a chemical to cause harm requires exposure to its hazardous properties, so legislation based solely on a chemical's hazardous properties, and not on the actual risk it poses, can and has led to a reduction in chemical diversity, which in turn can impact negatively on innovation. While organisations such as the RSC support the search for safer alternatives it must be remembered that chemical substances generally do not pose a single risk and in fact have a risk profile. Therefore, in the search for less harmful substitutes with equivalent functionality and utility, care must be taken to ensure that a reduction in one risk is not replaced by an increase in another. Furthermore, the search for safer solutions should be based on the principles of sustainability.

It is also necessary to monitor international chemicals control policy to ensure that UK companies have a level playing field regarding EH&S legislation. While appropriate chemicals control policies do contribute to increased safety and sustainability, and can be a source of competitive advantage, policies which are not based on scientific knowledge can create additional costs for business that do not contribute to reducing risk.

Another very important area is green procurement, where organisations take into account external environmental concerns alongside the procurement criteria of price and quality. Regulations requiring a proportion of public procurement to be green could create massive demand for green, sustainable products and help foster innovation.<sup>6</sup>

## 3. UNDERPINNING SCIENCE

### 3.1 Areas of underpinning science

To address the big global challenges mentioned in this report and maintain the flow of future breakthroughs it is critical to advance fundamental knowledge and to support curiosity driven research. This will be achieved by maintaining and nurturing areas of underpinning science. The areas outlined in this chapter are not an exhaustive list, but provide an indication of the critical role that chemical sciences play in partnership with other disciplines.

#### Analytical science

This '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.<sup>7</sup> Recent developments in this area have underpinned huge advances in the biosciences such as genome mapping and diagnostics.

#### Catalysis

'Catalysis is a common denominator underpinning most of the chemical manufacturing sectors. Catalysts are involved in more than 80 per cent 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. Biocatalysis is also becoming increasingly important.<sup>8</sup>

#### 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 devices.<sup>9</sup>

#### Computational chemistry

Computational chemistry plays a major role in providing new understanding and development of computational procedures for simulating, designing and operating systems ranging 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.

#### 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 these materials and understanding how the composition and structure of the new materials influence or determine their physical properties to optimise the desired properties.

#### Supramolecular chemistry and nanoscience

This involves 'devising a framework to understand and manipulate non-covalent interactions, and on the physico-chemical engineering of nanoscale materials and systems. Notable advances have been made in self-assembled molecular and biomolecular systems, synthetic molecular motors, biologically inspired nano-systems, nano-structured surfaces, hierarchically-functionalised systems and measurement at the nanoscale.<sup>9</sup>

#### Synthesis

'Synthesis is achieved by performing chemical transformations, some of which are already known and some of which must be invented.<sup>7</sup> One of the goals of the underpinning science of synthesis is to invent new types of transformations because novel transformations are the tools that make it possible to create interesting and useful new substances. Chemists also create new substances with the aim that their properties will be scientifically important or useful for practical purposes.

## 3.2 Examples of critical future developments

The following are four examples of areas of science where further developments in fundamental understanding could lead to a new generation of products and applications as well as deliver potential benefits for society.

### Controlled release and formulation

Formulation – creating multi-component, often multi-phase products – is an enabling capability exploitable across many global market sectors, for example home and personal care, cosmetics, food and beverages, fuel additives, lubricants, coatings, inks, dyes, agrochemicals, and pharmaceuticals. Relevant emerging high-value markets also include organic electronics and nanotechnology.

The combined global market for formulated products exceeds £1000 billion per annum and is growing. The drivers for this are varied but include a growing and ageing global population requiring new products for health, hygiene and food production. Globalisation is also opening up new market opportunities and generating a demand for products of novel and diverse performance and profile, such as environmental, ethical and premium products. In turn, there is an associated increase in competition, driving more efficient production, improved technology protection and new approaches to overcoming ever shortening product life-cycles.

To develop the science and technologies needed to exploit these opportunities and challenges, multidisciplinary and cross-sector teams will be needed with expertise in areas including colloids, particles, surfactants, polymers, crystallisation, high-throughput technologies, measurement, modelling and process engineering.

Consumers like products that are convenient to use and give good performance. A controlled-, sequential- or multifunctional-release product is likely to have an improved performance over a non-specific release formulation by requiring reduced amounts of active

ingredients and needing to be applied less frequently. Such technology may allow the design of site specific active substances. For example, cancer cells have a different pH and temperature to normal cells so designing-in pH and temperature functionality, together with incorporating biomarkers, may allow the development of novel formulation products that specifically target cancer cells, and hence are non-invasive, offering consumer convenience with reduced side effects.

Controlled release formulations may also be useful for agrochemical and pharmaceutical applications because they would allow the active ingredient to be delivered where and how it is needed, potentially leading to reduced non-target effects. New formulations will help us to develop drugs and agrochemicals against targets that were previously considered to be inaccessible. In personal care the sequential delivery of non-compatible active ingredients at specific time intervals during a wash cycle could lead to the improved cleaning performance of a washing powder; and in cosmetics controlled release may lead to improved topical cosmetic applications such as maximising the amount of time an active ingredient such as a sunscreen is present on the skin.

For the most part, existing technologies such as encapsulation, micro-encapsulation and polymeric systems do not allow sufficient levels of control of particle and formulation design. For process technology to evolve, understanding the individual particle characteristics of the active ingredient(s) (size, shape and functionality) and their relationship to the bulk properties that directly relate to product performance is important. Therefore, there is a need to develop a fundamental understanding of surface chemistry, individual particle attributes, process engineering and scale-up laws. Such knowledge would provide the scientific community with multibillion pound product opportunities and a market advantage due to 'first to market' and product differentiation. This knowledge would potentially impact on health, environment and sustainability.

## Intelligent synthetic design for effect

While our knowledge of chemical synthesis can be used to make increasingly complex molecular structures, another accolade for fundamental research would be to better understand how these structures relate to specific useful functional properties. Designing and building functionality into a 'final' form, such as a drug molecule, an adhesive or a coating, by understanding the necessary properties of the component parts should be the ultimate goal. A better understanding of the molecular basis of functionality would allow us to design more effective ingredients, including chemicals designed to impart more than one kind of functionality to a product. Equally, undesirable functionality such as toxicity and bio-persistence could be designed out at an early stage. Analysing known property data with computational approaches may offer insights into the structural basis for important bulk properties. This will have tremendous impact on the environment in terms of sustainability. Such an approach would enable a fundamental shift from 'make and test' approaches towards intelligence led design. Steps in this direction have been made with, for example, biomimicry research to understand how nature uses surface structure to control properties.

Retrosynthesis is a method that was developed, originally by E.J. Corey, to help the organic synthesis of target molecules in the pharmaceutical and agrochemical industries amongst others. Furthermore, retrosynthesis for materials is being developed to help design-in functionality in the materials chemistry field. This is described as 'combining concepts generally used in covalent organic synthesis such as retrosynthetic analysis and the use of protecting groups, and applying them to the self-assembly of polymeric building blocks in multiple steps. This results in a powerful strategy for self-assembling dynamic materials with a high level of architectural control'.<sup>10</sup>

One example of this is synthesising molecular motors, where the thermodynamics and kinetics of phase behaviour in polymer blends and block copolymers are applied to develop new processing methods based on self-assembly.

Thinking sustainably when looking at drug design<sup>11</sup> is another area that has become increasingly important. Attention has been given recently to the problems caused by pharmaceuticals in the environment. However, the environmental impact of pharmaceuticals is not just limited to their end-of-life. Each stage in the lifecycle of a pharmaceutical product will have an associated environmental impact, via, for example, resource consumption, energy use or waste disposal.

This presents an opportunity to apply new chemistry methods and technology to design pharmaceutical products that have improved overall sustainability. Efforts have been concentrated on improvements to processes and manufacturing, such as reducing waste and hazardous materials. The 12 *Principles of Green Chemistry* can be applied here:

- prevent waste;
- design safer chemicals and products;
- design less hazardous chemical syntheses;
- use renewable feedstocks;
- use catalysts, not stoichiometric reagents;
- avoid chemical derivatives;
- maximise atom economy;
- use safer solvents and reaction conditions;
- increase energy efficiency;
- design chemicals and products to degrade after use;
- analyse in real time to prevent pollution;
- minimise the potential for accidents.

## Synthetic biology

Synthetic biology seeks to reduce biological systems to their component parts and to use these to build novel systems or rebuild existing ones. This manipulation of living systems and their component parts in a rational way is equivalent to the way in which engineers design new machines, cars or planes. This manipulation has two major implications. First, in creating new functions from new combinations of component parts, and secondly in improving the understanding of existing biological systems through reverse engineering. Synthetic biology requires the contribution of expertise from across the sciences because it involves applying principles and tools provided by engineering and the physical sciences. This convergence of biology, engineering and the physical sciences in synthetic biology could result in the third industrial revolution over the next 50 years, similar to the development of steam power and electronics.

Biological systems can be viewed as a network of interacting modules. DNA elements are important functional modules as they encode and control the production of proteins that determine the outputs of the system. Furthermore, these DNA elements may be responsive to external cues through interactions with signalling pathways. DNA can be precisely manipulated to change the system's outputs or behaviour to external cues. Chemistry has a key role to play in synthetic biology by providing tools to analyse and modify DNA and other molecules in the required way. This includes advances in DNA sequencing technology and gene manipulation tools. The molecular modules are broadly similar across many species. For example, the chemical properties of DNA are universal and therefore developments provided by the chemical sciences will be widely applicable across synthetic biology.

A synthetic biology approach is being applied across a range of biological scales. This includes designing molecules, through to the engineering of novel organisms, and may eventually allow the integration of biological and non-biological components. Organisms and biomolecules with more uses in chemistry are likely

to benefit society through applications in healthcare, the environment and energy. For example, synthetic biology will allow the development of new materials, the synthesis of novel nucleic acid and protein-based drugs, and will create organisms with new functions, such as the targeted breakdown of harmful chemicals in the environment.<sup>12</sup>

Synthetic biology can provide new processes for producing chemicals and drugs.<sup>13</sup> In nature, cells contain enzyme pathways that make precise changes to molecules with great specificity. Synthetic biology now enables chemists to 'mix and match' enzymes from different organisms to create new functions that allow the synthesis of specific molecules. For example, artemisinin is a naturally occurring, anti-malarial drug that is currently extracted from a plant at high cost and with low efficiency. Research has led to the introduction of a new enzyme pathway into yeast cells to produce a precursor to the active drug. This method has the potential to produce the drug at high yield and consistent quality, reducing its costs and increasing availability. A more complex and distant application of synthetic biology to medicine is the potential to engineer microbes that are able to fight cancer, by sensing and destroying cancer tissue.

Synthetic biology may also be used to facilitate the production of bio-hydrogen for energy. In principle hydrogen can be produced by splitting water using hydrogenase enzymes found in plants and bacteria. However, these enzymes are inhibited by the oxygen by-product of the reaction, so the process is very inefficient. Synthetic biology may provide a solution to this problem by engineering bacteria that are able to split water to produce hydrogen for use as a fuel.

Synthetic biology has the potential to contribute to solving a range of global challenges. It is important that the public is well-informed of these advantages to ensure that synthetic biology can be used to the maximum benefit of society.

## 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 inter-converting electrical and chemical energy, but practically it can be applied as an analytical and synthetic tool.

The realisation of increased use of renewable electricity generation, including the reduction of CO<sub>2</sub> from transport, relies on developing energy storage devices. If future cars are to be run using batteries, energy storage devices need to be efficient, produce high power and ideally be recyclable at low cost. This requires further understanding and developments in electrochemical research, applied to batteries, supercapacitors, fuel cells and chemical energy storage.

Electrochemistry has a central role to play in producing energy from renewable sources. For example, solar cells are essentially electrochemical cells, and improvements in their efficiency will rely on an improved understanding of the electron transport process through the cells. Hydrogen, considered by some as the clean energy vector of the future, can be produced cleanly and renewably by electrolysing water. Direct fuel cells such as hydrogen or methanol cells, or cells built to run on alternative high energy clean chemical feedstocks, all require real technological breakthroughs in materials for electrodes, understanding electrode reactions and understanding electron transport mechanisms.

Another 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, and they have the advantage of producing electrical output signals compatible with microelectronic systems. 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 an animal's nose interfaced with the brain). This requires better and more flexible sensor systems than at present.

Another challenge is the need in healthcare to detect biomolecular species such as proteins, oligonucleotides (DNA and RNA) and cells, quickly, accurately and cheaply. In diagnostics this is driven by developing physical techniques, which include electrochemical transduction, to enable these measurements. Current applications include glucose and pregnancy testing kits, but in the future this will open up the real prospect of theranostics – using diagnostics in informing patient-specific therapies.

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 improve therapies for degenerative diseases such as Alzheimer's and Parkinson's.

There are also major technical challenges in electrochemical corrosion, which need further understanding. Corrosion is a major destructive process that results in costly, unsightly and destructive effects, such as the formation of rust and other corrosion products, and the creation of gaping holes or cracks in aircraft, automobiles, boats, gutters, screens, plumbing, and many other items constructed of every metal, except gold.

Finally, as an indispensable research tool, electrochemistry can be applied to understanding organic reaction mechanisms and reaction rates, in nanoscale imaging devices such as electrochemical scanning tunnelling microscopy (ESTM), and as an analytical tool to characterise electrochemical systems such as cyclic voltammetry, potential step voltammetry, and electrochemical impedance spectroscopy (EIS).

## 4. SOCIETAL CHALLENGES AND OPPORTUNITIES FOR THE CHEMICAL SCIENCES

### 4.1 Energy

**Creating and securing environmentally sustainable energy supplies, and improving efficiency of power generation, transmission and use**

An adequate and secure supply of energy is essential in almost every aspect of our lives, but this needs to be achieved with minimum adverse environmental impact. On current trends, global emissions are set to reach double pre-industrial levels before 2050, with severe impacts on our climate and the global economy.<sup>14</sup> At the same time, energy demand worldwide continues to increase, as the world's population grows and the developing world economies expand. On the basis of present policies, global energy demand will be more than 50 per cent higher in 2030 than today, with energy related greenhouse gas emissions around 55 per cent higher.<sup>15</sup>

Even if the potential for increasing low carbon sources of energy is realised, it is clear that remaining reserves of fossil fuels will play a significant part in meeting the world's energy needs for the foreseeable future, and ways of reducing emissions must be found. The International Energy Agency forecasts that \$20 trillion of investment will be needed to meet these challenges by 2030.<sup>15</sup>

As society moves from an economy based on fossil fuels to a more sustainable energy mix, scientists and engineers will be required not only to develop sustainable energy solutions but also to find more efficient ways of producing, refining and using fossil fuels during the transition.

This section defines the challenges that exist and identifies the key R&D areas for the chemical sciences that are needed to support the sustainable development of energy supply, distribution and use, and to assist in the transition to a sustainable energy future. The main challenges relate to energy efficiency, energy conversion and storage, fossil fuels, nuclear energy, nuclear waste and renewables.

#### 4.1.1 Energy efficiency

**Challenge: Improvements are needed in the efficiency with which electricity is generated, transmitted and energy is used.**

The European Commission set a target of saving 20 per cent of all energy used in the EU by 2020; improved energy efficiency is a crucial part of the energy puzzle.

It would save the EU around €100 billion and cut emissions by almost 800 million tonnes per year. It is one of the key ways in which carbon dioxide (CO<sub>2</sub>) emission savings can be realised.<sup>16</sup>

Estimates point to an energy shortfall of 14 terawatts (TW) across the planet by 2050. Collectively, individuals are responsible for over 40 per cent of the UK's energy use and CO<sub>2</sub> emissions.<sup>14</sup> The Energy Saving Trust estimates that at home we waste over £900 million per year by leaving appliances on when they are not being used. Through energy efficiency and behavioural measures to reduce waste, households, in the UK alone, could save a further nine million tonnes of CO<sub>2</sub> a year by 2020 and cut energy bills at the same time<sup>17</sup> (see also section 4.3.3 Home energy use). The chemical sciences have a role to play in improving the efficiency with which electricity is generated, transmitted and how the energy is used.

Major opportunities exist for improving the conversion of primary energy for transport, industrial energy use and in buildings and domestic applications. Innovation in these areas will be underpinned by the chemical sciences.<sup>18</sup> Materials chemistry has a significant role to play in meeting future requirements, for example:

- using nanotechnology to increase the strength to weight ratio of structural materials;
- developing better insulating materials and more efficient lighting for buildings (see also section 4.3.3 Home energy use);
- through improving fuel economy and reducing CO<sub>2</sub> emissions by developing advanced materials and components that can be used in conventional vehicles (see also section 4.3.5 Mobility).

In addition, there are undoubtedly developments in materials use and processing where the chemical sciences will play an important part in using energy more efficiently and improving manufacturing efficiency. Breakthroughs will be required in optimisation, process intensification and developing new process routes, including developing new catalysts and improving separation technologies. This must be linked to the application of Life Cycle Analysis (LCA) (see also section 4.6.1 Sustainable product design).

#### 4.1.2 Energy conversion and storage

**Challenge:** The performance of energy conversion and storage technologies (fuel cells, batteries, electrolysis and supercapacitors) needs to be improved to enable better use of intermittent renewable electricity sources and the development/deployment of sustainable transport.

In 2000, cars and vans accounted for 7 per cent of global CO<sub>2</sub> emissions. This proportion is rising as economic growth brings the benefits of widespread car use to the world's emerging and developing economies. Under a business-as-usual scenario global road transport emissions would be projected to double by 2050.<sup>19</sup>

According to the King Review,<sup>19</sup> it is essential to invest in renewable electricity generation technologies as well as technologies that allow transport decarbonisation. The realisation of both aims relies on developing energy storage devices that balance intermittent supply with consumer demand and addressing issues associated with security and quality of supply. Major technical challenges need to be met that require research into new areas of science, in particular the chemical sciences.

The major challenge is therefore to improve the performance of energy conversion and storage technologies (fuel cells, batteries, electrolysis and supercapacitors) to enable better use of intermittent renewable electricity sources and the development/deployment of sustainable transport.

Technology breakthroughs required include:

- improving power and energy densities;
- fundamental advances in new cheaper, safer electrode and electrolyte materials with better performance;
- reducing and replacing strategic materials to ensure security of supply (such as for platinum) and developing material recycling strategies.

Developments must be coupled with advances in the fundamental science of surface chemistry, electrochemistry and the improved modelling of thermodynamics and kinetics.

### 4.1.3 Fossil fuels

**Challenge: Current fossil fuel usage is unsustainable and associated with greenhouse gas production. More efficient use of fossil fuels and the by-products are required alongside technologies that ensure minimal environmental impact.**

The amount of the world's primary energy supply provided by renewable energy technologies will grow, but without further breakthroughs in technology, most estimates predict that it is unlikely to provide more than 10 per cent by 2050.<sup>18</sup> Fossil fuels will therefore remain part of our energy mix for some time to come. Currently the world relies on fossil fuels for around 80 per cent of its total energy supply and this energy use is responsible for around 85 per cent of anthropogenic CO<sub>2</sub> emissions.<sup>20</sup> Oil makes up 35 per cent of the total global energy source consumed, followed by 25 per cent gas and 21 per cent coal.<sup>20</sup> If some use of fossil fuels in the future is accepted, it is vital to use fossil fuels and their by-products more efficiently, alongside technologies that will ensure minimal environmental impact.

Crude oil is currently being produced from increasingly hostile environments. Enhanced oil recovery processes and the exploitation of heavy oil reserves require a detailed understanding of the complex physical and chemical interactions between oil, water and porous rock systems, and the development of novel chemical additives to improve water flooding and miscible gas injection. One of the main challenges facing the oil refinery industry is the cost effective production of ultra-low sulfur fuels. Input from the chemical sciences is needed to overcome this issue by developing improved catalysts and separation and conversion processes.

Natural gas has a higher hydrogen/carbon ratio than oil or coal and emits less CO<sub>2</sub> for a given quantity of energy consumed. It leaves virtually no particulate matter after burning. The potential benefits for improving air quality are therefore significant, relative to other fossil fuels. Chemical sciences will have a strategic role to play in up-grading and improving current systems, and in developing new technologies. Technology breakthroughs will be required in: developing cost effective gas purification technologies, improving high temperature materials for enhanced efficiency and performance, and developing advanced catalysts to improve combustion for a range of gas types and for emissions clean-up.

Coal-fired generation should have a long-term role in providing energy diversity and security, providing ways can be found to reduce CO<sub>2</sub> emissions in the longer term, while complying with other short to medium term barriers resulting from tightening environmental restrictions.<sup>18</sup> Short term technical needs in coal-fired power generation relate specifically to the control of SO<sub>2</sub>, NO<sub>x</sub> and carbon in ash. Research should be focused specifically on better 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 deposition. Improved process monitoring, equipment design and performance prediction tools to improve power plant efficiency are also required. Medium term challenges require improved materials for supercritical and advanced gasification plants as well as the development of gasification technologies themselves.

If we continue to use fossil fuels, it is vital that some means of capturing and safely storing CO<sub>2</sub> on a large scale is developed so that targets for CO<sub>2</sub> 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 per cent.<sup>14</sup> Capturing and storing CO<sub>2</sub> safely will rely on the skills of a range of disciplines, including the chemical sciences. The number of technical challenges to achieve CCS on the scale required is formidable. Amine scrubbing is currently the most widely used process for CO<sub>2</sub> capture, but the process is costly and inefficient. Further research is required into alternatives to amine absorption, including polymers, activated carbons or fly ashes for the removal of CO<sub>2</sub> from dilute flue gases. In addition, to optimise storage potential, research into the storage options for CO<sub>2</sub> is needed (such as in depleted gas and oilfields, deep saline aquifers or unmineable coal seams) and an improved understanding of the behaviour, interactions and physical properties of CO<sub>2</sub> under storage conditions is required. Research into the options for CO<sub>2</sub> as a feedstock is required, for example converting CO<sub>2</sub> to useful chemicals (see also section 4.6.4 Recovered feedstocks). To ensure uptake, it is essential that CCS technologies are integrated with new and existing combustion and gasification plants.

#### 4.1.4 Nuclear energy

**Challenge: Nuclear energy generation is a critical medium term solution to our energy challenges. The technical challenge is for the safe and efficient harnessing of nuclear energy, exploring both fission and fusion technologies.**

Nuclear power in 2005 accounted for 16 per cent of global electricity generation.<sup>20</sup> In 2007 nuclear power accounted for 18 per cent of the UK's electricity generation and 7.5 per cent of total energy supplies.<sup>14</sup> It is a low carbon source of electricity and makes an important contribution to the diversity of our energy supplies. Without our existing nuclear power stations, our carbon emissions would have been 5-12 per cent higher in 2004 than otherwise.<sup>21</sup> However, based on published lifetimes most of the existing stations are due to close in the next 15 years. Nuclear energy generation is therefore a critical medium-term solution to our energy challenge and is an important component of the energy mix. The technical challenge is for the safe and efficient harnessing of nuclear energy, exploring both fission and fusion technology.

Current nuclear energy capability uses nuclear fission. To improve further the efficient and safe utilisation of nuclear fission it is necessary to:

- undertake research to advance the understanding of the physico-chemical effects of radiation on material fatigue, stresses and corrosion in nuclear power stations;
- develop improved methods for spent fuel processing, including developing advanced separation technologies to allow unprecedented control of chemical selectivity in complex environments;
- study the nuclear and chemical properties of the actinide and lanthanide elements; and to improve our understanding of radiation effects on polymers, rubbers and ion exchange materials.

In addition, the new generation of advanced reactors, such as those being developed under the banner of Generation IV that use actinide-based fuels, have the potential to deliver step-change benefits. Opportunities exist in the design and demonstration of these new reactors.

In contrast, nuclear fusion is still at the development stage. Despite some progress, the challenge in fusion research is to generate more energy from fusion than is put in. Apart from the continued research into plasma physics, magnetics, instrumentation and remote handling, the development of high performance structural materials capable of withstanding extreme operating conditions is required.

#### 4.1.5 Nuclear waste

**Challenge: The problems of storage and disposal of new and legacy radioactive waste remain. Radioactive waste needs to be reduced, safely contained and opportunities for re-use explored.**

Globally about 270,000 tonnes of spent fuel are currently in storage and 10,000-12,000 tonnes are added each year.<sup>22</sup> The last published UK Radioactive Waste Inventory showed that the UK has approximately 476, 900 cubic metres of radioactive waste currently stored in repositories.<sup>23</sup> Only 0.3 per cent of that waste is considered of high radioactivity or 'high level waste'. The UK has a large variety of nuclear waste due to the different legacy reactors that were built across the country. It includes spent nuclear fuel, plutonium, uranium and general radioactive waste from running and decommissioned nuclear power plants. Published as part of the Managing Radioactive Waste Safely (MRWS) programme the UK's current strategy for dealing with higher activity radioactive waste in the long term is through geological disposal, coupled with safe and secure interim storage.<sup>23</sup>

The storage and disposal of new and legacy radioactive waste pose a number of challenges. Radioactive waste needs to be reduced, safely contained and opportunities for re-use explored. This must be coupled with decommissioning and contaminated land management. Processes for separating and reusing nuclear waste rely on developing areas of reprocessing chemistry, such as

recycling spent fuel into its constituent uranium, plutonium and fission products, and using separation chemistry in nuclear waste streams – for example using zeolites for sorption, membranes, supercritical fluids and molten salts. Improving the understanding of solids formation and precipitation behaviour will be key.

Using wasteform chemistry, which includes the fundamental science of materials used in immobilising nuclear waste, could help solve a number of waste management issues. But new and improved methods and means of storing legacy and new nuclear waste in the intermediate and long term are also required. Storage strategies will necessitate producing new materials, for example with high radiation tolerance. They will also require a greater understanding of the long term ageing of cements used for storage – and their microstructural properties – and understanding waste/cement interactions and the corrosion of metallic components in cement materials. Methods of waste containment for storage in geological sites require further research, as each site will have differences in the geological sub-strata.

The chemical sciences also have a role in developing methods for decommissioning nuclear plants and site remediation, including research into environmental chemistry – such as hydro-geochemistry, radio-biogeochemistry and biosphere chemistry, and methods for the effective and safe post-operational clean-out of legacy facilities.

#### 4.1.6 Biopower and biofuels

**Challenge: Fuels, heat or electricity must be produced from biological sources in a way that is economic (and therefore efficient at a local scale), energetically (and greenhouse gas) efficient, environmentally friendly and not competitive with food production.**

The proportion of solar radiation that reaches the Earth's surface each year is more than 10,000 times the current annual global energy consumption and about 0.2 per cent of it is fixed by plant life. Biomass is thought to contribute over 10 per cent of global primary energy and more than 80 per cent of this is used for cooking and heating in households in developing countries.<sup>20</sup>

In an attempt to alleviate fossil fuel usage and CO<sub>2</sub> emissions, developed nations are turning back to biomass as a fuel source. Crops such as sugar cane can grow very quickly and can fix sunlight with an efficiency of 2 per cent, 10 times higher than the planetary average for wild plants.

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. Biomass currently accounts for just 0.43 per cent of the UK's energy but it is seen as one way of meeting EU targets for reducing CO<sub>2</sub> emissions and increasing the use of renewable energy.<sup>24</sup>

Biomass is therefore a versatile and important fuel, and also a rich feedstock for the chemical industry (see also section 4.6.3 Conversion of biomass feedstocks). The potential for increased exploitation of biomass resources is very large. The chemical sciences have a role to play in producing fuels, heat or electricity from biological sources in a way that is economic (and therefore efficient at a local scale), energetically (and greenhouse gas) efficient, environmentally friendly and not competitive with food production.

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 using current technology. 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 produce appropriate waste products and high-value chemical products or they could be engineered to have more efficient

photosynthesis, increased yields and require lower carbon inputs. There could also be opportunities to develop methods of producing fuel from new sources such as algae, animal or other waste forms.

Biofuels are more expensive than conventional transport fuels<sup>18</sup> but developing improved and novel conversion technologies will broaden the range of feedstocks. For example, the cost effective hydrolysis of lignocelluloses will significantly increase the source of biomass for bioethanol. The drive to increase use of biomass and 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 products, in addition to biofuels. Gasification and thermochemical technologies are also important methods of converting biomass to transport fuels.

The chemical sciences have a significant role to play in improving bio-refinery processes through:

- advancing modelling and analytical methods;
- improving ways of hydrolysing diversified biomass and lignocellulose;
- improving the extraction of high value chemicals before energy extraction;
- developing thermochemical processes including developing better catalysts, microbes and enzymes;
- improving the flexibility of feedstock and output (electricity, heat, chemicals, fuel or a combination).

Breakthroughs also need to be made in developing better pre-treatment technologies to improve the handling and storage of biomass, and ways of managing bio-refinery waste streams so as to minimise environmental impact.

While there are significant opportunities, the challenges are considerable and will require developing novel biomass conversion technologies, a fundamental understanding of the chemistry of biomass production and the tools to measure the impacts of biofuels over the entire life-cycle. This will include analysing potential environmental issues related to impacts of land use change, water demand and biological diversity.

### 4.1.7 Hydrogen

**Challenge: The generation and storage of hydrogen are both problematic. Developing new materials and techniques so that we can safely and efficiently harness hydrogen will be required to enable its use as an energy vector, appropriately scaled to its applications.**

Hydrogen coupled with fuel cell technology offers an alternative to our current reliance on fossil fuels for transport and generating power. Despite the advantages, significant technical challenges exist in developing clean, sustainable, and cost-competitive hydrogen production processes to create a viable future hydrogen economy. Both generating and storing hydrogen are both problematic. The steam methane reforming process is used to produce 95 per cent of all hydrogen extracted today and liberates up to six times as much CO<sub>2</sub> as it does hydrogen.<sup>25</sup> Developing new materials and techniques so that we can harness and use hydrogen safely and efficiently will be required so that it can be used as an energy vector, appropriately scaled to different applications.

Energy is required to produce hydrogen, therefore hydrogen as a fuel is only as clean as the process that produces it in the first place.<sup>18</sup> The long-term goal is renewably produced hydrogen. The preferred renewable options include electrolysis, thermochemical water splitting, biochemical hydrogen generation and photocatalytic water electrolysis; but significant research is required before they 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 need to be made in efficiency by developing improved electrode surfaces for both types of electrolyzers and finding uses for the by-product, O<sub>2</sub>. Photocatalytic water electrolysis uses energy from sunlight to split water into hydrogen and oxygen. R&D must focus on the energetics of the light harvesting system to drive the electrolysis and the stability of the system in the aqueous environment.

Thermochemical water-splitting converts water into hydrogen and oxygen by a series of thermally driven reactions. Developing new heat exchange materials will be necessary to meet the required stability conditions. An improved understanding of fundamental high temperature kinetics and thermodynamics will be essential. Biochemical hydrogen generation is based on the concept that certain photosynthetic microbes produce hydrogen as part of their natural metabolic activities using light energy. To make this viable will require breakthroughs in:

- discovering new microorganisms or genetically modifying existing organisms;
- improving culture conditions for hydrogen production by fermentation or photosynthesis;
- using microorganisms in microbial fuel cells to generate hydrogen from waste and new efficient bio-inspired catalysts for use in fuel cells.

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 an advanced storage system to ensure a vehicle has enough on board to travel a reasonable distance. Technology breakthroughs required for alternative storage options include developing advanced materials, such as carbon nanotubes, or metal hydride complexes.

If hydrogen production and storage can be fully integrated with the development of advanced fuel cell systems for its conversion to electricity (see also section 4.1.2 Energy conversion and storage), it can provide fuel for vehicles, energy for heating and cooling, and electricity to power our communities.

### 4.1.8 Solar energy

**Challenge: Harnessing the free energy of the sun can provide a clean and secure supply of electricity, heat and fuels. Development of existing technologies to become more cost efficient and developing the next generation of solar cells is vital to realise the potential of solar energy**

The sun provides the Earth with energy at a rate of more than 100,000 TW (1 terawatt = 1 trillion watts =  $10^{12}$  W). This corresponds to more energy in an hour than the global fossil energy consumption in a year.<sup>26</sup> 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. There are a variety of technologies that have been developed to take advantage of solar energy. These include photovoltaic systems, concentrating solar power systems, passive solar heating and daylighting, solar hot water, and solar process heat and space heating and cooling. Developing these existing technologies, and specifically the next generation of solar cells, is vital to realising the potential of solar energy.

Solar cells offer an artificial means of utilising solar energy. The current generation of crystalline and amorphous silicon solar cells have efficiencies between 5 per cent and 17 per cent but their fabrication is expensive and consumes a lot of energy. The chemical sciences have a role to play in improving 'first', 'second' and 'third' generation photovoltaic cells.

The breakthroughs required to improve the design of current first-generation photovoltaic cells include:

- developing lower energy, higher yield and lower cost routes to silicon refining;
- lower CO<sub>2</sub>-emission process to the carbo-thermic reduction of quartzite;
- more efficient or environmentally benign chemical etching processes for silicon wafer processing;
- developing base-metal solutions to replace the current domination of silver printed metallisation used in almost all of today's 'first' generation devices.

Improvements to second-generation thin-film photovoltaics, such as amorphous silicon films and dye-sensitised solar cells, include:

- improving the reaction yield for silane reduction to amorphous silicon films and improving the efficiency of dye-sensitised solar cells;
- research into alternative materials and environmentally sound recovery processes for thin cadmium-containing films on glass and alternatives to indium;
- developing processes to improve deposition of transparent conducting film on glass.

The challenge for third-generation photovoltaic materials based on molecular, polymeric and nano-phase materials is to make the devices significantly more efficient and stable, and suitable for continuous deposition on flexible substrates.

The cost of photovoltaic power could also be reduced with advances in developing high efficiency concentrator photovoltaics (CPV) systems and improving the concentrated solar power (CSP) plants used to produce electricity or hydrogen. New thermal energy storage systems using pressurised water and low cost materials will enable on-demand generation day and night.

Breakthroughs will be required in developing the next generation of technologies that take advantage of biological methods of harvesting and storing energy from light. There is the potential to explore the idea of transferring concepts from natural photosynthesis to solid state devices. Research aimed at mimicking photosynthesis, but with increased efficiency over nature, to generate hydrogen or carbohydrates is required. The potential of artificial photosynthesis is huge as it offers a route to sustainable hydrogen production and also potentially to a process that removes CO<sub>2</sub> from the atmosphere and creates useful products. This must be linked to developing light harvesting, charge separation and catalyst technology. Another area of development is improving photobioreactors and photosynthetic organisms (algae and cyanobacteria) for generating hydrogen or for processing to biofuels (see also section 4.1.6 Biopower and biofuels).

#### 4.1.9 Wind and water

**Challenge:** Since power generation yields from tide, waves, hydro and wind turbines are intermittent and geographically restricted, effective energy supply from these natural world sources needs further development to minimise costs and maximise benefits.

Although in 2004 wind contributed only 0.5 per cent of global energy, its potential greatly exceeds this.<sup>20</sup> A 2 MW wind turbine in the UK will generate over 5.2 million units (kWh) of electricity each year. That is enough to make 170 million cups of tea, to run a computer for 1620 years, or to meet the electricity demands of more than 1100 homes.<sup>27</sup> With 3.1 GW of installed wind capacity, the UK is currently ranked fifth in Europe, which is the equivalent of running nearly two million UK homes on 'green' energy.

As an island nation with the best coastal resources in Europe it should be no surprise that the UK's emerging wave and tidal energy sector is a world leader.

The Carbon Trust *Future marine energy* report estimates that between 15 and 20 per cent of current UK electricity demand could be met by wave and tidal stream energy.<sup>28</sup> Around 1.3 GW of generating plant could be installed by 2020 and this would lead to significant industry expansion in the following decades.

Because power generation yields from tide, waves, hydro and wind turbines are intermittent, and geographically restricted, effective energy supply from these natural sources needs further development to minimise costs and maximise benefits.

In terms of wind energy, materials science will clearly play an important role in developing coatings, 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. Corrosion will also be a problem for offshore turbines exposed to salt, air pollution and UV radiation. The continued development of advanced long lasting protective coatings is required to reduce maintenance costs and prolong the operating life of wind energy devices.

To exploit fully the possibilities of electricity production from wave and tidal sources, further advances are required in the most developed ocean technologies including tidal barrages, tidal current turbines and wave turbines. This must be coupled with breakthroughs in less developed technologies that rely on salinity-gradient energy, also called blue energy, which work either on the principle of osmosis (the movement of water from a low salt concentration to a high salt concentration) or electro dialysis (the movement of salt from a highly concentrated solution to a low concentrated solution). This requires further developments that reduce the cost or improve the efficiency of membranes to significantly improve the economics of this process. Like wind energy, corrosion is also a problem for wave and tidal energy and will require the continued development of advanced long lasting protective coatings, to reduce maintenance costs and prolong operating life.

## ENERGY: FUNDAMENTAL SCIENCE CASE STUDY

### Photovoltaics

*One hundred and seventy years of research into fundamental photochemistry, theoretical physics, and new materials has resulted in a \$15 billion photovoltaic industry that is still growing and cleaning up the way the world produces energy.*

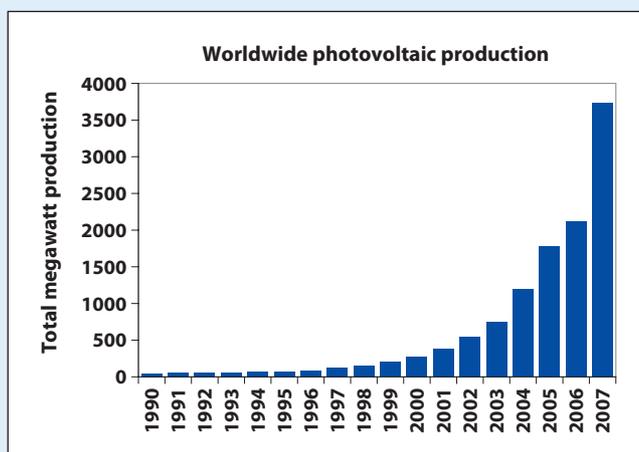
Photovoltaics, commonly known as solar cells, are used to harness energy from light. The first photovoltaic or solar cells were made in 1876 and were used by the emerging photographic industry in photometric light meters.

The history of photovoltaics can be traced back to 1839 when Alexandre-Edmond Becquerel conducted intensive fundamental research into phosphorescence, luminescence and photochemistry. Becquerel discovered the photovoltaic effect, a physical phenomenon that allows light–electricity conversion. He found that illuminating a beaker of dilute acidic liquid containing two metal electrodes produced a voltage. Further experimentation with wet cell batteries led to his eventual discovery that when metal electrodes are directly exposed to the sun, conductance increases significantly.

In 1896 Adams and Day studied the photovoltaic effect in solids by illuminating a junction between selenium and platinum.<sup>29</sup> They built the first photovoltaic cells from selenium which were just 1–2 per cent efficient. However, it was not until 1904 that quantum mechanical theory was conceived and a theoretical explanation of the photovoltaic effect was published by Albert Einstein.

In 1918 Jan Czochralski laid down the foundation for the formation of the first monocrystalline silicon photovoltaics. Czochralski accidentally discovered a technique for growing perfect single crystals when he dipped his pen into a crucible of molten tin rather than his inkwell. He immediately pulled it out to find that a thin thread of solidified metal was hanging from the nib.<sup>30</sup> Czochralski reproduced the technique using a capillary tube and was able to verify that the crystallised metal was a single crystal. This method for monocrystalline production was used in 1941 for the first generation of monocrystalline silicon photovoltaics,<sup>31</sup> and the same technique continues to dominate the photovoltaic industry today.

In 1932 further research into the properties of new materials led to the discovery of the photovoltaic effect in cadmium selenide (CdSe). CdSe remains an important material for modern day solar cells.



The increase in PV production from 1990 to 2007 (Kazmerski, National Center for Photovoltaics, USA)

Modern solar electric power technologies came about in 1954 when Bell Laboratories' experimentation with semi-conductors unexpectedly found silicon doped with certain impurities was very sensitive to light. The end result was the invention of the first practical solar modules with an energy conversion efficiency of around six per cent.

Photovoltaic cells continue to improve in efficiency (15 per cent efficiency cells are widely used today). This \$37 billion industry<sup>32</sup> is experiencing staggering growth because concerns over fuel supply and carbon emissions have encouraged governments and environmentalists to become increasingly prepared to off-set the extra cost of solar energy. Currently photovoltaics are around four times too expensive to compete with hydrocarbon fuels and therefore only generate a small part of total renewable energy supply. However, they offer by far the biggest potential to overcome the global energy crisis, because more energy from sunlight falls on the Earth every hour than is consumed in a whole year. Since their discovery, photovoltaics have developed to be used extensively in applications ranging from powering space satellites, parking meters and street lighting, to use in everyday objects such as calculators, watches and torches.

***“Sooner or later we shall have to go directly to the sun for our major supply of power. This problem of the direct conversion from sunlight into power will occupy more and more of our attention as time goes on, for eventually it must be solved.”***

**Edison Pettit, Wilson Observatory, 1932**

## 4. 2 Food

### Creating and securing a safe, environmentally friendly, diverse and affordable food supply.

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 by 1.7 billion to over eight billion.<sup>1</sup> 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, without permanently damaging the environment, is the greatest technological challenge humanity faces. The application of chemistry and engineering is a key part of the solution. This section looks at the opportunities that exist for the chemical sciences to supply healthy, safe and affordable food for all. The main challenges concern agricultural productivity, healthy food, food safety, process efficiency and supply chain waste.

#### 4.2.1 Agricultural productivity

**Challenge: 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.**

To meet the Millennium Development goals on hunger a doubling of global food production will be required by 2050.<sup>33</sup> This increase in food production is exacerbated by economic growth in the emerging 'BRIC' economies of Brazil, Russia, India and China. 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 products. The World Bank estimates that cereal production needs to increase by 50 per cent and meat production by 80 per cent between 2000 and 2030 to meet demand.<sup>34</sup> Furthermore, it estimates that by 2025 one hectare of land will need to feed five people whereas in 1960 one hectare was required to feed only two people.<sup>35</sup> 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.

#### Pest control

Up to 40 per cent of current agricultural outputs would be lost without effective use of crop protection chemicals.<sup>36</sup> Agriculture is facing emerging and resistant strains of pests. It is therefore essential that new crop protection strategies, chemical and non-chemical, are developed.

Research should be done into new high-potency, targeted agrochemicals with new modes of action that are safe to use, overcome resistant pests and are environmentally benign. New pest-specific biochemical targets will have to be identified and a more thorough understanding of the physico-chemical factors required for optimal agrochemical bioavailability. Computational and predictive tools developed for drug design could also be applied directly in designing agrochemicals. Other areas of interest include pest control strategies that use pheromones, semiochemicals and allelochemicals as starting points are also of interest.

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

The reliance of crop production on chemical protection strategies, for example agrochemicals, could be reduced by harnessing the full potential of modern biotechnology. Crops are being developed that are resistant to attack by pests and to environmental stresses, including drought and salinity.

## Plant science

Higher crop yields and controlling secondary metabolism should be sought through a better understanding of plant science.

Improving the efficiency of nutrient uptake and utilisation in plants is a major challenge in agricultural productivity. This must begin with improving the understanding of the roles of macro- and micro-nutrients together with carbon, nitrogen, phosphorus and sulfur cycling to help optimise nutrient sequestration. In addition, research should be undertaken to improve our understanding of the roles plant growth regulators can play in modulating plant water and nitrogen use efficiency. Similarly, a better understanding of plant biochemical signalling could facilitate the development of new crop defence technologies, with positive implications for crop yields.

A greater understanding of these and other areas should be exploited by biotechnology to generate, for example, transgenic crops with improved efficiency in nitrogen or water, or crops with improved yields of components desirable for producing biofuel and feedstock.

## 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. This should also include an understanding of the mechanical properties of soils and the flow of nutrients.

A lack of information on agro-ecology is a major barrier to the adoption of sustainable agriculture practices worldwide. Research should be done to improve the understanding of the biochemistry of soil systems. Specific examples include the chemistry of nitrous oxide emissions from soil and the mobility of chemicals within soil. Additionally, improved understanding of methane oxidation by soil methanotrophic bacteria would help in developing methane-fixing technologies. There is also scope for optimising how fertilisers are used. Fertilisers should be formulated to improve soil nitrogen retention and uptake by plants. Furthermore, low energy synthesis of nitrogen and phosphorus-containing fertilisers would increase the sustainability of agricultural production by reducing indirect input costs and resource requirements.

## Water

Maintaining an adequate, quality water supply is essential for agricultural productivity. 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'). Water-related challenges are dealt with in greater detail in section 4.7.

## Effective farming

To meet growing demand, agricultural productivity will need to be increased, minimising inputs and maximising outputs through sharing best agronomic practice. The universal implementation of existing and new technologies will result in greater productivity, and increased precision at the field level will impact positively on agricultural efficiency.

Chemical science will play a pivotal role in developing rapid *in situ* biosensor systems and other chemical sensing technologies. These sensors can be used to monitor a wide range of parameters, including soil quality and nutrients, crop ripening, crop diseases and pests, and water availability. This will allow farmers to pinpoint nutrient deficiencies, target agrochemical applications and improve the quality and yield of crops.

Tracking and understanding the impact of climate change parameters will facilitate the development of predictive climatic models, thus identifying changing conditions for agronomy and providing valuable data for the planting and targeted treatment of crops.

Improved engineering tools will result in greater efficiencies in on-farm practices such as grain drying, seed treatment and crop handling and storage.

## Livestock and aquaculture

In addition to crops, global livestock production faces enormous short-term challenges. Total world 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 2020.<sup>37</sup> Technologies are needed to counter the significant environmental impact and waste associated with rearing livestock.

Disease in farmed animals should be tackled with research into veterinary medicine, for such as developing effective vaccines. Nutrigenomics must be used to understand and guide improvements in efficient feed conversion. Modern biotechnology should be used to improve disease resistance, feed conversion and carcass composition.

Most wild fisheries are at or near their maximum sustainable exploitation level.<sup>38</sup> In 2004 43 per cent of the global fish supply already came from farmed sources.<sup>39</sup> The inevitable growth of aquaculture will involve further intensification. The chemical sciences will be able to provide improvements in productivity, modifications of the cultivated organism and disease control. Few effective drugs are available for treating diseases in fish because of environmental concerns and a relative lack of knowledge about many fish diseases.

### 4.2.2 Healthy food

**Challenge: We need to better understand the interaction of food intake with human health and to provide food that is better matched to personal nutrition requirements.**

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.<sup>40</sup>

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 obesity. In 2006 24 per cent of adults (aged 16 or over) in England alone were classified as obese.<sup>41</sup> 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/parallel supplies of 'healthier foods' with an improved nutritional profile. One of the main challenges is to produce food that reduces the fat, salt and sugar components that can be detrimental to health, while maintaining the customers' 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.

To achieve this requires technology breakthroughs such as:

- a better understanding of formulation science for controlled release of macro- and micro-nutrients and removing unhealthy content in food;
- novel satiety signals, for example, safe fat-replacements that produce the taste and texture of fat;
- producing sugar replacements and natural low calorie sweeteners to improve nutrition and combat obesity;
- using the glycaemic load of food in understanding nutrition and the role of glucose in health and the onset of type II diabetes;
- understanding the role of gut micro flora and probiotics, and prebiotics, in promoting health;
- developing and understanding fortified and functional food with specific health benefits, including minor nutrients.

Modern GM applications could be used to provide crops that are modified to meet specific nutritional shortfalls.

Research into the design of functional foods will need to be combined with *in vivo* approaches or techniques for evaluating their behaviour in the digestive tract. Similarly, nutrient requirements depend on factors including genetics. The availability of rapid methods in genomics, proteomics and metabolomics is allowing the study of the impact of gene expression in individuals, and individuals' genetic sensitivity to food intake. Nutrigenomics and nutrigenetics are also being used to provide routes to improved personal nutrition.

### 4.2.3 Food safety

**Challenge: Consumers need to be given 100 per cent confidence in the food they eat.**

Foodborne pathogens are a significant cause of global health problems. In England and Wales in 2000, the number of cases of foodborne illness was estimated at 1.34 million; there were 20,800 hospitalisations and 480 deaths.<sup>42</sup> In the EU campylobacteriosis remained the most frequently reported zoonotic disease in humans, with 175,561 confirmed cases in 2006.<sup>43</sup> In addition to zoonoses, physical, chemical and radiological contaminants can also pose risks to consumers.

Critical food hygiene and safety issues include those associated with microbiological contamination – the most common cause of health problems for consumers. This can be caused by poor hygiene at any stage of the food chain. This includes food spoilage caused by bacteria and fungi, which may secrete by-products that can be highly toxic, and via counterfeiting and adulteration, which can significantly undermine consumers' trust in the quality and safety of branded foods.

The chemical sciences have a role to play in both the detection and control of hygiene issues and food safety. Irradiation can be used to remove bacterial pathogens and prevent food spoilage. Technology breakthroughs in real-time screening and sensors are necessary to support rapid diagnostics to detect contaminants and ensure food authenticity and traceability; this includes detection of chemicals, allergens, toxins, veterinary medicines, growth hormones and microbial contamination of food products and on food contact surfaces. Technologies could be extended to address domestic food hygiene through visible hygiene indicators. More efficacy testing and safety of new food additives, such as natural preservatives and antioxidants is required, as is an understanding of the links between diet and diseases such as cancer. Further research should be done 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.

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. These might include microsensors to measure food quality, safety, ripeness and authenticity and to indicate when the 'best before' or 'use-by' date has been reached.

### 4.2.4 Process efficiency

**Challenge: 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.

#### Food manufacturing

To achieve the process efficiency goal, one of the main challenges is to build highly efficient and sustainable small scale manufacturing operations. This will require improvements in operational efficiency throughout the entire manufacturing process as materials are received, stored and transferred. Requirements include:

- intensifying food production by scaling down and combining process steps;
- improving process control to raise production standards and minimise variability;
- routes for by-product and co-product processing to reduce waste and recover value;
- milder extraction and separation technologies with lower energy requirements;
- technologies to minimise energy input at all stages of production, such as high pressure processing and pulsed electric fields;
- optimising the forces needed to clean food preparation surfaces in conjunction with developing new anti-fouling surface coating technologies to minimise energy requirements for cleaning;
- methods for synthesising food additives and processing aids;
- a greater understanding of inhibition of the chemistry of food degradation, and chemical stabilisation technologies for produce, including formulation and delivery.

In addition, 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.

## Food distribution

The chemical sciences also have a role to play in developing advanced storage technologies and in optimising methods to distribute foods with minimal energy requirements and environmental impact. In terms of storage, breakthroughs will be required in:

- 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;
- ambient storage technologies for fresh produce;
- improving food preservation methods for liquids and solids, including rapid chilling and heating and also salting.

In terms of distribution, the biggest opportunity for the chemical sciences lies in sustainable and efficient transport (see also section 4.3.5 Mobility). While shorter supply chains through local sourcing can cut emissions this must be balanced against possible increases in other emissions 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. Optimising food distribution will also require analytical techniques to ensure quality measurement and control of foodstuffs in transit.

## 4.2.5 Supply chain waste

**Challenge: There is an unacceptable amount of food wasted in all stages of the supply chain. We need to find ways to minimise this or use it for other purposes.**

The UK food industry alone accounts for about 10 million tonnes per year (10 per cent) of industrial and commercial UK waste.<sup>44</sup> Packaging and food waste are the two most significant waste issues for the industry. The main challenge is to find ways to minimise this waste or, within the context of lifecycle analyses, use it for other purposes.

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. These might include flexible thin films made from corn starch, polyacetic acid or cellulosic materials, which can withstand the chill-chain, handling and storage. There is also the possibility of developing food packaging that is compatible with anaerobic digesters.

There are many potential uses for food waste, including producing high value biochemicals, compost and energy. The chemical sciences have a role to play in:

- the efficient extraction and application of valuable ingredients from food waste and refinement to high value products, for example enzymes, hormones, phytochemicals, probiotics cellulose and chitin;
- using waste products as feedstock for packaging material, for example producing novel biodegradable plastic materials made from epoxides and CO<sub>2</sub>;
- efficient anaerobic treatment plants to process farm, abattoir and retail waste, thus generating renewable energy from biomass in the form of biogas.

## FOOD: FUNDAMENTAL SCIENCE CASE STUDY

### Saccharin

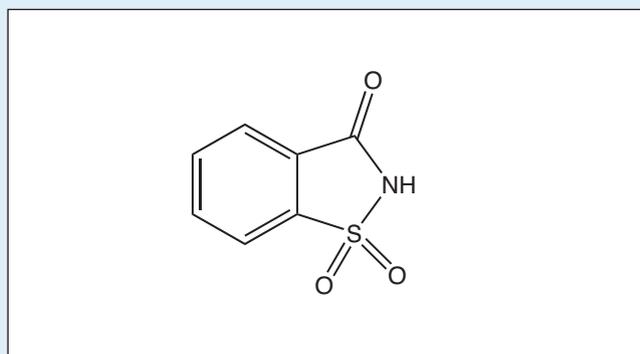
*Basic research into the chemical reactivity of toluene over a hundred years ago led to the serendipitous discovery of the world's first artificial sweetener; the global sweetener market is now worth \$1.1 billion.*

Saccharin was the first artificial sweetener to be discovered and it represented a significant development in the use of artificial chemicals to control the human diet. Saccharin is 300 times sweeter than sugar and as it is not metabolised by the body it has no calorific value.

Saccharin was discovered in 1879 by Constantin Fahlberg, a researcher in Ira Remsen's lab at Johns Hopkins University, US. Fahlberg. He was investigating the fundamental reactivity of toluene, a chemical found in coal tar. As toluene provides a useful starting point for generating synthetic chemicals, Fahlberg and Remsen were curious about what new compounds they could make. At dinner one evening, Fahlberg had not thoroughly washed his hands after leaving the lab, and realised that he had a very sweet taste on his hands. He was able to trace the taste back to a new compound that he had synthesised: benzoic sulfinide.<sup>45</sup> Fahlberg was excited by the prospect of this new chemical and published a paper on the subject with Remsen. However, although Remsen was curious he did not show interest in commercialising the product and Fahlberg alone patented the compound as 'saccharin'.

Saccharin was produced commercially in Germany from 1886, initially as a food preservative and later marketed for diabetics. The company Monsanto was set up in 1901 by a drug salesman who saw the potential market in the US and started trading with saccharin as his first product. Saccharin was seen as such a threat by the sugar industry that sugar manufacturers lobbied governments to regulate its use. However, it was not until the sugar shortages of WWI that it became widespread; saccharin use increased further during WWII.

A more efficient synthesis was developed by chemists in the 1950s that used anthranilic acid rather than toluene as the starting material, and the popularity of saccharin continued to grow through the 1960s. Health concerns over saccharin have been raised during its history but research has now shown that it is not harmful and it is approved by the UK Food Standards Agency.



Structure of Saccharin

Saccharin has a long shelf life and is stable when heated, which makes it an ideal cooking ingredient. Furthermore, to achieve the same amount of sweetness saccharin is 20 times cheaper than the natural sugar sucrose.<sup>46</sup> These attributes mean that although other artificial sweeteners have been discovered, saccharin is still in widespread use today.

Artificial sweeteners have been useful in times of natural sugar shortage, but also have additional benefits. Saccharin can be used to reduce calorie and sugar intake while still making enjoyable sweet foods; therefore it is particularly valuable for diabetics and calorie-controlled diets, for example, saccharin is the active compound in Sweet'N Low sweetener. Unlike sugars, artificial sweeteners do not promote tooth decay and saccharin is routinely used to sweeten toothpaste and mouthwash. Although Saccharin is the oldest of all the artificial sweeteners and has been used for over 100 years it still shares around 10 per cent of the \$1.1 billion global sweetener market. Its valuable properties mean that saccharin use is also likely to continue in the foreseeable future.

## 4.3 Future cities

### Developing and adapting cities to meet the emerging needs of citizens

Half of humanity now lives in cities, up from 30 per cent in the 1950s, and within two decades, nearly 60 per cent of the world's people will be urban dwellers. Urban growth is most rapid in the developing world where cities gain an average of five million residents every month.<sup>47</sup>

The challenges that have to be faced in providing enough food, water, shelter, energy and security are huge, especially when exacerbated by climate change.

This section looks at the role for chemists in addressing the challenges cities face due to the pressures they place on resources, concerning: their creation and continued growth, energy generation and use in buildings and homes, public safety and security, ICT, and transport.

#### 4.3.1 Resources

**Challenge: Cities place huge demands on waste, water and air quality management. We need technologies that help provide healthy, clean, sustainable urban environments.**

Many cities already live beyond their means and their ecological footprint is enormous. Cities cover only two per cent of the Earth's surface, but they use 75 per cent of the planet's natural resources.<sup>48</sup> These include fresh water, fuels, land, food, construction materials and raw materials. The chemical sciences have a role to play in reducing the ecological footprint through reducing the tendency for cities to transfer environmental costs to its surroundings, reducing resource use and reducing waste.

There is a need for technologies that provide healthy, clean, sustainable urban environments. As cities expand, air pollutant emissions are likely to increase dramatically. Measuring and understanding air pollution provides a sound scientific basis for its management and control. Technological advances need to be made in developing low cost, localised sensor networks for monitoring atmospheric pollutants, which can be dispersed throughout developed and developing urban environments. This must be coupled with improving catalysts for destroying pollutants and converting greenhouse gases with high global warming potential to less harmful products.

Waste is a serious issue for cities. Population, urbanisation and affluence are linked to waste generation and high income countries generate more waste per capita than low income countries.<sup>49</sup> The EU generates 1.3 billion tonnes of waste each year, equivalent to 3.5 tonnes of solid waste per capita.<sup>50</sup> The UK generates about 100 million tonnes of waste from households, commerce and industry<sup>51</sup> and uses over five million tonnes of plastic each year.<sup>52</sup> The majority of all waste is deposited in landfill sites. The chemical sciences have an important role to play in reducing, recycling, re-using and disposing of waste. For example, recycling plastics is problematic due to the wide variation in properties and chemical composition among the different types of plastics. Adopting current and evolving technologies in pyrolysis, catalytic conversion, depolymerisation and gasification for recycling plastic waste into fuels, monomers, or other valuable materials could significantly reduce this burden; as will developing plastic derivatives from non-petrochemical based materials, such as corn starch.

The technological breakthroughs required to reduce the burdens placed on food, energy, raw materials and water are covered in their respective sections. The role of the chemical sciences in reducing the pressures that buildings and transport place on the ecological footprint of cities are referred to in sections 4.3.3 Home energy use and 4.3.5 Mobility.

### 4.3.2 Home energy generation

**Challenge:** Most homes rely upon inefficient energy technologies. We need to develop new technologies and strategies for local (home) energy generation and storage with no net CO<sub>2</sub> emissions.

Projections for global carbon emissions from buildings, including electricity use, is predicted to rise from 8.6 GtCO<sub>2</sub> in 2004 up to 15.4 GtCO<sub>2</sub> by 2030, contributing around 30 per cent of total emissions.<sup>53</sup> Most homes rely upon inefficient energy technologies. Forty per cent of total UK carbon emissions come from buildings and the largest contributor to this total is our homes, with domestic property accounting for 27 per cent of total UK carbon emissions.<sup>54</sup> Technological advances and resource management techniques have now made it possible to cut energy consumption by up to 90 per cent.<sup>3</sup> If in addition energy efficient buildings can draw their energy from zero or low carbon technologies, and therefore produce no net carbon emissions from all energy use, it will be possible to reduce the environmental impact of homes to virtually zero.

A range of renewable energy technologies already exist, including solar, offshore wind, wave and tidal stream, and geothermal energy. Some domestic energy generation technologies are tried and tested, such as using solar photovoltaic cells, to generate electricity. However, technology breakthroughs are needed to maximise cost effective energy collection from the sun, and opportunities also exist for developing domestic versions of other alternative energies. Renewable energy is covered in more depth in section 4.1.

With the wider use of renewable resources the need for energy storage will increase by orders of magnitude. Superior battery technology and alternative energy storage approaches with high energy density optimisation, flexibility and portability will be required to sustain a continuous supply of energy. Energy needs to be stored at times of high generation for release at times of high demand. To achieve this, the technology breakthroughs required include superior electrodes, electrolytes and fuel cells. Developments in materials chemistry will also be pivotal in driving the breakthroughs needed for micro-sized batteries and for mobile and portable devices. Energy storage is also covered in detail in section 4.1.

### 4.3.3 Home energy use

**Challenge:** Current and evolving technologies could significantly reduce the burden of buildings/homes on energy consumption.

Space heating corresponds to about 30 per cent of residential building energy use in both the US and China, with water heating the next greatest single energy use.<sup>48</sup> In developing countries traditional biomass is still commonly used for heating and cooking and these uses represent 80 per cent of global biomass use.<sup>20</sup> In western countries the energy used to heat residential and commercial buildings alone represents around 43 per cent of total energy use, generating the second highest amount of greenhouse gases after transportation. A typical family with two children spends 70 per cent of its yearly energy consumption in the home.<sup>3</sup> Current and evolving technologies in energy efficiency and use can significantly reduce this burden, and are central to efforts to mitigate climate change.

The chemical sciences already contribute to developing and installing energy efficiency measures in homes. However, to make a significant step change technology breakthroughs are required. These include:

- superior building materials (see also section 4.3.4 Construction materials);
- nanocoatings for decorations;
- photochromic coatings for glass;
- the integration of intelligent ICT components and sensors requiring new conductive/non conductive polymers and flat lightweight displays, that are able to respond to changes in temperature and light intensity.

This will need to be coupled with improved energy efficiency of household appliances, lighting, heating and cooling. Technologies such as LEDs and OLEDs based on conjugated polymers with nanoscale controlled deposition on thin films, along with integration into products like self cleaning surfaces, will be key.

#### 4.3.4 Construction materials

**Challenge:** We need to use materials for construction (such as for roads and buildings), which consume fewer resources in their production, and confer additional benefits in their use, and may be used for new build and for retrofitting older buildings.

Each year, 420 million tonnes of materials are used in construction in the UK. The construction and demolition industries produce over four times more waste than the domestic sector, over a tonne per person living in the UK.<sup>55</sup> The environmental impact of extracting, processing and transporting these materials and then dealing with their waste are major contributors to greenhouse gas emissions, destroying habitats and depleting resources. For example, concrete is used throughout the world and contributed to around 5 per cent of global CO<sub>2</sub> emissions in 2003.<sup>56</sup> Consumption of concrete is growing by about 2.5 per cent per year, with the majority of growth occurring in developing countries.<sup>51</sup>

Chemical science has a role in developing construction materials, such as for roads and buildings *etc.*, which consume fewer resources in their production, confer additional benefits in their use and can be used for new buildings and for retrofitting older buildings. The technology breakthroughs required for this include:

- developing superior building materials for designing new buildings and structures, and retrofitting older buildings;
- developing intrinsically low energy materials, for example low temperature/low CO<sub>2</sub> emission cement compositions based on recycled materials;
- reduced dependence on strategic materials;
- developing recycling methodologies.

The environmental impact of the materials used in a house's construction account for just 2–3 per cent of the UK's CO<sub>2</sub> emissions, whereas domestic household energy consumption accounts for 27 per cent.<sup>45</sup>

The chemical sciences already contribute to the development and installation of energy efficiency measures in households (see also section 4.3.3 Home energy use). However, to make a significant step change these technologies must be coupled with breakthroughs in developing superior building materials. Materials that provide improved insulation are available today but new materials will significantly increase performance, for example new high performance insulating materials, including aerogel nanofoams.

Eco-efficiency in the home will also be achieved with technology breakthroughs in:

- the development of building materials that are also functionalised to offer additional benefits, for example, building materials/surfaces that decompose volatile organic compounds;
- functional textiles with superior energy balance;
- the development of flexible anechoic building materials to provide non-flammable sound insulation and reduce urban stress.

### 4.3.5 Mobility

**Challenge: Urban transport is fuel inefficient and environmentally damaging. Enormous societal benefits will flow from scientific and technological solutions to these problems.**

Urban transport is fuel inefficient and environmentally damaging. In 2004 transport made up 23 per cent of global emissions, of which almost three quarters was produced by road transport.<sup>57</sup> Total energy use and carbon emissions are predicted to rise to 80 per cent more than current values by 2030. One factor contributing to this rise will be the increased transport energy use of non-OECD countries, from 36 per cent to 46 per cent by 2030. Tackling CO<sub>2</sub> emissions from transport is therefore an increasingly important part of a strategy to avoid climate change and enormous societal benefits will therefore flow from scientific and technological solutions to these problems.

To reduce emissions there will need to be significant developments and advances in the materials and components used in conventional vehicle design, allowing for a two or threefold improvement in fuel economy. The chemical sciences have a vital responsibility to progress developments in lightweight and safe vehicles.

The technology breakthroughs required in this area include:

- developing innovative elastomeric and thermoplastic products for structural parts (thermoplastic foams, organic fillers based-thermoplastic composites), including alternative assembly and disassembly methodologies that don't compromise safety;
- new tyre technologies;
- engine oils and additives that save fuel;
- ceramic engine technology that reduces engine wear and friction;
- developing improved sensor technologies for engine management and pollution/emission gas detection.

Alongside this, eco-efficient hybrid vehicles will require new energy storage systems (enhanced lithium batteries and supercapacitors), which provide the required power peaks during acceleration and energy recovery during braking.

### 4.3.6 ICT

**Challenge: Public and business demand outstrips the current capacity of the existing ICT infrastructure, creating opportunities for the successful commercial application of technological innovations.**

Public and business demand outstrips the current capacity of the existing ICT infrastructure, creating opportunities for the successful commercial application of technological innovations. The chemical sciences have a role to play in data storage, miniaturisation for device size and speed, power management and in the reducing, recycling and reusing materials.

New applications, more complex business analytics and the need to meet regulatory requirements stimulate demand for developing materials and technologies, which are able to deliver ultrahigh density and ultrafast data storage. The chemical sciences have a role to play in meeting these requirements, through developing highly innovative storage options. The technological breakthroughs in this area include developing information storage holographics by using new molecular and polymeric materials, along with DNA- and protein-based biological switches, molecular switches, and photoresponsive devices.

As computing speeds and power consumption continue to increase, increased focus will be placed on power management: reducing power consumption by switching off components that are not being used and rapidly activating the same components when necessary. Because batteries and power supplies are very slow, ultrafast capacitors will be needed. This will require research into identifying mechanisms for self-assembling low resistance interconnects and high-k dielectric materials with low electrical leakage.

With process geometries approaching physical limits and the adoption of new materials, there will be fundamental changes in the concepts and design of integrated circuits to ensure future electronic devices will be smaller, operate faster and be cheaper to produce. Fundamental research is required, particularly into the materials that will be needed in future devices. Research must be done into:

- integrating nanostructures in device materials;
- self-assembling biological and non-biological components to produce complex devices such as biosensors, memory devices and switchable devices;
- selecting polymers for high density fabrication that meet resolution, throughput and other processing requirements;
- printed electronics;
- high density, low electrical resistance interconnect materials to enable ultra high speed, low power communication.

### 4.3.7 Public safety and security

**Challenge: Technology must increase its role in ensuring people feel and are safe in their homes and the wider community. High population densities increase the potential impact of environmental and security threats.**

High population densities increase the potential impact of environmental and security threats. Technology must increase its role in ensuring people feel and are safe in their homes and the wider community. Defence and national security does not fall under the remit of this project.

Developing effective and rapid analytical techniques for the early detection of a wide range of potential environmental and security threats is essential. Chemical and biological sensors need to be developed that are remote, rapid, miniaturised and reactive. Opportunities exist for developing sensor networks, such as a chemical analogue of CCTV that could trace chemical and biological threats, narcotics, explosives and potential pandemics. Similar technologies could be adapted for use as home security networks.

To make this a reality technological breakthroughs are required in developing nano-structured materials that can achieve sensitivity and selectivity for detecting minute sample quantities. The ability to analyse and detect a multiple number of species, including both inorganic and organic species in one sensor, is the goal but achieving this will require significant research effort. The ability to detect potential threats must be coupled with the development of decontamination and remediation technologies.

Advances in detecting crime require technological breakthroughs that can provide evolutionary, real-time information-rich crime scene profiles. This must be coupled to advances in chemical biometrics for example DNA profiling and fingerprint technology, and advances in 'Lab on a chip' technology. Increases in the amount of information generated at a scene will require advances in methods of data storing and handling, for example chemometrics. Developments of this nature will require breakthroughs in ICT (see section 4.3.6 ICT) and in advanced and sustainable electronics (see section 4.5.4).

The growth and proliferation of counterfeit products, which are of inferior quality and are potentially dangerous, pose an additional threat to people. Novel technologies are required to identify counterfeit products, including pharmaceuticals, money and high value products. This will necessitate advances in analytical and materials chemistry.

In addition to developing technologies for detecting and preventing environmental and security threats, the chemical sciences have a role in developing high performance protective materials for those involved in civil protection, such as the police. This will require advances in materials science (see section 4.5.5 Textiles).

## FUTURE CITIES: FUNDAMENTAL SCIENCE CASE STUDY

### DNA fingerprinting

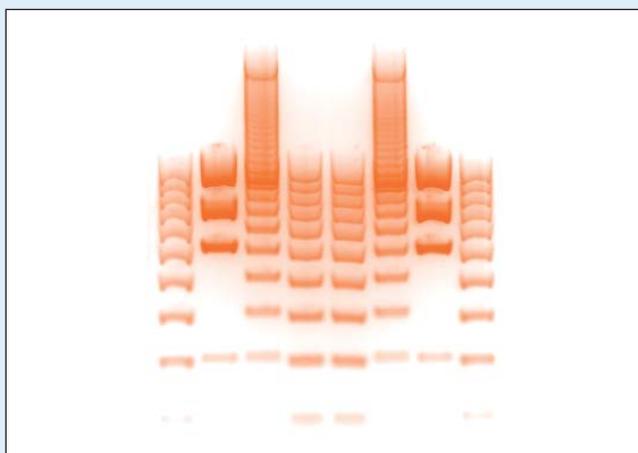
*The elucidation of the structure of DNA in the 1950s and the development of the polymerase chain reaction (PCR) were major breakthroughs in fundamental science that have led to DNA fingerprinting and a safer, more secure society.*

A DNA fingerprint is unique for every individual and consequently DNA fingerprinting is rapidly becoming the primary technique employed by forensic scientists for identifying and distinguishing individual human beings. DNA fingerprinting has become an indelible part of society, helping to prove innocence or guilt in criminal cases, resolving immigration arguments and clarifying paternity.

DNA fingerprinting is built upon several decades of fundamental research into the properties of DNA and advances in molecular techniques. A major breakthrough was the elucidation of the structure of DNA in 1953, involving the work of Watson, Crick, Wilkins and Franklin.<sup>58</sup> Another essential development was the invention of gel electrophoresis, a method of separating DNA molecules according to their size.

DNA fingerprinting is the analysis of regions of the human genome that are highly variable between individuals. This ensures that one person can be clearly identified from another. As all individuals' genes are very similar they are not an appropriate target for DNA fingerprinting. However, during the 1970s Alec Jeffreys showed that some regions of the human genome in between genes contain many short repeated sequences. Importantly for DNA fingerprinting, he found that the number of repeats is inherited between generations and that the overall number of repeats varies between people. Repeats such as these are found at many sites throughout the genome. By analysing the number of repeats at different sites you can construct a DNA fingerprint.

By the end of the 1980s, DNA fingerprinting had established itself as an international gold standard for genetic testing. However, the technique was slow and not very sensitive; the polymerase chain reaction (PCR)



Electrophoresis gel showing DNA fragments

revolutionised DNA fingerprinting. PCR, invented in 1983 by Kary Mullis, is a method of rapidly and accurately isolating and amplifying a specific DNA sequence using only a small amount of starting material.<sup>59</sup> In PCR a template piece of DNA is mixed with small DNA fragments that bind at the ends of the sequence to be amplified and a DNA replication enzyme from bacteria is used to fill in the gaps. Because PCR amplifies DNA, PCR can be used to analyse extremely small amounts of sample, which is often critical for forensic analysis, when only a trace amount of DNA is available as evidence.

DNA fingerprinting offers security to society. In addition to its use in solving criminal cases, paternity and immigration issues, DNA fingerprinting has also secured future generations because it has been used successfully for controlling the spread of tuberculosis. Furthermore DNA fingerprinting can be used to fight fraud by identifying counterfeit drugs, unauthentic wine and adulterated meat.

On a global scale, the availability of this technique and its refinement to a stage where it would become virtually foolproof could act as a deterrent to certain kinds of crime. Experts now think that DNA fingerprinting, when combined with rapid detection methods, could give rise to better authentication tools than the ones in use today.

## 4.4 Human health

### Improving and maintaining accessible health, including disease prevention

On the whole, people are healthier, wealthier and live longer today than 30 years ago.<sup>60</sup> 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 day.<sup>61</sup> 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.<sup>60</sup>

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 provided by the chemical sciences. This section covers the challenges that exist relating to ageing, diagnostics, hygiene and infection, materials and prosthetics, drugs and therapies, and personalised medicine.

#### 4.4.1 Ageing

**Challenge: With an ageing population, we need to enhance our life-long contribution to society and improve our quality of life.**

In 2007 almost 500 million people worldwide were 65 and older. Increased longevity and falling fertility rates mean that by 2025 that total is projected to increase to 835 million; this will account for over one in 10 of the Earth's inhabitants.<sup>62</sup> By 2031 there will be two million more people aged over 65 in England and Wales who will require assistance with daily life if current disability rates continue.<sup>63</sup> Between 1991 and 2031 the total population of England and Wales is expected to increase by 8 per cent. However, the growth of the older population will far exceed this. The numbers of people aged 60–74 are predicted to rise by 43 per cent, those aged 75–84 by 48 per cent and those aged 85 and over by 138 per cent.<sup>63</sup> Yet the largest number of older people will live in the transitional and developing regions. Sixty two percent (three fifths) of the world's older people live in less developed countries. By 2050 this will increase to 78 per cent.<sup>62</sup>

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, for example nutraceuticals, on future health and quality of life (see also section 4.2.2 Healthy food). 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. Technology breakthroughs will be required in identifying relevant biomarkers and sensitive analytical tools for early diagnosis, 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 (see also section 4.4.2 Diagnostics). There will also be a need to develop new materials for cost effective, high performance prosthetics, for example artificial organs, tissues and eye lenses (see also section 4.4.4 Materials & prosthetics).

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 (see also section 4.5.3. Sporting technology) and in designing living space and communities.

#### 4.4.2 Diagnostics

**Challenge: Recognising disease symptoms and progress of how a disease develops is vital for effective treatment. We need to advance to earlier diagnosis and improved methods of monitoring disease.**

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 diseases.<sup>64</sup> Screening and early detection of breast, cervical, colorectal and possibly oral cancers can reduce mortality<sup>48</sup> but in the UK less than half of cancer cases are diagnosed at a stage when cancer can be treated successfully. Cancer Research UK has set a target that two thirds of cancer cases are to be diagnosed at a stage when the cancer can be treated successfully by 2014.<sup>65</sup>

Globally there are 33.2 million people living with HIV, but only 10 per cent are aware that they are infected. There are also 8.8 million new cases of TB annually, many of which are undiagnosed. These diseases, along with one million deaths from malaria per year, place a huge burden on developing countries.<sup>66</sup> To overcome this, better systems are required that can be used in resource-limited settings to detect diseases as early as possible and to monitor the effectiveness of treatments.

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 and predisposition along with other genetic traits for an individual. In combination with basing treatment on targeted genotype rather than mass phenotype, and an increased focus on chemical genetics, this could result in personalised treatment and medication tailored to the specific needs of the individual (see also section 4.4.6 Personalised medicine).

In addition to detection, 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 also 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.

### 4.4.3 Hygiene and infection

**Challenge:** To prevent and minimise acquired infections, we need to improve the techniques, technologies and practices of the anti-infective portfolio.

Infectious diseases account for over a fifth of human deaths and a quarter of ill-health worldwide.<sup>67</sup> In 2004, 12.6 million people died globally from major infectious diseases: lower respiratory tract, HIV, diarrhoeal disease, TB, malaria and childhood infections.<sup>54</sup> These diseases disproportionately affect the poor, and in some African countries they have contributed to reducing life expectancy to less than 40 years.<sup>54</sup> Climate change is expected to exacerbate the severity of infectious diseases particularly in Africa, by providing more favourable conditions for insect-borne parasites that cause diseases, including malaria and sleeping sickness.<sup>54</sup>

In addition to the appearance of new infectious diseases, such as SARS, and the worsening of current diseases through climate change, we also face the challenge of antibiotic resistance. Some strains of bacteria are now resistant to the antibiotics that have previously been used to treat them. In the UK alone Methicillin-resistant *Staphylococcus aureus* (MRSA) contributed to over 1593 deaths in 2007, an increase from 51 deaths in 1993.<sup>68</sup>

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. 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 paints and coatings;
- 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.

### 4.4.4 Materials and prosthetics

**Challenge:** Orthopaedic implants and prosthetics need to be fully exploited to enhance and sustain function fully.

In the UK more than 3000 people received organ transplants in 2007/08. However, 1000 died while on the waiting list, which currently numbers around 8000.<sup>69</sup> The scale of the problem is even larger than these figures suggest, as many patients are never put on the waiting list and it is estimated that need for organs is 50 per cent more than currently available.<sup>56</sup>

In addition to the continued demand for developing advanced materials to use in orthopaedic implants such as hips, knees, ankles, *etc.* and traditional prosthetics such as artificial limbs, there is a need to develop new materials for cost effective, high functional prosthetics, for example, artificial organs, tissues and eye lenses. The challenge is to exploit replacement organs to enhance sustained function fully.

Materials breakthroughs will be required in polymer and bio-compatible material chemistry for surgical equipment, implants and artificial limbs, developing smarter and/or bio-responsive drug delivery devices for diabetes, chronic pain relief, cardiovascular disease and asthma, and in researching 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.

In addition, 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.

#### 4.4.5 Drugs and therapies

**Challenge: Basic sciences need to be harnessed and enhanced to help transform the entire drug discovery, development and healthcare landscape so new therapies can be delivered more efficiently and effectively for the world.**

Chronic diseases, including cardiovascular, cancer, chronic respiratory, diabetes and others including mental health problems and joint problems, caused 35 million deaths globally in 2005.<sup>70</sup> 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 per cent between 2005 and 2015.<sup>70</sup> Developing drugs and therapies that can target these diseases have the potential to save a huge number of lives worldwide.

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 therapies can be delivered more efficiently and effectively for the world. To achieve this, a number of breakthroughs are required in applying systems biology in:

- identifying new biological targets;
- improving the knowledge of the chemistry of living organisms, including structural biology;
- designing and synthesising small molecules that attenuate large molecule interactions, for example 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.

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 underpinned 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 *in vivo* 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. It is also necessary to develop model systems to improve understanding of extremely complex biological systems and how interventions affect these living systems over time.

Increased understanding of the chemical basis of toxicology and the derivation of 'Lipinski-like' 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.

#### 4.4.6 Personalised medicine

**Challenge: We need to be able to deliver specific, differentiated prevention and treatment on an individual basis.**

Technological advances in the past 10 years have reduced the cost of sequencing the whole human genome by a staggering 1000-fold or more.<sup>71</sup> George M. Church, Professor of Genetics at Harvard, predicts that the '\$1000 genome' milestone, that is the ability to sequence a whole human genome for less than a \$1000, will be a reality before the end of 2009.<sup>72</sup> 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 individual. Commercial kits are already available to assess an individual's genome for disease traits for only \$399.<sup>73</sup> In addition, 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.

Technological advancement is therefore leading to personalised treatment and medication tailored to the specific needs of individuals. 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. It is imperative that research advances are translated into robust, low cost techniques.

## HUMAN HEALTH: FUNDAMENTAL SCIENCE CASE STUDY

### Beta-blockers

*Building on the fundamental and groundbreaking medical theory of drug-receptor interactions, pharmacologist Sir James Black worked in collaboration with chemists to synthesise Propranolol, the first beta-blocking drug for treating hypertension.*

Beta-adrenoreceptor blocking drugs, or beta-blockers for short, are adrenaline receptor-blocking drugs that reduce the effects of the sympathetic nervous system on the cardiovascular system. Adrenaline, the fight-or-flight hormone secreted at times of stress and exercise, binds to beta-adrenoreceptors causing the arteries to constrict and the heart to work harder. In some patients this increases the risk of having a heart attack.

Beta-blockers work by binding to beta-adrenoreceptors and preventing the binding of adrenaline, therefore avoiding the effects that lead to heart attacks.

Beta-blockers have been used routinely to treat high blood pressure since the 1970s and are also given to relieve angina, correct irregular heartbeats and reduce the risk of dying after a heart attack.

The first successful beta-blocker, Propranolol, was discovered in 1962 by Sir James Black, who was awarded the Nobel Prize for medicine in 1988.<sup>74</sup> Black believed he would not have started his work on the subject without the fundamental research done by his predecessors including Paul Ehrlich, John Langley and Raymond Ahlquist.

**// Science is a gradual progression that requires building on the work of others. //**

#### James Black

The groundbreaking work of Paul Ehrlich, pioneer of many aspects of modern medicine, and physiologist John Langley in the late 19th and early 20th century introduced the concept that drugs bind to targets, we now call receptors, and affect their activity.<sup>75</sup> In 1948, Raymond

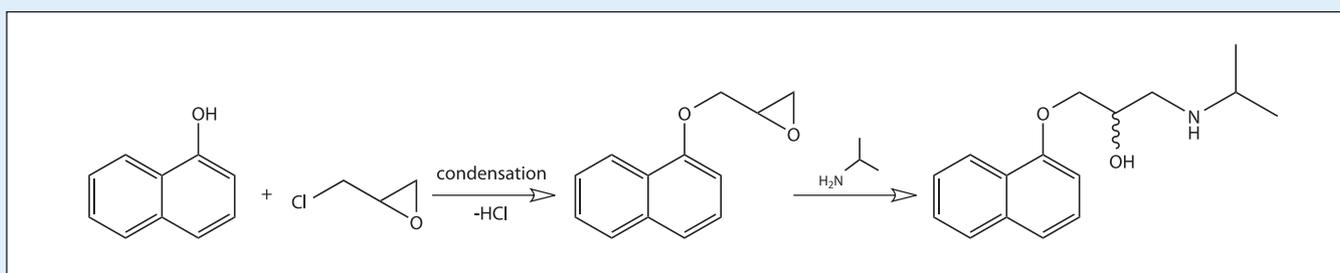
Ahlquist published his adrenergic 'receptor' theory that adrenaline binds specific receptors to bring about its effects. However, the theory was not widely accepted by influential scientists, such as Henry Dale. It was not until the 1950s when, while looking for a long-acting bronchodilator compound, Powell and Slater from Eli Lilly accidentally discovered the adrenoreceptor blocking compound dichloroisoproterenol (DCI). They found that DCI competed with adrenaline and isoprenaline for adrenergic receptor sites. Subsequently, in 1958, Neil Moran and Marjorie Perkins showed that DCI antagonised the changes in heart rate and muscle tension produced by adrenaline, proving Ahlquist's receptor theory.

From this, Black realised that a drug that could block the effect of adrenaline on the heart would be effective in treating cardiovascular conditions. Black collaborated with a chemist at ICI, John Stephenson, in his search for such a drug. Using DCI as a lead compound Stephenson synthesised an analogue where the two chlorine atoms in DCI were substituted with a phenyl ring. This compound, Pronethalol, had promising clinical activity but had long-term toxicity problems. Further analogue-based design and fundamental organic chemistry led to the synthesis of a compound, that would become known as Propranolol, by chemists Leslie Smith and Albert Crowther. Clinical trials soon confirmed that Propranolol was a safe and effective drug for hypertension and cardiac arrhythmias.

The effects of adrenaline are mediated through different beta-adrenoreceptor subtypes that are located in different tissues, for example in the heart. The first generation of beta-blockers, including Propranolol, were non-selective and blocked all types of adrenoreceptors. However, second generation beta-blockers are specific to different receptor subtypes and are therefore suitable to treat different conditions.

Since its discovery as a beta-blocker, Propranolol has proven effective in managing a number of medical conditions, including migraine prophylaxis in children. It may even have potential future uses as an antimalarial drug by preventing the parasite from entering red blood cells.

Propranolol has annual sales around \$215 million in the US.<sup>76</sup>



The reaction scheme for the synthesis of Propranolol

## 4.5 Lifestyle and recreation

### Providing a sustainable route for people to live richer and more varied lives

Lifestyle and recreation contribute to the quality of life and bring a sense of wellbeing to citizens and communities. Everything from the museums, galleries, archives, libraries and historic buildings that surround us, to the clothes we wear, the household and personal care products that we use and the latest advances in sporting and digital technology that we purchase, promote convenience and perceptions of well being.

One of the key challenges we face is to reconcile the need to reduce the levels of energy and environmental resources that we consume, while at the same time maintaining and improving quality of life for all, thus enabling people to live richer, more varied lives.

#### 4.5.1 Creative industries

##### **Challenge: Continued innovation is necessary to give new options to designers, artists and architects.**

Society is underpinned by its understanding of history. This understanding is profoundly influenced by the survival of the physical artefacts that embody much of our cultural heritage – buildings, artefacts, works of art, books, film and so on. The conservation of these physical objects presents a fascinating, rich and diverse range of scientific challenges. Equally, the chemical sciences can make a huge contribution, not only to preserving our cultural heritage, but to providing a continual supply of innovative options for the designers, artists and architects of the future.

Pollutants are having a major impact on our historic buildings. Scaffolding moves continuously around York Minster in a 100-year cycle as stonemasons restore decayed and weathered limestone. York Minster recently revealed that a five-year programme to restore the East Front and half of the Great East Window will cost £12 million.<sup>77</sup> The chemical sciences are vital for understanding why previous materials have either decayed or survived, and in helping to develop new materials for restoring and protecting both new and historical buildings. In addition, changes in climate could affect the indoor environment.

Temperature and humidity could cause extensive damage to art collections, books and other artefacts. Chemical science can provide an increased understanding of the threat to these materials, which will help to minimise damage and aid preservation. In addition, restoration of paintings and other cultural treasures will require the development of improved analytical techniques to identify the compounds comprising the materials and colour pigments used. In this way the piece can be preserved or restored as close to its original state as possible.

In contrast to preserving our cultural heritage, the designers, artists and architects of the future will require the chemical sciences to provide a continual supply of innovative materials for a whole range of new applications. Examples include developing new materials for use in the design of new buildings and structures and new materials and applications for creative designers – for example, dynamic systems that change colour or texture as desired, new dyes that are more stable and less toxic, and sustainable and renewable packaging incorporating emerging active and intelligent materials with time, temperature, spoilage and pathogen indicator technologies.

### 4.5.2 Household

**Challenge:** Household and personal care products that promote convenience and perceptions of well-being, or that deliver household functionality, need to combine efficacy with safety and sustainability/ longevity.

Everything, from household and personal care products right up to the materials used to furnish and build homes, relies on developments from the chemical sciences. It is important that these products, which promote convenience and perceptions of well-being, or that deliver household functionality, combine efficacy with safety and sustainability.

To achieve this further fundamental research is required to understand the complex interactions that take place during formulation of products for the home and personal care sector. This will require research into the disciplines of physical and colloid chemistries, as well as elements of analytical chemistry, chemical engineering, pharmaceutical and biological sciences.

The chemical sciences also have a significant role in facilitating the re-formulation of household and consumer products to address safety and environmental concerns, along with the legislative requirements, for example, REACH (EU legislation concerning Registration, Evaluation, Authorisation and restriction of Chemicals). This must be linked to a better understanding of the effects of dermatology and cosmetic ingredients at a molecular and cellular level, and an improved understanding of the chemical basis of toxicology in new and novel products, and their breakdown in the environment. This will require, for example, using computational chemistry to develop good predictive models for human and eco-toxicity.

Breakthroughs will also be required in developing improved recyclable materials and building technologies, including new materials and innovations for constructing houses and their contents, for example floor coverings and furniture, which combine efficacy with safety and sustainability (see also section 4.3.4 Construction materials). Developments could include self-cleaning materials for homes and more efficient laundry processes, to reduce the amount of detergents used and waste produced. There could also be advances in developing innovative technologies such as controlled switchable surface adhesion, which could lead to self assembly furniture or self hanging pictures and wall paper which, at the flick of a switch, can be disassembled, removed or replaced.

### 4.5.3 Sporting technology

**Challenge:** We need to develop new materials that enable higher performance as an ultimate sporting goal, and bring a sense of well-being to the wider and ageing population.

Physical activity not only contributes to well-being, but is also essential for good health. People who are physically active reduce their risk of developing major chronic diseases such as coronary heart disease and type II diabetes by up to 50 per cent, and their risk of premature death by about 20–30 per cent. The annual costs of physical inactivity in England are estimated at £8.2 billion; this includes the rising costs of treating chronic diseases such as coronary heart disease and diabetes, but does not include the contribution of inactivity to obesity – an estimated further £2.5 billion cost to the economy each year.<sup>78</sup>

New materials, to enable higher performance as an ultimate sporting goal and to bring a sense of well-being to the wider and ageing population, will be required. Advances and developments in materials chemistry for sporting equipment that confers additional benefits in weight, strength and accuracy will be essential, as will developments in functional textiles (see also section 4.5.5 Textiles). Advances in materials chemistry have already been used in developing lightweight supports and braces that can be used during physical activity without hindering performance. In addition, technology breakthroughs will be required for the next generation of protective clothing and sportswear.

Advances in equipment and clothing will be coupled with developing and using active diagnostics and monitoring to assist personal performance – for example, monitoring hormone levels.

The health benefits of physical activity are even more pronounced in older adults, increasing an older person's ability to maintain an independent lifestyle. In addition to advances in equipment and clothing, the chemical sciences can help keep sport and recreation accessible to the wider population, especially the ageing population, through advances in healthcare - notably in the development of an array of new technologies for managing chronic illness and promoting active lifestyles.

#### 4.5.4 Advanced and sustainable electronics

**Challenge:** Miniaturised electronic devices, with faster computer speeds and denser storage, need to be produced. This should be coupled with developing sustainable electronic devices, which are recyclable, and have little dependence on materials in increasingly short supply.

According to the UN environment programme, some 20–50 million metric tonnes of e-waste, including lead, cadmium, mercury and other hazardous substances, are generated worldwide every year as a result of the growing demand for computers, mobile phones, TVs, radios and other consumer electronics. In the US alone, 14–20 million PCs are thrown out every year. In the EU the volume of e-waste is expected to increase by 3–5 per cent per year. Developing countries are expected to triple their output of e-waste by 2010.<sup>79</sup>

Electronic products have a great positive impact on our lives, however, their increasing availability and affordability means that they also present a growing environmental problem. The challenge is to produce miniaturised electronic devices with faster computer speeds and denser storage. This must be coupled with the need for sustainable electronic devices, which are recyclable and have little dependence on materials in increasingly short supply (see also sections 4.6.1 and 4.6.2).

To develop miniaturised electronic devices with faster computer speeds and denser storage, key requirements in the future will include:

- advances in display technology, such as flat lightweight and rollable displays for a variety of applications;
- controlled deposition (microcontact printing, nanotemplate patterning *etc*) onto thin films and integration into printed electronics;
- advances in flexible, printable electronics based on new molecular technologies (allowing dynamic re-configuration);
- design concepts and new materials for micro-sized batteries for mobile and portable electronic devices (see also sections 4.3.2 Home energy generation and 4.5.4 Advanced and sustainable electronics).

Enhancing information storage technology will also be required – for example, molecular switches with the potential to act as a molecular binary code is one possibility. Molecular switches have the potential to reduce the size of information storage by a factor of 100,000 and increase the speed of information storage by a factor of 1,000,000.<sup>3</sup> Technology advances will also be required in the development of biological and/or molecular computing, in understanding bio-mimicking self-assembling systems and in developing the ability to exploit the interface between molecular electronics and the human nervous system - for example, using the brain to switch on a light.

### 4.5.5 Textiles

**Challenge:** There is a need to move away from a conventional, low-cost, disposable fashion culture to new systems which provide design scope, colour, feel, sustainability, longevity and new, low-cost fabrication routes.

Textiles surround us in our daily lives.

They are manufactured from natural fibres, manmade fibres, or a mixture of both. Textiles and clothes are getting cheaper. They follow fashion more rapidly and we are buying more and more of them. In 2000 the world's consumers spent around \$1 trillion worldwide buying clothes. Around one third of sales were in Western Europe, one third in North America and one quarter in Asia.<sup>60</sup> The total UK consumption of textile products is approximately 2.15 million tonnes per year, equivalent to approximately 35 kg per UK capita.

The combined waste from clothing and textiles in the UK is about 2.35 million tonnes per year.<sup>64</sup>

The challenge is to move away from this conventional, low cost, disposable fashion culture to new systems, which provide design scope, colour, feel, sustainability, longevity and new low cost fabrication routes. Chemical science will be crucial in developing technological innovations and sustainable textiles by:

- helping to improve resource usage (water, energy) during fabrication;
- substituting harmful chemicals used during production processes and in the fabrics themselves;
- developing environmentally sensitive production techniques, particularly for cotton;
- increasing the re-use of materials;
- producing biodegradable textiles, allowing for better disposal solutions;
- developing synthetic fibres from sustainable sources.

In addition to traditional textiles, developing functional textiles (materials and products that are manufactured mainly for their technical performance and functional properties, rather than their aesthetic characteristics such as colour or style) will require input from the chemical sciences. Technology breakthroughs are needed to develop functional textiles with superior energy balance, strength and flexibility for future use in clothing, in the home and in the construction, automotive, aerospace, health, leisure and defence sectors. Opportunities include developing textiles incorporating self-healing and self-cleaning dynamic pigmenting technologies – for example, biotherapeutic textiles for use in wound dressings.

## LIFESTYLE & RECREATION: FUNDAMENTAL SCIENCE CASE STUDY

### Liquid crystal displays

*A chemical curiosity with 'no application', liquid crystals (now worth £40 billion per year) only became commercially useful after years of developing an understanding of structure-property relationships and novel materials.*

Liquid crystals exhibit a phase of matter that is between that of a liquid and that of a crystal. A liquid crystal may flow like a liquid, but contain molecules, typically rod-shaped organic moieties about 25 Å in length, oriented like they would be in a crystal. The molecular orientation, and hence the material's optical properties, can be controlled by changing the temperature and by applying an electric field. The most common application of liquid crystal technology is in liquid crystal displays (LCDs).

Liquid crystalline mesophases – called nematic, smectic and chiral phases – were discovered in 1888, through the initial work of Friedrich Reinitzer on naturally-occurring cholesterol derivatives, and his subsequent collaboration with Otto Lehmann. When determining the purities of esters of cholesterol Reinitzer noticed that they seemed to exhibit a 'double melting' transition. For example, a sample changed from a solid into a liquid at 145.5 °C and then at 178.5 °C this opaque liquid suddenly turned transparent. Reinitzer sent samples to Otto Lehmann for crystallographic studies and he intuitively deduced from his data that the liquids' optical properties were due to elongated molecules oriented parallel to each other.<sup>81</sup>

By the early 1900s, Daniel Vorländer had synthesised a wide range of liquid crystalline compounds to investigate the connection between molecular structure and liquid crystalline behaviour. George Friedel also investigated liquid crystalline phases and classified the phases according to their molecular ordering.<sup>82</sup>

During the late 1940s and 1950s, George Gray at the University of Hull in the UK did fundamental research to better understand the influence of molecular structure on liquid crystalline characteristics. Other chemists synthesised novel materials with similar goals, and interdisciplinary work with physicists and mathematicians provided a good understanding of the physical properties of liquid crystal materials and their phases. During the early 1960s, many scientists concluded that although liquid crystals were most unusual, they were now well-understood and had no potential applications.

However, in 1963 Richard Williams of Radio Corporation of America (RCA) recognised that liquid crystals responded to electric fields; this led to the invention of the first LCD



Nematic phase liquid crystal

by his colleague George Heilmeyer in 1968.<sup>83</sup> Unfortunately the material he used was unstable and was not liquid crystalline until 83 °C, making the device impractical. Following this, in 1971, Martin Schadt and Wolfgang Helfrich at Hoffman-la Roche in Switzerland invented a new class of LCDs, the Twisted Nematic Liquid Crystal Display (TNLCD).

Since the UK had to pay licensing fees to RCA for producing shadow mask displays for radar (greater than the cost of developing Concorde), John Stonehouse, Minister for Trade and Industry, encouraged the MoD to set up a contract with George Gray in Hull to develop new liquid crystals for the TNLCD. By 1973 Gray had developed cyano-biphenyl liquid crystals,<sup>84</sup> which were stable, colourless and operated at room temperature. These were quickly patented and mixtures of the various homologues were formulated to generate an acceptable blend for commercial displays. Remarkably for a new invention, the materials were commercially available in devices within two years of the discovery.

With rapid increases in technological inventions, the need for more elaborate, quality displays in colour became important. Hence, research into liquid crystal materials and properties has grown enormously. A significant portion of research has been targeted at improved displays, but a lot has been fundamental research to improve understanding of the structure-property relationships.

LCDs are used in a variety of everyday objects, from watches and calculators, mobile phones, digital cameras and MP3 players through to computer monitors and high-definition televisions with large area screens. Such displays, combined with the product they facilitate, have revolutionised people's lives. The market value of LCDs is currently £40 billion per year and there are now more LCDs in the world than there are people.

There is still scope for developing liquid crystal technologies. Current ferroelectric liquid crystal technology offers extremely fast switching devices for microdisplays and telecommunications. Liquid crystals of a different type to those in displays are attracting attention for their potential applications in biological and medical fields due to their similarity to cell membranes and biological fluids and processes.

## 4.6 Raw materials and feedstocks

### Creating and sustaining a supply of sustainable feedstocks, by designing processes and products that preserve resources

In the developed world we live in a time of unprecedented mass affluence and convenience. However, this comfortable lifestyle comes at a cost. Society is profligate in its use of materials with one source estimating that 93 per cent of production materials do not end up in saleable products and 80 per cent of products are discarded after a single use.<sup>85</sup>

At the same time, the global population continues to increase and with it, the affluence and expectations of the developing world. For the whole world to share the living standards currently enjoyed in the UK, the resources of three planet Earths would be required.<sup>86</sup> For a more equitable world in which developing countries may hope to share our living standards, it is clear we all must do more with less material resource. It is estimated that 50 per cent of the products which will be needed in the next 10–15 years have not yet been invented, so the opportunities are both real and substantial.<sup>87</sup>

Industry will respond by becoming increasingly focused on selling 'solutions' rather than ingredients, and developing innovative, added value components. There will be a shift from material intensive products to knowledge intensive products. This section focuses specifically on the challenges we face in sustainable design, conservation of scarce natural resources, conversion of biomass feedstocks and recovered feedstocks.

#### 4.6.1 Sustainable product design

**Challenge:** Our high level of industrial and domestic waste could be resolved with increased downstream processing and re-use. To preserve resources, our initial design decisions should take more account of the entire life-cycle.

The environmental impact of a product is determined largely at the design stage and mistakes made here can embed unsustainable practice for the lifetime of the product. Life-cycle thinking needs to be developed and applied across entire supply chains to understand where the highest environmental impacts are incurred and which interventions are necessary to reduce these. This includes closing the recycling and remanufacturing loop. In addition to formal life-cycle analysis (LCA), the chemical sciences will be needed to develop flexible and agile tools to allow life-cycle thinking to be applied throughout the innovation process.

Chemists have a huge role to play in applying best practice technologies (such as metal recycling) throughout the life-cycle of products, setting clear standards for LCA methods and data gathering, and developing tools to aid the substitution of toxic substances, which can be particularly problematic. For example, The British Coatings Federation has estimated that if it was necessary to reformulate the resin that binds an aircraft topcoat to the primer, as a result of the withdrawal of one ingredient, the effort required for substitution would lead to approximately nine man years of work.<sup>88</sup>

An understanding of sustainable design and the principles of reduction, remanufacture, reuse and recycle (4Rs) must be applied widely by chemical scientists. Concepts such as water and atom efficiency, alongside green chemistry and chemical engineering, should be standard approaches in intensifying and optimising manufacturing processes – developing process modelling and process analytics will be key. Additional technological breakthroughs include:

- developing methods for tagging polymers to aid recycling;
- designing biodegradability into finished products;
- developing smart coatings;
- developing improved recovery processes;
- developing new composites that are readily recyclable.

As limits are placed on raw materials, substitution based on functionality will become increasingly important. Improvements in the processing of recyclates will help, but a fundamental understanding of how structure relates to property will enable an improved understanding of eco-toxicity and the intelligent design of substances.

## 4.6.2 Conservation of scarce natural resources

**Challenge: Raw material and feedstock resources for both existing industries and future applications are increasingly scarce. We need to develop a range of alternative materials and associated new processes for recovering valuable components.**

Mineral commodities are essential to our way our life. For example, the average car contains over 30 mineral components, including almost a tonne of iron and steel, over 100 kg of aluminium, 22 kg of carbon and nearly 20 kg of both silicon and zinc.<sup>89</sup> Chemical scientists rely on precious metallic elements that have applications in many industries. However, it is difficult to estimate the amounts in extractable reserves and to predict global demand for specific elements as technologies change. In modern technologies many of the elements are used in small amounts and some are dispersed into the environment. These factors can make it difficult to recover and recycle the elements for future use.

A recent assessment, based on data from the US Geological Survey's annual reports and UN statistics on global population, considered the per capita use of elements and performed basic calculations to estimate how soon we may exhaust known reserves.<sup>90</sup> To sustain the quality of life of the modern developed world and its extension to the entire global population, new technologies may have to use elements more efficiently or use substitutes in place of those used in contemporary technologies<sup>91</sup> – for example, indium is used in the manufacture of LCDs for flat-screen TVs. The substance indium gallium arsenide is crucial for a new generation of more efficient solar cells but insufficient resource is available for this technology to make a useful impact on global energy needs. As such, alternative technologies will have to be sought. Tellurium is used increasingly in semiconductors and solar panels, with the concomitant increase in demand leading to a price increase of 25-fold in 2006.<sup>92</sup>

The chemical sciences must apply the principles of sustainable design to this issue. In particular innovations to reduce, replace, and recycle elements will be needed. Achieving 'more with less' is vital and reducing material intensity through applying nanotechnology to increase activity per unit mass and reducing raw material use through processes such as thrifting are key areas. Replacing precious metals with more common metals in applications will continue to be a key strategy, as will improved fertiliser management of nitrogen and phosphorus and reduced dependence on finite metal resources. Efficient methods for recovering metals from electronic scrap (so-called e-waste) and landfill will also be needed.

### 4.6.3 Conversion of biomass feedstocks

**Challenge: Biomass feedstocks (whether they are agricultural, marine or food waste) for producing chemicals and fuels are becoming more commercially viable. In the future, integrated bio-refineries using more than one biofeedstock will yield energy, fuel and a range of chemicals with no waste being produced.**

In the future, chemicals will be based increasingly on biomass, which will also be used to help meet our energy needs. Tomorrow's chemical industry will be built on the concept of a 'bio-refinery', where regional facilities will take in a diverse range of crops and plant matter and process them into biofuels, materials and 'platform molecules'.

Sugars, oils and other compounds in biomass can be converted into 'platform' chemicals directly, or as by-products from fuel in processes analogous to the petrochemical industry. These building block chemicals have a high transformation potential into new families of useful molecules. To produce platform chemicals, the chemical sciences will be vital in providing novel separation technologies, such as membranes and sorbent extraction of valuable components from biological media, and in developing pre-treatment methods for biomass component separation.

The chemical sciences will also provide enzymes tolerant to oxygen and inhibitors, and new synthetic approaches to adapt oxygen-rich starting feedstocks, which will help to convert platform molecules into valuable products.

Biomass is not just available from agriculture, but is also available in the form of industrial and municipal waste streams. Global reserves of sustainable biomass are estimated to be 200 billion tonnes (oven-dried material), of which only 3 per cent is currently utilised.<sup>93</sup> One billion tonnes of biomass is equivalent in energy to over two billion barrels of crude oil.

For bio-based renewable chemicals to compete with fossil-fuel based feedstocks there are several key areas of technology that must be developed and this offers huge potential for the chemical sciences.

Fundamental bioprocessing science will have to mature. Homogeneous feedstocks with metabolically engineered properties will be required, as will a greater variety and yield of products through advances in fermentation science. Introducing novel catalysts and biocatalysts will be valuable for breaking down lignin into aromatic substrates, in pyrolysis and gasification techniques that increase the density of biomass, and in technologies that exploit biomethane from waste. Technological breakthroughs will also be required in microbial genomics to improve micro-organisms, and in developing catalysts for upgrading pyrolysis oil.

Robust and transparent methods for assessing the life-cycle impact of renewables and comparing alternative routes is a priority. The few comprehensive life-cycle assessments performed to date indicate that using renewable chemicals has good potential for energy and greenhouse gas savings. Improvements in the efficiency of production are considered to be highly likely in the near future, providing there are economic incentives for development.

#### 4.6.4 Recovered feedstocks

**Challenge: There are limits to the current supply of chemical and fuel feedstocks from alternative sources. The conversion of readily available, cheap feedstocks and waste into useful chemicals and fuels is an opportunity for chemical scientists.**

The supply of chemical and fuel feedstocks currently used for energy generation is severely limited. Finding and enabling alternative energy sources is a challenge for the chemical sciences.

Each person in the UK generates around 170 kg of organic waste each year and approximately 33 per cent of food bought by consumers, including £10.2 billion of perfectly good food, is thrown away each year in the UK.<sup>94</sup> Most of this discarded waste ends up in landfills, producing the harmful greenhouse gas methane, which is 25 times more powerful than CO<sub>2</sub>. Organic waste offers a cheap and readily available alternative feedstock, thus converting waste to useful chemicals and fuels is an opportunity for chemical scientists. Not only would this provide an alternative energy source, but it would also reduce greenhouse gas emissions generated in landfill sites.

Anaerobic digestion and advanced thermal processing are established technologies, used to treat organic waste and produce renewable energy in the form of biogas or gas for electricity or heat generation. However, a raft of new chemical, thermal and biological processes are beginning to emerge as methods to convert biomass waste into a variety of fuels including hydrogen, bio-crude oil and solid fuel. Energy recovery from waste will become increasingly important in providing on-site power generation for industry and therefore technologies to process waste must evolve. There needs to be a general shift in opinion to view waste as a 'raw material'.

Efficient recovery and recycling of feedstocks is also important. Novel separation and purification technologies for economic recycling need to be developed. Upcycling plastic is an important aspect of this and developing genuine, innovative recycling technologies to allow, for example, monomers to be recovered from mixed plastics must be facilitated by the chemical sciences.

Plants successfully convert sunlight to energy through photosynthesis. The ultimate challenge for the chemical sciences would be to mimic this, by inventing 'artificial photosynthesis' to harness light. The chemical sciences could also provide future energy sources through other biomimetic processes, such as converting small molecules – such as CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub> – to chemicals, and by the catalytic conversion of simple alkanes to alcohols – for example, the production of 1,4-butanediol from butane. It is currently possible to use CO<sub>2</sub> as a feedstock to produce chemicals, fuels and polymers; however, there are a number of potential technologies that require further R&D – for example photochemical conversion of CO<sub>2</sub>.

## RAW MATERIALS & FEEDSTOCKS: FUNDAMENTAL SCIENCE CASE STUDY

### The Haber process

*The fundamental understanding of reaction equilibria established by Le Chatelier gave hope to chemists seeking to develop conditions for converting abundant supplies of hydrogen and nitrogen feedstocks to ammonia – a vital component of agricultural fertilisers.*

The Haber process is used to produce ammonia from nitrogen and hydrogen at high temperature and pressure with an iron catalyst. Ammonia can be processed into nitrates, which are important components of fertilisers and explosives. Developing a process to synthesise ammonia was vital because it provided independence from limited global deposits of nitrates and meant that ammonia could be produced using common atmospheric gases as feedstocks. The rapid industrialisation of the Haber process is indicative of the importance of ammonia synthesis.

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 Henry Louis 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.<sup>95</sup>

***“I let the discovery of the ammonia synthesis slip through my hands. It was the greatest blunder of my scientific career.”***

**Le Chatelier**

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 insoluble. The baton was taken up by Walther Hermann 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 catalyst.<sup>96</sup> 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. The ability to synthesise large quantities of a nitrogen rich compound from abundant atmospheric nitrogen freed countries from depending on limited nitrate deposits. Ammonia synthesis played a strategic part in WWI. The large scale production of ammonia allowed Germany to continue producing explosives after their supplies had run out, thus prolonging the war.

The industrialised Haber process is still important almost 100 years after its initial use. 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'. Although there are environmental risks involved in intensive fertiliser use, these chemicals remain essential for the sustainable production of food, and while the world population continues to grow it appears that there will always be an important place for the Haber process in producing fertiliser.

## 4.7 Water and air

### Ensuring the sustainable management of water and air quality, and addressing societal impact on water resources (quality and availability)

Water and air are essential constituents of life.

Providing sufficient quantities of water in a sustainable way at an appropriate standard to satisfy domestic, industrial, agricultural, and environmental needs is a global challenge.<sup>97</sup> Estimates predict that by 2025 more than half of the world population will potentially be facing some level of water-based vulnerability.<sup>98</sup>

These challenges are exacerbated in the face of an increasing population, climate change and man-made pollution. This section focuses on the challenges that exist in the areas of drinking water quality, water demand, waste water, contaminants, air quality and climate.

#### 4.7.1 Drinking water quality

**Challenge: Poor quality drinking water damages human health. Clean, accessible drinking water for all is a priority.**

Access to safe drinking water and adequate sanitation varies dramatically with geography and many regions already face severe scarcity. Current population forecasts suggest that an additional 784 million people worldwide will need to gain access to improved drinking water sources to meet the UN Millennium Development Goal target:<sup>99</sup> to halve the proportion of people without sustainable access to safe drinking water and basic sanitation by 2015.<sup>100</sup> The World Health Organization estimates that safe water could prevent 1.4 million child deaths from diarrhoea each year.<sup>101</sup>

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.

Technology breakthroughs required include:

- energy efficient desalination processes;
- energy efficient point of use purification, for example disinfection processes and novel membrane technologies;
- developing low cost portable technologies for analysing and treating contaminated groundwater that are effective and appropriate for use by local populations in the developing world, such as for testing arsenic-contaminated groundwater.

#### 4.7.2 Water demand

**Challenge: Population growth means greater demand on water supply. Household, agricultural and industrial demands are in competition. Management and distribution strategies must ensure that clean water of an appropriate quality remains economically accessible.**

With 71 per cent of the Earth's surface covered in water<sup>102</sup> there is no physical shortage, but most of the resource is saline (97 per cent) and therefore non-potable. The remaining 3 per cent is freshwater of which two thirds are locked away in glaciers and the polar ice caps. Humanity's growing needs must therefore be met with only 1 per cent of the Earth's total water. With household, agricultural and industrial demands in competition, the chemical sciences, alongside engineering, have an important role to play in ensuring management and distribution strategies make certain that clean water of an appropriate quality remains economically accessible.

To achieve this, products must be designed to minimise water and energy use during their production and use (water footprinting). This can be achieved by adopting, for example, the principles of green chemistry and integrated pollution prevention and control to industrial manufacture, with the aim of reducing waste, energy and water use. Household products and appliances must be designed to work effectively with minimal water and energy demands, and include better water re-cycle systems. Efficient, safe and low maintenance systems need to be developed for industrial water recycling and better strategies for water use and re-use for agriculture systems. In addition, efficient water supply systems and anti-corrosion technologies for pipework are needed, including development of materials for preventing leakage and water quality maintenance.

### 4.7.3 Wastewater

**Challenge:** Wastewater treatment needs to be made energy neutral and we need to enable the beneficial re-use of its by-products.

Every day in the UK alone, about 347,000 km of sewers collect over 11 billion litres of wastewater.<sup>103</sup> With the future threat of water scarcity there will be an increased interest in the recycling and re-use of water. These sources have a wide range of contaminants that require removal, which is currently energy intensive. The challenge is to make waste water treatment energy neutral and to enable the beneficial re-use of its by-products.

To make a breakthrough, advanced, energy efficient, industrial wastewater treatment technologies are needed, for which there is the potential to exploit novel membrane, catalytic and photochemical processes. In addition, more efficient ways are needed for treating domestic wastewater, to avoid the high energy input and sludge generation associated with using biological processes. Opportunities exist for developing a foul sewer network that can be considered part of the treatment plant and works as a long, continuously monitored pipe reactor that treats water *in situ* and maintains quality to the point of delivery.

Further technology breakthroughs are required in membrane technology for microfiltration, ultrafiltration and reverse osmosis to reduce costs and improve process efficiency significantly in removing particulates, precipitates and micro-organisms. Novel coatings and chemicals for minimising corrosion in pipe-work, biofilm growth and deposition of solids such as iron and manganese during water and wastewater treatment are also required.

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.

### 4.7.4 Contaminants

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

Human activity has resulted in the emergence of chemical contaminants in the environment, typically mobilised by water. Further research is required into the measurement, fate and impact of existing and emerging contaminants. This will help determine and control the risks of contaminants to the environment and human health.

Our understanding of the major fate processes for many contaminants is well developed. Experimental and modelling approaches are available to determine how a substance is going to 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 transformation products. The chemical sciences are crucial in assessing the risks of mixtures of chemicals at low concentrations to the environment and human health. This must be coupled with further research into understanding the impact of contaminants on and their interaction with biological systems.

Temperature and precipitation changes due to global warming may affect input of chemicals into the environment, and their fate and transport in aquatic systems. There is a need for the chemical sciences to identify the potential impact of climate change on fate and behaviour of contaminants.

#### 4.7.5 Air quality and climate

**Challenge: Increasing anthropogenic emissions are affecting air quality and contributing to climate change.**

**We need to understand the chemistry of the atmosphere to be able to predict the impact of this with confidence and to enable us to prevent and mitigate further changes.**

Global greenhouse gas emissions due to human activities have grown since pre-industrial times, with an increase of 70 per cent between 1970 and 2004.

World CO<sub>2</sub> emissions are expected to increase by 1.8 per cent annually between 2004 and 2030.<sup>104</sup>

Increasing anthropogenic emissions are affecting air quality and contributing to climate change.

Scientists have an important role to play in understanding the chemistry of the atmosphere to be able to predict with confidence the impact of these emissions and to prevent and mitigate further changes.

To achieve this, the chemical sciences will need to:

- develop novel techniques for studying reactive molecules that occur at ultra-low concentrations in the atmosphere and are the agents of chemical change;
- understand, through developing novel techniques for studying sub-micron particles, how aerosols form and change in the atmosphere, and their impacts on human health and climate;
- study geo-engineering solutions to climate change – such as ocean fertilisation to draw down CO<sub>2</sub>, or increasing the Earth's albedo by enhancing stratospheric aerosols to modify the Earth's climate in response to rising greenhouse gas levels – looking both at the effectiveness and undesirable environmental side-effects of these solutions;
- develop new modelling methodologies for treating the enormous chemical complexity that occurs on regional and global scales.

This must be coupled with developing novel analytical techniques, such as low-cost sensors for the detecting of atmospheric pollutants (ozone, nitrogen oxides, particulates *etc*), which can be dispersed throughout both developed and developing urban areas for fine-scale measurement of air quality, and can be used in developing atmospheric models. In addition, technology breakthroughs will be required in space-borne techniques for measuring major pollutants, including particulate aerosols, with sub-20 km horizontal resolution and the capacity to resolve vertically within the lower troposphere.

## WATER AND AIR: FUNDAMENTAL SCIENCE CASE STUDY

### Ion exchange

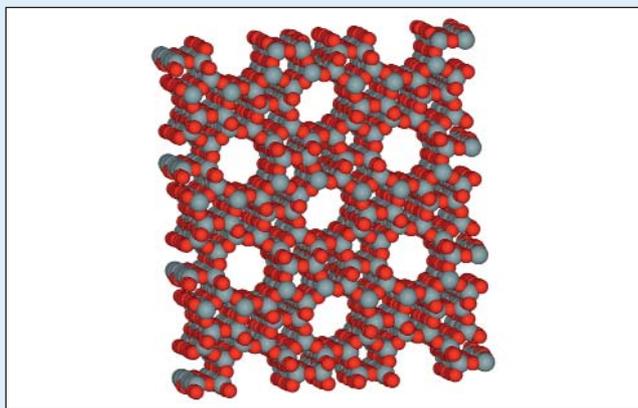
*Building on the discovery of ion exchange by soil chemists, drinking water standards have been improved globally by a new generation of chemists seeking a better fundamental understanding of materials that soften and purify water.*

Ion exchange is the transfer of charged particles (ions) between a solid and a solution. This process was first observed in soils. However, it took almost 100 years to develop into a practical tool for water purification and ion exchange techniques are still being developed today.

The phenomenon of ion exchange was first documented in 1850 by two English chemists, John Thomas Way and Harry Stephen Thompson.<sup>105</sup> They confirmed that ion exchange occurs naturally in soil. Experimentation proved that it was possible to release calcium ions by treating various clays with ammonium sulfate or carbonate in solution.

After ion exchange was observed in soil, research was done in an attempt to understand the material properties that were causing the effect. Zeolites, along with other minerals, were identified as being capable of ion exchange. Zeolites are aluminium based minerals with a porous structure, which allows them to trap ions such as sodium and calcium. However, the ions are only held weakly by the mineral, allowing them to be exchanged readily with other positively charged ions in surrounding solutions. Hard water contains high concentrations of minerals including calcium<sup>2+</sup> and magnesium ions, leading to limescale build up and poor soap lathering. Scientists wondered if they could use these ion exchange properties of zeolite to soften water. To test this possibility hard water was mixed with zeolite 'charged' with sodium ions. In 1905 German chemist Robert Gans achieved this goal: the water was softened because calcium and magnesium ions in the water were exchanged with sodium ions in the zeolite.<sup>106</sup>

Although zeolites were used for ion exchange as early as 1905, the material properties that caused the effect were poorly understood. To create synthetic ion exchangers with different functions, understanding of the materials had to be improved. A major step towards this was made in 1935 when English chemists Basil Albert Adams and Eric Leighton Holmes discovered that crushed phonograph records were capable of ion exchange.<sup>107</sup>



The micro-porous molecular structure of a zeolite, ZSM-5

An improved understanding of synthetic materials that were capable of ion exchange meant that novel ion exchange materials could be produced. This discovery was soon put into practice and in 1937 the first synthetic ion exchange resin was used in a commercial water softening plant in the UK.

Armed with a better fundamental understanding of material properties, further improvements to ion exchange materials were made over the following decades. Properties such as capacity were improved and resins could be designed to have specificity for different ions. Current ion exchange resins are usually based on polystyrene beads conjugated with different chemical groups that determine their ion exchange properties.

In addition to water softening, ion exchange can also be used to remove toxic metal ions, which can be detrimental to human health, from water. The global water treatment industry is worth around \$30 billion. This includes ion exchange technology, which is often in parallel with other water purification methods that remove micro-organisms and organic material to ensure that drinking water is safe. Ion exchange in water treatment can be used on both a large scale in water treatment plants and in homes. Water filter jugs, kettles and plumbed in systems, such as those made by BRITA, contain ion exchange resin and these products are popular because of the improvement in the taste of the water. In addition, ion exchange is used to produce ultrapure water for the pharmaceutical industry.

Our understanding of ion exchange is contributing to developing sophisticated membranes that may be able to produce drinking water from salt water sources. In the future these membranes may be used for desalination to produce safe, secure and sustainable drinking water supplies around the world.

## Appendix

### A1 Study methodology

The process consisted of a number of different stages, which are outlined below.

April 2008	<b>Scoping group workshop</b> – A workshop to develop clear visions and issues for each priority area, as defined by the steering group, and to explore new lines of enquiry.
May 2008	<b>Exploration workshops</b> – Facilitated workshops that allowed the RSC to better understand the potential of a series of new lines of inquiry, which encompassed and expanded the initial priority areas.
June 2008	<b>Crafting and articulating workshop</b> – A workshop to bring together all the big thoughts and themes that emerged throughout the scoping group and exploration workshops and current RSC policy work. These defined the challenges and potential opportunities for the chemical sciences for each priority area.
June–July 2008	<b>Online consultation 1</b> – Online consultation to comment on the challenges and potential opportunities for chemical sciences for each of the priority areas.
September 2008	<b>Online consultation 2</b> – Online consultation to review responses to the first session and subsequent revised challenges and opportunities for the science focused Priority Areas. To comment on a series of identified priorities mapped against a timeline for each priority area and provide input to the implementation phase.
November 2008	<b>Online evaluation</b> – Participants were given the opportunity to evaluate the process.
December 2008	<b>Prioritisation exercise</b> – Online survey to determine which of the 41 challenges relating to the seven priority areas identified during the project the RSC should lead on.

The main output from the process was identifying the seven priority areas, which encompass the key global issues facing the world today and in the future.

Across the seven priority areas 41 major challenges society face are highlighted, as are a selection of the hundreds of opportunities where chemistry and the chemical sciences have a role to play in contributing to the delivery of solutions. The main opportunities for the chemical sciences have been mapped to a 15 year time horizon for each thematic area.

A total of seven workshops, incorporating over 150 experts took place during 2008; these were leaders in their field, including chief scientists and Nobel Prize winners. In addition, the expertise, attitudes and opinions of the wider community were incorporated via an open three-stage web based consultation. All RSC members and key stakeholders were invited to participate in June 2008, September 2008 and November 2008. Stakeholder and public engagement specialists Dialogue by Design were commissioned to carry out and manage the online consultation process on behalf of the RSC. Over 1300 individuals registered their interest to participate and submitted over 2000 comments.

In the first stage participants were invited to comment on, contest and add depth to a series of key societal challenges and potential opportunities for the chemical sciences that were identified during earlier workshop stages. In the second stage participants were invited to review all the submissions to the first phase. For each priority area participants were also asked to comment on a series of timelines, where the main opportunities for the chemical sciences have been mapped to a 15 year time horizon. The final phase gave participants the opportunity to evaluate the process.

This was supplemented by the views of our substantial and varied member network groups, which were collected during various stages of the project and at the RSC's Annual General Assembly in Birmingham in November 2008. At the General Assembly members helped determine which of the 41 challenges the RSC would be best placed to lead. This list was further prioritised by an online survey in December 2008, where 1350 people participated. A total of 10 challenges were identified for the RSC to focus on over the coming years.

## A2 Energy

### Energy efficiency

#### Challenge

Improvements are needed in the efficiency with which electricity is generated, transmitted and energy is used.

#### Potential opportunities for the chemical sciences

- Further developments in materials chemistry
  - Develop superconducting materials which operate at higher temperatures
  - Develop cheaper, better insulating materials, including recycled materials
  - Use nanotechnology and other methods to increase the strength to weight ratio of structural materials
  - Develop more efficient lighting – *eg* OLEDs
  - Develop smart windows
- Developing novel/more efficient coatings, lubricants and composites
- Improve energy intensive processes through process optimisation; process intensification; new process routes, including developing new catalysts; and improved separation technologies
- Improve fuel economy: develop high performance catalysts and next generation fuels

### Energy conversion and storage

#### Challenge

The performance of energy conversion and storage technologies (fuel cells, batteries, electrolysis and supercapacitors) needs to be improved to enable better use of intermittent renewable electricity sources and the development/deployment of sustainable transport.

#### Potential opportunities for the chemical sciences

- Reduce production and material costs
  - Use self assembly methods
  - Replace expensive materials
- Increase calendar and cycle lives, recyclability and durability
- Improve modelling of thermodynamics and kinetics
- Improve power density
- Improve energy density
- Advance the fundamental science and understanding of surface chemistry
- Replace strategic materials to ensure security of supply – *ie* platinum
- Develop enzymatic synthesis of nanomaterials
- Improve safety of devices – *ie* problems associated with overheating
- Decrease the cycle time of batteries – *ie* charging time needs to be reduced
- Develop material recycling strategies

## Fossil fuels

### Challenge

Current fossil fuel usage is unsustainable and associated with greenhouse gas production. More efficient use of fossil fuels and the by-products are required alongside technologies that ensure minimal environmental impact.

### Potential opportunities for the chemical sciences

- Further research and development of carbon capture and storage (CCS) technologies
  - Research alternatives to amine absorption, including polymers, activated carbons or fly ashes for removing CO<sub>2</sub> from dilute flue gases
  - Further research the storage options for CO<sub>2</sub> – *ie* in ageing oilfields, saline aquifers or unmineable coal seams
  - Advance the understanding of corrosion and long term sealing of wells
  - Improve understanding of the behaviour, interactions and physical properties of CO<sub>2</sub> under storage conditions
  - Research the options for CO<sub>2</sub> as a feedstock – *ie* converting CO<sub>2</sub> to useful chemicals
  - Research the integration of CCS technologies with new and existing combustion and gasification plants
- Further research into extracting and processing crude oil is required
  - Improve the understanding of the physical chemistry of oil, water and porous rock systems for enhanced oil recovery technology
  - Develop novel chemical additives to improve water flooding and miscible gas injection
  - Utilise unconventional oil reserves by better understanding the chemistry and physics of reservoirs and petroleum fluids
  - Develop improved catalysts and separation and conversion processes for production of ultra-low sulfur fuels
  - Develop tailored separation technologies for clean, atom efficient refineries
- Further research and development of clean coal technologies is required
  - Short term: develop advanced materials for plant design – *ie* corrosion resistant materials for use in flue gas desulfurisation (FGD) systems
  - Develop better catalysts for emissions control, particularly SO<sub>2</sub> and NO<sub>x</sub>
  - Improve understanding of corrosion and ash deposition
  - Improve process monitoring, equipment design and performance prediction tools to improve power plant efficiency
  - Develop advanced coal products – *ie* improved briquetted domestic fuel with lower emissions for use in domestic dwellings
  - Medium term: improved materials for supercritical and advanced gasification plants
  - Develop gasification technologies
  - Interface various power generation plants with fuel cells and carbon capture and storage technologies to move towards zero emissions technology
- Further research and development of natural gas processing
  - Develop gas purification technologies
  - Improve high temperature materials for enhanced efficiency and performance
  - Develop catalysts for improved combustion and emissions clean-up

## Nuclear energy

### Challenge

Nuclear energy generation is a critical medium term solution to our energy challenges. The technical challenge is for the safe and efficient harnessing of nuclear energy, exploring both fission and fusion technology.

### Potential opportunities for the chemical sciences

- Research methods for the efficient and safe utilisation of nuclear fission
  - Advance the understanding of the physico-chemical effects of radiation on material fatigue, stresses and corrosion in nuclear power stations
  - Improve methods for spent fuel processing including developing advanced separation technologies, which will allow unprecedented control of chemical selectivity in complex environments
  - Design and demonstrate the new generation of advanced reactors including GEN IV based fuel cycles using actinide-based fuels
  - Study the nuclear and chemical properties of the actinide and lanthanide elements
  - Improve understanding of radiation effects on polymers, rubbers and ion exchange materials
- Nuclear fusion
  - Develop high performance structural materials capable of withstanding extreme operating conditions

## Nuclear waste

### Challenge

The problems of storage and disposal of new and legacy radioactive waste remain. Radioactive waste needs to be reduced, safely contained and opportunities for re-use explored.

### Potential opportunities for the chemical sciences

- Improved processes for nuclear waste separation and reuse
  - Develop areas of reprocessing chemistry – *ie* recycling of spent fuel into its constituents of U, Pu and fission products
  - Use actinide separation chemistry in nuclear waste streams – *eg* zeolites for sorption, membranes, supercritical fluids, molten salts
  - Understand solids formation and precipitation behaviour and a reduction in the number and volume of secondary waste streams through developing non-aqueous processes
- Research into the UK's legacy and new nuclear waste storage options
  - Use wastefrom chemistry (including the science of materials used in immobilising nuclear waste materials) to solve waste management issues
  - Develop new and improved methods and means of storing waste in the intermediate and long term, including new materials with high radiation tolerance
  - Improve understanding of long term ageing and development of microstructural properties of cements, waste/cement interaction and the corrosion of metallic components in cement materials used in storing intermediate level waste
  - Study methods of waste containment for storage in a geological site
- Methods for nuclear plant decommissioning and site remediation
  - Research into environmental chemistry (hydro-geochemistry, radio-biogeochemistry and biosphere chemistry) issues
  - Methods for effective and safe post-operational clean-out of legacy facilities

## Biopower and biofuels

### Challenge

Fuels, heat or electricity must be produced from biological sources in a way that is economic (and therefore efficient at a local scale), energetically (and green-house gas) efficient, environmentally friendly and not competitive with food production.

### Potential opportunities for the chemical sciences

- Develop tools to measure impacts of biofuels over entire life cycle (Life cycle analysis) – ie impacts of land use change
- Genetically engineer plants to produce appropriate waste products and high value chemical products
- Genetically engineer plants to grow on land (or sea) that is unsuitable for any food crops
- Genetically engineer plants with increased efficiency of photosynthesis, increased yields and requiring lower carbon inputs
- Develop better pre-treatment technologies to improve the handling/ storage of biomass
- Improve bio-refinery processes
  - Improve modelling and analytical methods
  - Improve ways of hydrolysing diversified biomass and lignocellulose
  - Improve extraction of high value chemicals before energy extraction
  - Improve thermochemical processes, including developing better catalysts, microbes and enzymes
  - Improve flexibility of feedstock and output (electricity, heat, chemicals, fuel or a combination)
- Develop methods of producing fuel from new sources such as algae or animal and other wastes
- Develop ways of managing the bio-refineries waste streams so as to minimise environmental impact
- Develop engine technology and improve understanding of surface technology to improve efficiency of biofuels for transport

## Hydrogen

### Challenge

The generation and storage of hydrogen are both problematic. Developing new materials and techniques so that we can safely and efficiently harness hydrogen will be required to enable its use as an energy vector, appropriately scaled to different applications.

### Potential opportunities for the chemical sciences

- Improve efficiency of splitting water via electrolysis, using electricity preferably from renewables
  - Develop improved electrode surfaces for electrolyzers and materials of construction
  - Find uses for the by-product  $O_2$
- Investigate methods of photocatalytic water electrolysis
  - Light harvesting systems must have suitable energetics to drive the electrolysis
  - Systems must be stable in an aqueous environment
- Improve efficiency of  $H_2$  production from the thermochemical splitting of water
  - Research into new heat exchange materials
  - Improve the understanding of the fundamental high temperature kinetics and thermodynamics
- Research the production of biochemical hydrogen generation
  - Discovery new microorganisms or genetically modify existing organisms and improve culture conditions for hydrogen production by fermentation or photosynthesis
  - Develop using microorganisms in microbial fuel cells to generate hydrogen from waste
  - New efficient bio-inspired catalysts for use in fuel cells
- Research into the safe and efficient storage of hydrogen
  - Fuel cells (see Energy conversion & storage)
  - New nanostructured materials, such as carbon nanotubes, or metal hydride complexes
- Research methods of implementing a hydrogen national infrastructure
  - Better materials for fuel cells and for on-board hydrogen storage
  - Large-scale  $H_2$  production processes using renewable or low-carbon energy sources

## Solar energy

### Challenge

A source of energy many more times abundant than required by man, harnessing the free energy of the sun can provide a clean and secure supply of electricity, heat and fuels. Development of existing technologies to become more cost efficient and developing the next generation of solar cells is vital to realise the potential of solar energy.

### Potential opportunities for the chemical sciences

- Improvements to the design of current 'first generation' photovoltaic cells
  - Develop lower energy, higher yield and lower cost routes to silicon refining
  - Develop a lower CO<sub>2</sub>-emission process to the carbo-thermic reduction of quartzite
  - Develop more efficient or environmentally benign chemical etching processes for silicon wafer processing
  - Base-metal solutions to replace the current domination of silver printed metallisation used in almost all of today's first-generation devices
- Improvements to 'second generation' thin-film photovoltaics
  - Improve the reaction yield for silane reduction to amorphous silicon films
  - Research alternative materials and environmentally sound recovery processes for thin cadmium-containing films on glass
  - Research sustainable alternatives to indium
  - Develop processes to improved deposition of transparent conducting film on glass.
- Develop third-generation photovoltaic materials based on molecular, polymeric and nano-phase materials for significantly more efficient and stable devices, suitable for continuous deposition on flexible substrates.
- Develop high efficiency concentrator photovoltaic (CPV) systems
- Improve Concentrated Solar Power (CSP) plants used to produce electricity or hydrogen.  
New thermal energy storage systems using pressurised water and low cost materials will enable on-demand generation day and night.
- Research into producing 'Solar fuels'
  - Improve photoelectrochemical cells in which photovoltaics are coupled to the electrolysis of water to generate hydrogen
  - Research aimed at mimicking photosynthesis to generate hydrogen or carbohydrates.  
Requires developing light harvesting, charge separation and catalyst technology
  - Improve photobioreactors and photosynthetic organisms (algae and cyanobacteria) for generating hydrogen or for processing to biofuels

## Wind and water

### Challenge

Since power generation yields from tide, waves, hydro and wind turbines are intermittent and geographically restricted, effective energy supply from these natural world sources needs further development to minimise costs and maximise benefits.

### Potential opportunities for the chemical sciences

- Develop embedded sensors/sensing materials, which allow instant safeguarding of wind towers
- Develop lightweight durable composite materials, coatings and lubricants
- Develop technologies for salinity-gradient energy, also called blue energy, working either on the principle of osmosis (the movement of water from a low salt concentration to a high salt concentration) or electrodialysis (the movement of salt from a highly concentrated solution to a low concentrated solution). This requires further developments that reduce the cost or improve the efficiency of membranes to improve significantly the economics of this process
- Further develop ocean technologies for producing electricity including tidal barrages, tidal current turbines and wave turbines
- Develop long lasting protective coatings, required to reduce maintenance costs and prolong operating life of wave, wind and tidal energy devices

## A3 Food

### Agricultural productivity

#### Challenge

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.

#### Potential opportunities for the chemical sciences

Agricultural productivity is broken down into six sub-challenges:

##### 1. Pest control

Challenge: Up to 40 per cent of agricultural productivity would be lost without effective use of crop protection chemicals. Agriculture is facing emerging and resistant strains of pests. The development of new crop protection strategies is essential.

- New high-potency, more targeted agrochemicals with new modes of action that are safe to use, overcome resistant pests and are environmentally benign
- Formulation technology for new mixtures of existing actives, and to ensure a consistent effective dose is delivered at the right time and in the right quantity
- Develop better pest control strategies, including the using pheromones, semiochemicals and allelochemicals, as well as GM and pesticides
- Pesticides tailored to the challenges of specific plant growth conditions – *eg* hydroponics
- Reduce chemical crop protection strategies through GM crops

##### 2. Plant science

Challenge: Increasing yield and controlling secondary metabolism by better understanding plant science.

- Understand and exploit biochemical plant signals for developing new crop defence technologies
- Improve the understanding of carbon, nitrogen, phosphorus and sulfur cycling to help optimise carbon and nitrogen sequestration and benefit plant nutrition
- Understand plant growth regulators
- Develop secondary metabolites for food and industrial use
- Understand the impact of nutrients at the macro and micro level
- Exploit the outputs of this understanding using biotechnology
- Nitrogen and water usage efficiency – *eg* drought resistant crops for better water management
- Better yields of components for biofuels and feedstocks through the use of modern biotechnology

##### 3. Soil science

Challenge: Understanding the structural, chemical and microbiological composition of soil and its interactions with plants and the environment.

- Develop fertiliser formulations able to improve the retention of nitrogen in soil and uptake into plants
- Optimise farming practices by understanding the biochemistry of soil ecosystems, for example, the chemistry of nitrous oxide emissions from soil, the mobility of chemicals within soil, and partition between soil, water, vapour, roots and other soil components
- Improve the understanding of methane oxidation by bacteria (methanotrophs) in soil to help in developing methane-fixing technologies
- Understand soil structure – mechanical properties of soils and nutrient flow
- Low energy synthesis of nitrogen and phosphorus-containing fertilisers – alternatives to Haber–Bosch

#### 4. Water

Challenge: Coping with extremes of water quality and availability for agriculture.

- Use grey water in agriculture
- Targeted use of water in agriculture (drip delivery)

#### 5. Effective farming

Challenge: Minimising inputs and maximising outputs through agronomic practice

- Develop rapid *in situ* biosensor systems that can monitor soil quality and nutrients, crop ripening, crop diseases and water availability to pinpoint nutrient deficiencies, target applications and improve the quality and yield of crops
- Analyse climate change parameters – *eg* greenhouse gases and seawater salinity, generates input for predictive models, which can identify changing conditions for agronomy providing valuable data for planting new crops
- Precision agriculture at the field level
- Engineering tools for on farm practices – *eg* grain drying, seed treatment and crop handling

#### 6. Livestock and aquaculture

Challenge: Optimised feed conversion and carcass composition.

- Develop new vaccines and veterinary medicines to treat the diseases (old/new/emerging) of livestock and farmed fish – *ie* zoonoses
- Aquaculture production for food and industrial use (including algae)
- Understand feed in animals: feed conversion via nutrigenomics of the animal and bioavailability of nutrients
- Formulation engineering for delivery and minor component release and reduced waste – *ie* phosphorus in pigs & fish
- Genetic engineering
- Genetic analysis for conventional breeding – Qualitative Trait Loci (QTL)

## Healthy food

### Challenge

We need to better understand the interaction of food intake with human health and to provide food that is better matched to personal nutrition requirements.

### Potential opportunities for the chemical sciences

- Understand the chemical transformations taking place during processing, cooking and fermentation processes, that will help to maintain and improve palatability and acceptance of food products by consumers
- Develop novel satiety signals, for example, safe fat-replacements that produce the taste and texture of fat
- Technology to produce sugar replacements and natural low calorie sweeteners to improve nutrition and combat obesity
- Model the whole digestive tract to research the digestion of new food and ingredients
- Understand the role of gut microflora in sustaining health and the role of probiotics and prebiotics in promoting health
- Further develop and understand fortified and functional food with specific health benefits, and the impact of minor nutrients on health
- Better understand formulation technology for the controlled release of macro- and micronutrients and removing unhealthy content in food
- Nutrigenomics and nutrigenetics to satisfy individual genotype, optimise nutrition and health, protect against disease and identify allergenic responses
- Develop diets for specific groups, such as neonates, adolescents and the elderly
- Use of the glycaemic load of food in understanding nutrition and the role of glucose in health and the onset of type II diabetes
- Better understand the nutritional content of all foods so that we can produce food more efficiently for the life-stage nutritional requirements of humans, livestock and fish
- Formulate for sensory benefit
- Formulation science to increase nutritional content of food
- More nutritious crops through GM technologies
- Target food composition for immune health

## Food safety

### Challenge

Consumers need to be given 100 per cent confidence in the food they eat.

### Potential opportunities for the chemical sciences

- Better understand the links between diet and cancer. For example, research into naturally occurring carcinogens in food such as acrylamide and mutagenic compounds formed in cooking
- Develop microsensors in food packaging to measure food quality, safety, ripeness and authenticity and to indicate when the 'best before' or 'use-by' date has been reached
- Harness analytical chemistry to design rapid, real-time screening methods, microanalytical techniques and other advanced detection systems to screen for chemicals, allergens, toxins, veterinary medicines, growth hormones and microbial contamination of food products and on food contact surfaces
- Efficacy testing and food safety of new food additives, such as natural preservatives and antioxidants
- Domestic hygiene – visible signalling
- Irradiation for removing bacterial pathogens and preventing food spoilage
- Chemical labelling to enable traceability – rapid fingerprint methods
- Understand the effects of prolonged exposure to food ingredients

## Process efficiency

### Challenge

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

### Potential opportunities for the chemical sciences

Process efficiency is broken down into two sub-challenges:

#### 1. Food manufacturing

Challenge: Building highly efficient and sustainable small scale manufacturing operations.

- Storage technologies
  - Develop new, more efficient refrigerant chemicals that will help avoid environmental damage and save energy
  - Increase efficiency of refrigeration technology at all stages in the supply-chain – *eg* super-chilling as an alternative to freezing
  - Develop ambient storage technologies for fresh produce
  - Develop improved food preservation methods for liquids and solids, including rapid chilling and heating, and salting
- Intensify food production processes by scaling down and combining process steps
- Improve process control to raise production standards and minimise variability
- Develop routes for by-product and co-product processing to reduce waste and recover value
- Develop milder extraction and separation technologies with lower energy requirements
- Develop technologies to minimise energy input at all stages of production – *eg* high pressure processing and pulsed electric fields
- Optimise the forces needed to clean surfaces during food processing – new surface coating technologies to minimise fouling and to minimise energy requirements for cleaning
- Methods for the synthesis of food additives and processing aids
- Understand and inhibit the chemistry of food degradation
- Chemical stabilisation technologies for produce, including both their formulation and delivery

#### 2. Food distribution

Challenge: Optimising methods to distribute foods by minimising energy requirements and environmental impact.

- Life cycle analysis – mapping carbon footprints
- Sensors to monitor food stuffs in transport
- Quality measurement and control: analytical techniques to detect pesticide residues, adulteration and confirm traceability

## Supply chain waste

### Challenge

There is an unacceptable amount of food wasted in all stages of the supply chain. We need to find ways to minimise this or use it for other purposes.

### Potential opportunities for the chemical sciences

- Use analytical methods to support Lifecycle Analyses of the environmental impact of individual food products, packaging and materials
- Extract and apply valuable ingredients from food waste – *eg* enzymes, hormones, phytochemicals, probiotics cellulose and chitin
- Polymer chemistry to develop new biodegradable, recyclable or multifunctional packaging materials, to reduce environmental damage and the quantity of packaging used in the supply-chain
- Understand the biochemical processes involved in produce ripening and food ageing, enabling shelf-life prediction and extension
- Develop new methods for the efficient use, purification and cost-effective recovery of water in food processing, leading to water-neutral factories
- Develop efficient anaerobic treatment plants to process farm, abattoir and retail waste, to generate biogas
- Use waste products as feedstock for packaging material, for example, the producing a novel biodegradable plastic material made from epoxides and CO<sub>2</sub>
- Develop biodegradable or recyclable, flexible films for food packaging – *eg* corn starch, polylactic acid or cellulose feedstock, able to withstand the chill-chain, consumer handling, storage and final use – *eg* microwave or conventional oven
- Develop functional and intelligent packaging films providing specific protection from moisture, bacteria and lipids, improving texture and acting as carriers for various components – *eg* nanotechnologies
- Packaging for food that is compatible with anaerobic digestors
- Recycle mixed plastics used in food packaging to recover monomers
- Sensors to replace inaccurate sell-by dates

## A4 Future cities

### Resources

#### Challenge

Cities place huge demands on waste, water and air quality management. We need technologies that help provide healthy, clean, sustainable urban environments.

#### Potential opportunities for the chemical sciences

##### Monitoring and improving air quality

- Catalysts for efficient conversion of greenhouse gases with high global warming potential (in particular  $\text{N}_2\text{O}$ ,  $\text{CH}_4$  and  $\text{O}_3$ ), including those that occur in dilute process streams
- Develop low cost, localised sensor networks for monitoring atmospheric pollutants, which can be dispersed throughout developed and developing urban environments
- Improve catalysts for destroying pollutants, in particular  $\text{CO}$ ,  $\text{NO}_x$ , hydrocarbons, VOC, particulate matter
- Advanced end of pipe treatment, including separation methods, catalysis and using plasma surface etching *etc*
- Healthy buildings:
  - Air quality management (sensor technologies coupled to ventilation system)
  - Functionalised surfaces for decomposing VOCs in homes

##### Monitoring and improving the quality of and conserving water

- Purify drinking water, targeting the conversion and removal of a wide variety of substances at low concentrations
- Increase local use of grey water
- Detergents designed for grey water reuse
- Treatments for grey water remediation

##### Reducing waste

- Increase the proportion of city waste to be recycled – *eg* improve processes for recycling plastics, electronics and organic matter – *ie* composted or processed to become a fuel
- Use/develop low environmental impacting materials – *eg* recyclable or easily disposable plastics, which are designed to be compatible with recycling methods
- Soil remediation through applying (bio) catalysts
- Synthetic biology application of bioremediation for the clean up of toxic spills

##### Generic issues

- Smart devices that can sense, intervene and 'correct'
- Environmental monitoring
- Sensors for checking for 'leaks' in distribution systems

## Home energy generation

### Challenge

Most homes rely upon inefficient energy technologies. We need to develop new technologies and strategies for local (home) energy generation and storage with no net CO<sub>2</sub> emissions.

### Potential opportunities for the chemical sciences

- Using alternative energy sources
  - More flexible low cost photovoltaics based on 'first generation' silicon materials
  - New solar panel production approaches, hybrid materials, new electrodes, photovoltaic paints
  - Biogas fuel cells
  - CHP units for small residences/homes using a variety of fuels – *ie* renewables/waste
  - Harnessing thermal energy – *eg* excess heat from car engines
  - Harvesting geothermal energy through improved heat transfer and anti-corrosion materials
- Superior domestic batteries and alternative energy storage approaches
  - Lithium batteries based on alternative electrodes/electrolytes and polymers – *eg* nanostructured electrode materials of high specific capacity, mesoporous carbon electrodes and electronically conducting polymer electrodes
  - Develop design concepts and new materials for microsized batteries for mobile and portable electronic devices
  - Fuel cells: PEM & DMFC; mesoporous carbon supported catalysts; electronically conducting polymer supported catalysts; novel catalysts containing low or no noble metal content. Develop thin film deposition and patterning techniques
  - Hydrogen storage
- Technology approaches such as supercapacitors

## Home energy use

### Challenge

Current and evolving technologies could significantly reduce the burden of buildings/homes on energy consumption.

### Potential opportunities for the chemical sciences

- Ubiquitous on-board power sources for low energy-density devices
- Intelligent ICT components and sensors able to respond to parameter changes in temperature, light intensity *etc* requiring new conductive/non conductive polymers and flat lightweight displays
  - Nanocoatings for decorations
  - Photochromic coatings for glass
- Appliances with improved energy efficiency
- Light and energy management technologies
- Develop LEDs and OLEDs
- Nanoscale controlled deposition (microcontact printing, nanotemplate patterning *etc*) on thin films and integration into products like self-cleaning surfaces

## Construction materials

### Challenge

We need to use materials for construction (such as for roads and buildings), which consume fewer resources in their production, and confer additional benefits in their use, and may be used for new build and for retrofitting older buildings.

### Potential opportunities for the chemical sciences

- New materials for designing new buildings and structures
- Functionalised materials
  - Functionalised building materials/surfaces that perform detoxification: low temperature nanoscale catalysts designed to decompose volatile organic compounds
  - Functional textiles requiring lightweight and low cost nonporous systems, and self-healing and self-cleaning nanocoatings
  - Anechoic building materials to provide non-flammable sound insulation and reduce urban stress
  - Smart building materials integrated with intelligent ICT components and sensors able to respond to parameter changes (such as changes in temperature)
- Insulating materials
  - Develop new high performance insulating materials – eg aerogel nanofoams
- Develop self-cleaning materials
- Develop intrinsically low energy materials
  - Develop innovative (low temperature/low CO<sub>2</sub> emissions) cement compositions based on recycled materials
- Recyclability and reduced dependence on strategic materials

## Mobility

### Challenge

Urban transport is fuel inefficient and environmentally damaging. Enormous societal benefits will flow from scientific and technological solutions to these problems.

### Potential opportunities for the chemical sciences

- Reduce CO<sub>2</sub> emissions from transport
- Eco-efficient hybrid vehicles will require new energy storage systems (enhanced lithium batteries and supercapacitors)
- Catalysts for CO<sub>x</sub>, NO<sub>x</sub>, SO<sub>x</sub> decomposition
- Develop lubricant and fuel formulations that increase the fuel economy of vehicles
- Develop new recyclable materials for the lightweight construction of vehicles (thermoplastic foams, organic fillers-based thermoplastic composites) including alternative assembly/disassembly methodologies without compromising safety
- Improve the internal combustion engine through developing and using new materials to reduce wear and friction, and combustion/additive chemistry
- Smart polymers as actuators – integrating the power source and the machine movement
- New tyre technologies to reduce fuel consumption and reduce noise
- Improve sensor technologies for engine management and pollution/emission gas detection
- Reduce pollution from air transport
- Alternative catalyst technologies compatible with jet engines
- Catalysts for fuel quality and emissions control for ships
- Coatings for reducing friction

## ICT

### Challenge

Public and business demand outstrips the current capacity of the existing ICT infrastructure, creating opportunities for the successful commercial application of technological innovations.

### Potential opportunities for the chemical sciences

- Data storage
  - Information storage: holographic storage, by means of new molecular and polymeric materials; DNA-based and protein-based biological switches; molecular switches and photoresponsive devices
- Miniaturisation for device size and speed
  - Integrate nanostructures in device materials
  - Self assembly of biological and non-biological components to produce complex devices such as biosensors, memory devices, switchable devices that respond to the environment, enzyme responsive materials, nanowires, hybrid devices, self assembly of computing devices, smart polymers
  - Polymers for high density fabrication: identify suitable materials meeting resolution, throughput and other processing requirements
- Printed electronics
- High density, low electrical resistance, interconnect materials to enable ultra high speed, low power communication: metallic nanowires; metallic carbon nanotubes
- Lightweight materials for ICT
- Power management
  - Nanomaterials for power management; identify mechanisms for the self assembly of low resistance interconnects, and high-k dielectric materials with low electrical leakage
- Reduce, recycle and reuse of materials used in information and communication technology
- Reduce dependence on strategic materials

## Public safety and security

### Challenge

Technology must increase its role in ensuring people feel and are safe in their homes and the wider community. High population densities increase the potential impact of environmental and security threats.

### Potential opportunities for the chemical sciences

- Chemical and biological sensors: remote, rapid, miniaturised and reactive sensors; sensor networks; chemical analogue of CCTV that could for example trace narcotics or the geographical movements of suspects; home security networks; miniaturised analytical detectors to carry out range of functions as components of portable consumer articles; hybrid biological devices, such as cheap biosensors that can communicate the information needed made from the self assembly of biological and non-biological components
- Crime: evolutionary, real time information rich crime scene profiles; advances in DNA profiling/fingerprint technology, 'Lab on a chip'
- Develop high performance protective materials for civil protection practitioners – *eg* police
- Novel detection technologies to identify counterfeit products: drugs; money; high value products
- Data handling and sharing – chemometrics
- Chemical biometrics
- Early detection of potential pandemic diseases through developing effective and rapid analytical techniques

## A5 Human health

### Ageing

#### Challenge

With an ageing population, we need to enhance our life-long contribution to society and improve our quality of life.

#### Potential opportunities for the chemical sciences

- Prevent, treat and control chronic diseases – *eg* cancer, Alzheimer's, diabetes, dementia, obesity, arthritis, cardiovascular, Parkinson's, osteoporosis)
- Focus on preventative intervention – *eg* statins, flu jab – what next?
- Improve the understanding of the impact of nutrition and lifestyle – *eg* nutraceuticals – on future health and quality of life
- Develop practical non-invasive bio-monitoring tools – *eg* 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 – *eg* artificial organs, tissues, eye lenses *etc*

### Diagnostics

#### Challenge

We need to enable earlier diagnosis and develop improved methods of monitoring disease.

#### Potential 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, detect infection and respond to attack

## Hygiene and infection

### Challenge

To prevent and minimise acquired infections, we need to improve the techniques, technologies and practices of the anti-infective portfolio.

### Potential 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 – *eg* paint, coatings
- Detect and reduce airborne pathogens – *eg* 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

## Materials and prosthetics

### Challenge

Orthopaedic implants and prosthetics need to be fully exploited to enhance and sustain function fully.

### Potential 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 – *eg* 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

## Drugs and therapies

### Challenge

We need to harness and enhance basic sciences to help transform the entire drug discovery, development and healthcare landscape so new therapies can be delivered more efficiently and effectively for the world.

### Potential opportunities for the chemical sciences

- Chemical tools for enhancing clinical studies – *eg* non-invasive monitoring *in vivo*, biomarkers, contrast agents *etc*
- Design and synthesise small molecules that attenuate large molecule interactions *eg* protein–DNA interactions
- Understand the chemical basis of toxicology and hence derive 'Lipinski-like' 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

### Effectiveness and safety

- Understand communication within and between cells and the effects of external factors *in vivo* to combat disease progression
- Monitor the effectiveness of a therapy to improve compliance
- 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 – *eg* 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

## Personalised medicine

### Challenge

We need to be able to deliver specific, differentiated prevention and treatment on an individual basis.

### Potential opportunities for the chemical sciences

- Apply advanced pharmacogenetics to personalised treatment regimes
- Use an individual's genetic profile for diagnosis and treatment
- 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

## A6 Lifestyle and recreation

### Creative industries

#### Challenge

Continued innovation is necessary to give new options to designers, artists and architects.

#### Potential opportunities for the chemical sciences

- Develop new materials for restoring and protecting new and historical buildings
- Develop new materials for use in architecture, in designing new buildings and structures
- Developing new materials and applications for creative designers – *eg* dynamic systems that change colour, texture or feel as desired
- Sustainable and renewable packaging coupled with emerging active and intelligent materials – *eg* developing time, temperature, spoilage and pathogen indicator technologies
- Develop new dyes that are more stable and less toxic
- Better preservation & protection of materials, *eg* film and magnetic materials
- Use chemical science in preserving/restoring paintings and other cultural treasures: develop analysis techniques to determine the compounds that comprise the colour pigments and materials

### Household

#### Challenge

Household and personal care products that promote convenience and perceptions of well-being, or that deliver household functionality, need to combine efficacy with safety and sustainability/ longevity.

#### Potential opportunities for the chemical sciences

- Continue to move formulation of household and personal care products from 'black art' to a more scientific basis
- Facilitate reformulation of household and consumer products to address safety and environmental concerns
- Further develop recyclable materials and building technologies including new materials for constructing houses and their contents (floor covering, furniture *etc*)
- Develop self-cleaning materials for homes
- Reduce waste by rethinking systems and usage – *eg* less detergent in the water means less to dispose of
- Improved understanding of the chemical basis of toxicology in new/novel household products and their breakdown in the environment to a level where good predictive models can be developed and used, such as computational chemistry (safety assessment without the use of animals) for human and eco-toxicology
- Better understanding of the effect of dermatology and cosmetic ingredients at a molecular and cellular level
- Controllable surface adhesion at a molecular level. Switchable adhesion – *eg* self assembly furniture, self cleaning materials, self hanging pictures and wall paper, which at the flick of a switch you can remove, replace or disassemble

## Sporting technology

### Challenge

We need to develop new materials that enable higher performance as an ultimate sporting goal, and bring a sense of well-being to the wider and ageing population.

### Potential opportunities for the chemical sciences

- Advance/develop materials chemistry for sporting equipment including protective wear
- Use active diagnostics and monitoring to assist personal performance – *eg* hormone levels
- Keeping sport and recreation accessible to the wider population, especially the ageing population through the chemistry underlying healing, flexibility, aerobic performance *etc*

## Advanced and sustainable electronics

### Challenge

Miniaturised electronic devices, with faster computer speeds and denser storage, need to be produced. This should be coupled with developing sustainable electronic devices, which are recyclable, and have little dependence on materials in increasingly short supply.

### Potential opportunities for the chemical sciences

- Improve controlled deposition (microcontact printing, nanotemplate patterning *etc*) on thin films and integrate into printed electronics
- Develop design concepts and new materials for micro-sized batteries for mobile and portable electronic devices
- Further enhance information storage technology – *eg* molecular switches with the potential to act as a molecular binary code
- Develop biological and/or molecular computing
- Understand biomimicking self-assembling systems
- Printable (allowing dynamic re-configuration) electronics based on new molecular technologies
- Exploit the interface between molecular electronics and the human nervous system – *eg* using the brain to switch on a light
- Advance display technology – *eg* flat lightweight and rollable displays – for a variety of applications

## Textiles

### Challenge

There is a need to move away from a conventional, low-cost, disposable fashion culture to new systems which provide design scope, colour, feel, sustainability, longevity and new, low-cost fabrication routes.

### Potential opportunities for the chemical sciences

- Functional textiles with superior energy balance and flexible use for garments, in the home and construction industry, requiring lightweight and low cost systems, and self-healing and self-cleaning dynamic pigmentation technologies
- New synthetic fibres from sustainable sources
- Biotherapeutic textiles – *eg* in wound dressing – building on currently available technology
- Textiles that respond to their environment
- New fabrication technologies (*cf* spray-on T-shirt)

## A7 Raw materials and feedstocks

### Sustainable design

#### Challenge

Our high level of industrial and domestic waste could be resolved with increased downstream processing and re-use. To preserve resources, our initial design decisions should take account of the entire life cycle.

#### Potential opportunities for the chemical sciences

- Wider role of chemistry in product design for 4Rs (reduction, remanufacture, reuse, recycle)
  - Technology for designing biodegradability into finished products
  - Methods for tagging of polymers to aid recycling
  - Wider training of chemists in sustainable design
  - New composites that are readily recyclable
  - Develop and apply smart coatings
  - Develop improved recovery processes
- Manufacturing process intensification and optimisation
  - Atom efficiency
  - Green chemistry and chemical engineering
  - Process modelling, analytics and control
- Improve life cycle assessment (LCA) tools and metrics
  - Clear standards for LCA methods and data gathering
  - Methods to assess recycled materials
  - Tools to aid substitution of toxic substances
- Improve the understanding of ecotoxicity
  - Better understand structure-property relationships

### Conservation of scarce natural resources

#### Challenge

Raw material and feedstock resources for both existing industries and future applications are increasingly scarce. We need to develop a range of alternative materials and associated new processes for the recovery of valuable components.

#### Potential opportunities for the chemical sciences

- Recovery of metals
  - Methods to recover metals from 'e-waste'
  - Extract metals from contaminated land/landfills
- Substitute key materials
  - Select the most effective metal in high volume applications
  - Improve fertiliser management of N and P
  - Improve battery design and reduce dependence on finite metal resources – eg lithium
- Reduce material intensity
  - Apply nanoscience to increase activity per unit mass
  - Reduce raw material – ie thrifting

## Conversion of biomass feedstocks

### Challenge

Biomass feedstocks (whether they are agricultural, marine or food waste) for the production of chemicals and fuels are becoming more commercially viable. In the future, integrated bio-refineries using more than one biofeedstock will yield energy, fuel and a range of chemicals with no waste being produced.

### Potential opportunities for the chemical sciences

- Develop bioprocessing science for producing chemicals
  - Methods for generating homogeneous feedstocks
  - Improve biocatalytic process design
  - Develop fermentation science to increase the variety and yield of products
  - Metabolic engineering for improved biomass feedstock properties
- New separation technologies
  - Membranes and sorbent extraction of valuable components from biological media
  - Pre-treatment methods for biomass component separation
- Novel catalysts and biocatalysts for processing biomass
  - New techniques for lignin and lignocellulose breakdown
  - Microbial genomics to produce improved micro-organisms
  - Pyrolysis and gasification techniques for pre-treatment and densification of biomass
  - Catalysts for upgrading pyrolysis oil
  - Technologies to exploit biomethane from waste
- Convert platform chemicals to high value products
  - Oxygen and poison tolerant catalysts and enzymes
  - New synthetic approaches to adapt to oxygen-rich, functional starting feedstocks

## Recovered feedstocks

### Challenge

There are limits to the current supply of chemical and fuel feedstocks from alternative sources. The conversion of readily available, cheap feedstocks and waste into useful chemicals and fuels is an opportunity for chemical scientists.

### Potential opportunities for the chemical sciences

- Small molecule activation
  - CO<sub>2</sub> as a feedstock – producing amino acids, formic acid and methanol
  - Catalytic conversion of simple alkanes as a feedstock
  - Biomimetic conversion of CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub> to chemicals
  - Artificial photosynthesis/solar energy conversion
- Recycling processes
  - Novel separation and purification technologies for economic recycling
  - Shift to viewing 'waste' as a raw material
  - Genuine, innovative recycling technologies – *ie* not downcycling – especially for plastics

## A8 Water and air

### Drinking water quality

#### Challenge

Poor quality drinking water damages human health. Clean, accessible drinking water for all is a priority.

#### Potential opportunities for the chemical sciences

- Energy efficient point of use purification such as using disinfection processes and novel membrane technologies
- Develop portable technologies for analysing and treating contaminated groundwater that are effective and appropriate for use by local populations – *ie* for testing arsenic contaminated groundwater
- Develop new instruments, sensors and analytical approaches and techniques to ensure consistent and comparable measurement globally. For example, ongoing development of sensors for real time water quality monitoring in distribution systems
- Develop energy efficient desalination technology

### Water demand

#### Challenge

Population growth means greater demand on water supply. Household, agricultural and industrial demands are in competition. Management and distribution strategies must ensure that clean water of an appropriate quality remains economically accessible.

#### Potential opportunities for the chemical sciences

- Products designed to minimise water and energy use during their production and use through water footprinting. This can be done by adopting, for example, the principles of green chemistry and the principles of integrated pollution prevention and control, to industrial manufacture, with an aim of reducing waste, and energy and water use
- Household products and appliances designed to work effectively with minimal water and energy demands and include better water recycle systems
- Efficient, safe and low maintenance systems developed for industrial recycling of water
- Efficient water supply systems and anticorrosion technologies for pipework, including developing materials to prevent leakages and water quality maintenance
- Better strategies for water use and re-use for agriculture systems

## Waste water

### Challenge

Wastewater treatment needs to be made energy neutral and we need to enable the beneficial re-use of its by-products.

### Potential opportunities for the chemical sciences

- More energy efficient industrial waste water treatment technologies are needed potentially exploiting novel membrane, catalytic and photochemical processes
- More efficient ways are needed of treating domestic waste water (to avoid the high energy input and sludge generation associated with using biological processes). For example, developing a foul sewer network that can be considered part of the treatment plant and works as a long, continuously monitored pipe reactor that treats water *in situ* and maintains quality to the point of delivery
- Breakthroughs in membrane technology for microfiltration, ultrafiltration and reverse osmosis to reduce costs significantly and improve process efficiency for removing particulates, precipitates and micro-organisms
- Novel coatings and chemicals for minimising corrosion in pipe-work, biofilm growth and deposition of solids such as iron and manganese during water and wastewater treatment
- Develop processes for localised treatment and re-use of waste water to ensure that appropriate quality water is easily accessible. Standards for rainwater and grey water identified so that coupled to appropriate localised treatment rain/grey water can be harvested and used for secondary purposes such as toilet flushing or crop irrigation

## Contaminants

### Challenge

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

### Potential opportunities for the chemical sciences

- Study the breakdown of and transport of substances in the aquatic environment, including emerging contaminants such as pharmaceuticals and nanoparticles
- Research into understanding the impact of contaminants on, and their interaction with biological systems
- Research into how, if possible, to assess the risk to the environment and human health of mixtures of chemicals at low concentrations
- Identify the potential impact of climate change on contaminant fate and behaviour

## Air quality and climate

### Challenge

Increasing anthropogenic emissions are affecting air quality and contributing to climate change. We need to understand the chemistry of the atmosphere to be able to predict the impact of this with confidence and to enable us to prevent and mitigate further changes.

### Potential opportunities for the chemical sciences

- Develop novel techniques for studying reactive molecules that occur at ultra-low concentrations in the atmosphere and are the agents of chemical change
- Understand, through developing novel techniques for studying sub-micron particles, how aerosols form and change in the atmosphere, and their impacts on human health and climate
- Develop new chemical sensors for atmospheric gases and aerosols, which are cheap enough for widespread deployment
- Provide the underpinning knowledge from laboratory studies to advance atmospheric chemistry models
- Develop new modelling methodologies for treating the enormous chemical complexity that occurs on regional and global scales
- Study geo-engineering solutions to modify the Earth's climate in response to rising greenhouse gas levels, looking both at the effectiveness and undesirable environmental side-effects of these solutions

## A9 Glossary of key terms

### Priority Areas

Priority Areas are the key societal concerns on a national and global level, where the RSC and the chemical sciences can have a role to play in providing innovative solutions.

### Challenges

Within each priority area, 41 challenges for scientists, engineers and wider society have been defined as a result of the workshops.

### Opportunities

For each challenge, potential opportunities for the chemical sciences have been identified; these will be key in helping to provide solutions.

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**Royal Society of Chemistry**

Burlington House  
Piccadilly, London  
W1J 0BA, UK  
**Tel:** +44 (0)20 7437 8656  
**Fax:** +44 (0)20 7437 8883

Thomas Graham House  
Science Park, Milton Road  
Cambridge CB4 0WF, UK  
**Tel:** +44 (0)1223 420066  
**Fax:** +44 (0)1223 423623

**Email:** [roadmap@rsc.org](mailto:roadmap@rsc.org)  
**www.rsc.org**