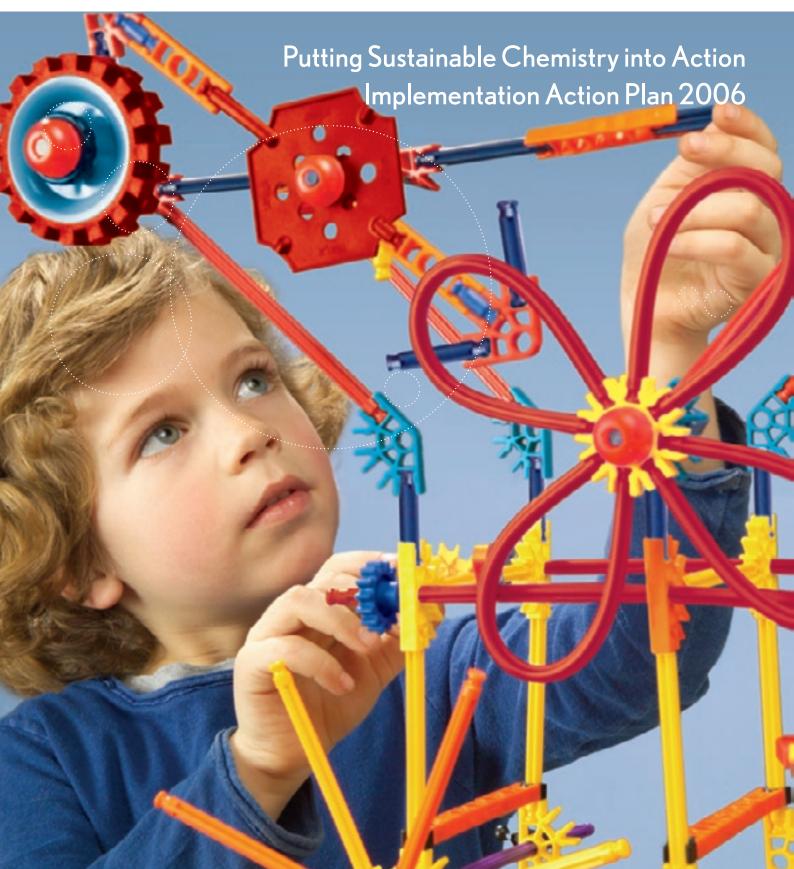
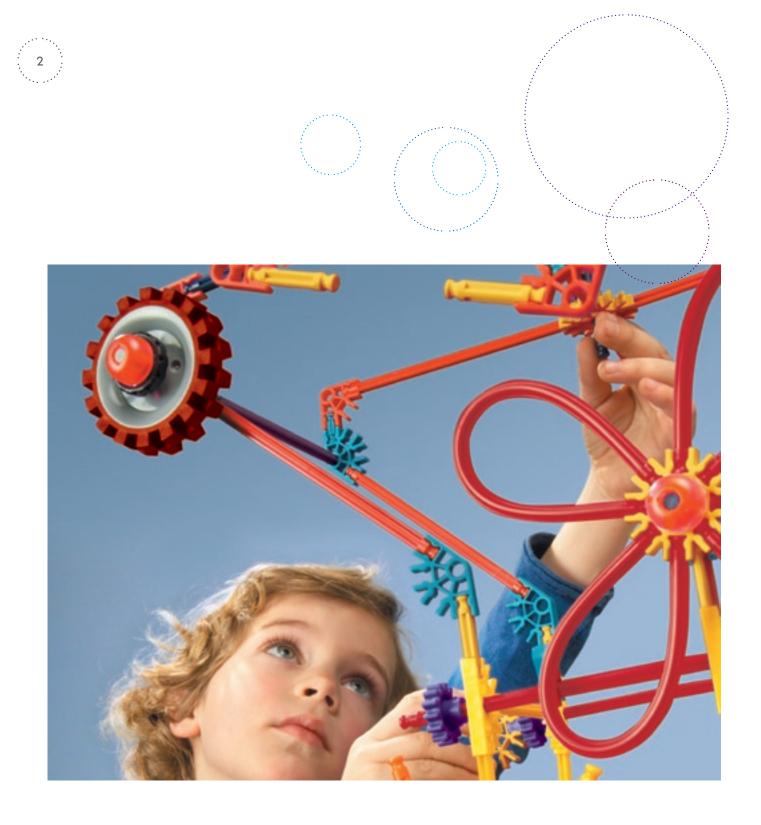


# Innovating for a Better Future





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### Up-to-date information

SusChem communicates via its own website, <u>http://www.suschem.org</u> Regular newsletters are published and can be found at <u>http://www.suschemsolutions.org</u>



Welcome to the SusChem Implementation Action Plan: this is the third document produced by SusChem and in some senses is the most important.

The European Technology Platform for Sustainable Chemistry was initiated jointly by Cefic and EuropaBio in 2004 to help foster and focus European research in chemistry, chemical engineering and industrial biotechnology. That partnership was expanded to include Dechema, ESAB, the GDCh and the RSC. In addition many other stakeholders have joined SusChem activities since then. The first output from SusChem, the vision document, was published in March 2005. It painted a picture of a sustainable European chemical industry with enhanced global competitiveness, providing solutions to critical societal demands and powered by a world-leading technological innovative drive.

SusChem then produced a Strategic Research Agenda (SRA) in November 2005 outlining the future priorities for European research efforts. The SRA identified key areas of research as well as the limitations and hurdles faced by researchers. In its foreword I called for the European Commission, Member States, industry and academia to implement the SRA. The present document represents the output of the discussion and consultation that followed that call.

This Implementation Action Plan (IAP) explains how the research priorities that were identified in the SRA can be implemented. For each research theme it describes in detail the issues that need to be addressed to realise its respective potential. It also illustrates activities required by SusChem, its stakeholders and other parties to facilitate this process. While the SRA focused on topics and themes, the IAP focuses on activities and actions.

The time horizon of the IAP is obviously shorter than that of the SRA as it focusing on the most pressing issues. However, SusChem will monitor progress in achieving the IAP and update it from time to time considering achievements made and new topics that need to be included.

SusChem continues to unite a wide variety of stakeholders around its vision. It is an open and transparent grouping of stakeholders: new stakeholders interested in chemistry, industrial biotechnology and chemical engineering research, development and innovation can join at any time.

My fellow SusChem Board members and I are committed to SusChem continuing its highly valuable work during the implementation phase of the research agenda. The SusChem partners have already agreed on supporting SusChem beyond 2006. Future SusChem activities are described in this IAP. SusChem's further evolution into the future is also very much up to its stakeholders so please get involved and help to shape the future of European research.

1. alung

**Alfred Oberholz** Chairman SusChem Board Deputy Chairman of the Board of Management, Degussa

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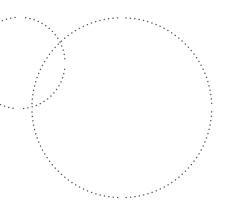
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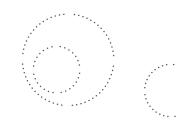
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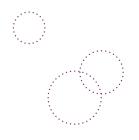


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Chemistry has a clear role in delivering technological solutions to the challenges facing society today. It will be at the heart of stimulating the European economy, providing new opportunities and creating wealth that will benefit all citizens.

# The way forward



# The way forward



# Sustainable Chemistry – goals and strategic research agenda

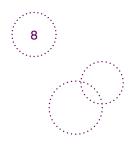
The European Technology Platform for Sustainable Chemistry (SusChem) vision responded to the societal needs for chemistry\* in Europe by:

- Providing the innovative drive for Europe: chemistry does not just deliver raw materials – it is a major source of innovation in areas from clothing to energy and pharmaceuticals.
- Being at the heart of the new technologies that underpin the knowledge-based economy: chemistry is the core science of nanotechnology, biotechnology and environmental technology.
- Investing for sustainable development: chemistry is improving the eco-efficiency of products and processes to optimise the use of resources and minimise waste and environmental impact.
- Protecting and extending employment, expertise and quality of life: chemistry is providing the innovation for knowledge-based enterprise across Europe; it is already a knowledge-led sector with a highly trained workforce stimulating significant growth and wealth creation across Europe.

Having established a vision SusChem prepared a Strategic Research Agenda (SRA) outlining the future priorities for European research efforts. The document comprised of the contributions from four working groups (industrial biotechnology, material technologies, reaction and process design and horizontal issues) tasked with identifying key areas of research and the limitations and hurdles faced by researchers, and with starting the process of proposing future activities.

One point is clear throughout: sustainable chemistry is a key driver for innovation in many technologies and disciplines, providing the knowledge to improve the benefits of traditional technologies and combine them with nano- and biotechnologies, leading to new and improved products. A clear interdisciplinary approach within the three technology areas, supported by cross-cutting actions in areas such as education and training, stakeholder dialogue including public engagement activities, and measures to create a Europe with the appropriate regulatory and financial environment for innovation (for Europe to become the preferred location for innovation activities), is needed for successful implementation of these challenges.

\*SusChem considers chemistry in its broadest sense, including industrial biotechnology, polymers and other synthetic materials and indeed all the products and services covered by the SusChem SRA and IAP.



The Industrial Biotechnology section of the SRA details the approach needed to make Europe's industries' leaders in biotechnology processes and technologies in a number of sectors, including chemicals, food and nutrition, textiles, leather, animal feed, pulp and paper, energy and waste processing. Industrial biotechnology plays a key role in increasing the sustainability of the European economy. From a business perspective the main themes for R&D in industrial biotechnology are the development and production of novel, innovative products and processes in a cost- and eco-efficient manner using increasingly renewable raw materials, through the discovery and optimisation of microorganism strains and biocatalysts.

The *Materials Technology* section focuses on materials for mankind's future surroundings, which will be designed to enhance the quality of life while at the same time minimising the use of resources and limiting environmental impact. These materials will make life simpler, easier, safer, better, and, more importantly, place mankind at the centre of technology. One important factor will be the role of nanoscience, and related nanotechnologies, in providing the knowledge necessary to lead to innovative products and process methods. Nanotechnology is an important enabling technology for the development of new material technologies. Reaction and Process Design is essential to achieve sustainable development: the *Reaction and Process Design* section considers the processes that will be used in the development, design and production of the appropriate products. These fundamental enabling technologies will contribute to the entire lifecycle from product development via catalyst and process development, plant development and operation to product handling and logistics. Reaction and process design integrates the complementary approaches of chemical synthesis, and process design and engineering, providing key contributions to all relevant steps from reaction to viability of process plants, and is applicable to all areas of chemistry and biotechnology.

The Horizontal Issues section takes into account the necessary political, social and structural reforms needed to maintain and increase Europe's edge within the increasingly global world of innovation. The top level goal is to ensure that the citizens of the EU benefit from the development and use of innovations based on the SusChem SRA. In particular there is a need to ensure that SusChem technologies lead to wealth and job creation within the EU. Priority areas for further work within the horizontal arena fit into two themes: stimulating support for innovation; and addressing societal concerns associated with new products and processes. These include the evaluation and improvement of funding models for innovation, new communication and dialogue approaches with all stakeholders including the public, and means to develop the appropriate skills sets to enhance the human capacity that will underpin these innovations.



# The Implementation Action Plan

The Implementation Action Plan (IAP) is the third in the series of SusChem documents. After presenting the vision for the future and the Strategic Research Agenda (SRA) focusing on research topics and themes, the next logical step is to explain how exactly the research themes defined in the SRA are to be implemented and to describe what SusChem and its stakeholders need to, and will, do to facilitate this process, and which other parties to involve. Thus, the IAP focuses on activities and actions.

The Implementation Action Plan describes more precisely for each research theme identified in the SRA the issues that need to be addressed in the short term to realise the full potential of research and innovation. This is followed by a definition of the next steps which are necessary to progress each topic and of the prerequisites, if any, that need to be fulfilled (requirements, constraints) before this next step can be taken. This process leads to a further prioritisation, an ordering of topics and activities and detailed roadmaps.

The IAP also includes a general perspective on the framework necessary (such as policy, capacity building, and

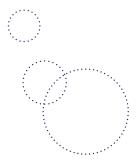
public acceptance) to speed up innovation in chemistry, biotechnology and chemical engineering, and a description of the actions needed to achieve these conditions.

The actors who will eventually perform the activities described in the IAP are manifold. They include a variety of SusChem stakeholders (academia, industry, authorities) as well as the platform itself and the partners involved in the organisation of SusChem, now and in the future. The future role of SusChem in the implementation phase and within the network of related and relevant European initiatives is described in the final section of this document.

The IAP is written from today's perspective and sets a time horizon shorter than that of the SRA. SusChem will monitor progress in achieving the IAP and revise the plan on a regular basis taking into account progress against targets, and adding new targets and topics from the SRA. SusChem will also revise the SRA albeit less frequently.

For easy reference the structure of the IAP is depicted in the diagram below to show the various horizontal and vertical parts.

The way forward	Introdu	ction						
Realising the SRA	Bio-based economy	Energy	Healthcare	Information and communication technologies	Nanotechnology	Sustainable quality of life	Sustainable product and process design	Transport
	Requirements Novel resources and business models							
с	INovel r	esources a	nd busines	s models				
Supportive environment	Innovat	ion framew	vork					
	Public engagement, capacity building							
	Visionary projects: Smart Energy Home Biorefinery F <sup>3</sup> Factory							
Strengthening foundations								
	Future SusChem role and activities							



The SusChem Implementation Action Plan defines activities to turn dialogue into actionable outcome moving towards the vision of sustainable chemistry in Europe. Significant funding and alignment of European and national research programmes is needed for success.

# Realising the SRA

Actions for research, networking and training.

Eight themes for the **future** 

Superior novel products and processes.

# **Realising the SRA**

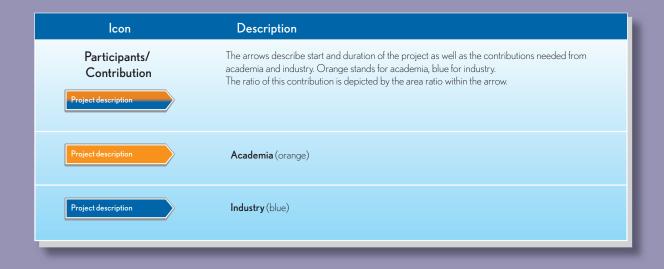


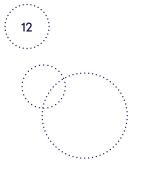
The IAP defines priority research areas for several themes that are of major importance for sustainable chemistry in terms of market expectations, societal demand and impact, or for the sustainability of different industrial sectors. These themes are:

- Bio-based economy.
- O Energy.
- Healthcare.
- Information and communication technologies.
- Nanotechnology.
- Sustainable quality of life.
- Sustainable product and process design.
- Transport.

Priorities are already defined in the SusChem Strategic Research Agenda. However, the IAP focuses on those which require the most immediate steps to be taken. For each priority, a set of activities is proposed that need to be followed to enable the goals set forth in the SusChem Vision and Strategic Research Agenda to be achieved.

The requirements and the time frame for each activity are also presented in graphical form in order to allow easy visualisation. Beyond the graphical summary of activities, the following chapters will also provide reasons for choosing a specific activity, the expected outcomes, the contribution to gap closure and other valuable information. For the diagrams, the following symbol keys are used:

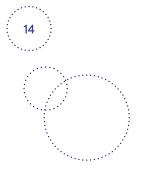




lcon	Description
Project type	Different types of projects might be needed depending on the envisaged activity:
	<b>Research projects:</b> Projects ranging from frontier/basic research to applied, pre-competitive research the primary aim of which is to generate scientific and technical knowledge that can be further used for the development of new innovative products and/or improving the sustainability of existing production. These projects will benefit from collaborative efforts and networks.
	<b>Demonstration/Pilot project:</b> Projects with the aim of demonstrating the industrial and economic feasibility, and the sustainability of a concept.
	<b>Studies:</b> These projects, including surveys, feasibility studies, LCA or eco-efficiency analysis, aim at generating knowledge/information allowing stakeholders and decision-makers to make informed choices.
	<b>Network/Coordination:</b> Networks and coordination projects will allow better coordination between stakeholders in a field, interdisciplinary cooperation, exchange of information and alignment between European and Member States levels.
	<b>Training:</b> Exchange/Mobility of researchers, courses and projects influencing curricular programmes in the Member States.
Funding resources	Activity funding might come from different sources. While a general overview of available funding resources required for different project types is given in <i>Resources - ways and means</i> , the pie charts present the envisaged distribution of funding sources for each activity. Possibilities for venture capital, if they exist, will be addressed in the text.
	Private or industry funding (dark blue)
	European Union funding (white)
$\diamond$	National funding (light blue)
Funding amount	The monetary symbols give a scale for the resources required during the total duration of the activity.
-	<10 Million €
	10 - 50 Million €
	> 50 Million €



lcon	Description
Human resources	Activities require human resources with adequate training and expertise.
Ŕ	A blue symbol depicts that sufficient research expertise is, or is likely to be, available in Europe.
<b>İ</b>	An orange symbol means that such a skill base needs to be actively developed for a sufficient number of researchers.
Relations to other sections in the IAP	Certain activities might not be specific to one of the sections chosen within the SusChem IAP. To avoid unnecessary duplication in the document and to show the importance of activities for other areas the areas of importance for each activity are clearly indicated.
Bioeconomy	Bio-based economy
Energy	Energy
Healthcare	Healthcare
ICT	Information and communication technologies
Nano	Nanotechnology
QoL	Sustainable quality of life
SPPD	Sustainable product and process design
Transport	Transport
Existing activities	For the SusChem IAP activities were selected based on the importance of the issue and the relevance to the overall SusChem goals. It is often the case that other research and networking activities of relevance are already ongoing. New projects must build on such ongoing activities to achieve the best value. The puzzle pieces indicate whether significant, related and currently ongoing activities exist within the EU (FP6), at national level, in ERAnets, and/or in other regions of the world. More details of su activities are given in the description for each activity. Related technology platforms are mentioned the text and are summarised in <i>Integration, cooperation and networking</i> .
FP6	Within the EU (FP6)
National	National level
ERAnet	ERAnets
Inter national	In other regions of the world
	Out of all IAP priorities a few have been chosen as early priorities,



# **Bio-based economy**

Industrial biotechnology is a key technology required to realise the Knowledge Based Bioeconomy (KBBE) and to transform life sciences knowledge into new sustainable,

eco-efficient and competitive products, through an optimised combination of classical and new biochemical processes, especially in the chemical, biopolymers and biofuels sectors. However technological advances still need to be made.

The following three topics have been identified as the top priorities to facilitate the harmonious development of industrial biotechnology in Europe:

- Biocatalysis novel and improved enzymes and processes.
- Development of the next generation of high efficiency fermentation processes.
- Process eco-efficiency and integration: the biorefinery concept.

# BIOCATALYSIS – NOVEL AND IMPROVED ENZYMES AND PROCESSES

Enzymes are increasingly used to perform a range of chemical reactions. These catalysts from nature are sustainable, selective and efficient, and offer a variety of benefits such as environmentally friendly manufacturing processes, reduced use of solvents, lower energy requirement, high atom efficiency and reduced cost. However, natural biocatalysts are often not known or not optimally suited for industrial applications. To develop this research area, and especially the use of enzymes in industrial processes, it is important to expand the range of reactions catalyzed by enzymes and to improve their properties for industrial applications. Currently hydrolases are mainly being employed. Specific types of enzymes are needed to expand the scope and to reduce the number of synthetic steps. In this respect ligases, isomerases and oxidoreductases, are of particular interest for the development of sustainable industrial processes. This programme is aimed at the discovery, evolution and development of novel, robust and selective biocatalysts suitable for industrial use, and builds on Europe's strong position in enzyme manufacturing and utilisation and will allow Europe to attain leadership in industrial biotechnology.

# Goals

The aim of research in biocatalysis is to:

- Employ nature's toolkit to foster a shift in chemical manufacturing to enable cleaner, safer and more cost efficient processes.
- Assure the basis for continued innovation in industry by addressing the increasing need for selectivity, stability and efficiency in the use of enzymes as catalysts.
- Enable novel chemo-enzymatic processes with the integrated use of biocatalysts by the discovery, evolution and/or design of enzymes.
- Solve reaction and process problems of industrial relevance and support the move to sustainable chemistry through the search for novel biocatalytic functions and the selection of new high performance process configurations.

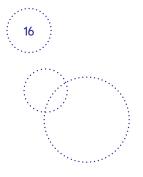
# Key activities

- Novel and improved biocatalysts
- Biocatalytic process design



# Novel and improved biocatalysts: discovery of new functions and properties of enzymes via new tools and technologies

Biocatalysis – novel and improved enzymes and processes							
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities	
	Novel an	d improved bio	ocatalysts				
0 5 Years				-10-			
Screen nature's diversity for novel biocatalysts.	X					National	
Improve target-oriented screening technologies.	X					Industry National	
New tools and technologies for novel and improved enzymes.	X					Industry National	
Understand catalytic enzyme/substrate interactions.	X				SPPD	National	
Novel enzymes for specific applications.	ľ				Health SPPD	National	
Improvement of biocatalysis.	Ť				SPPD	Industry National	



This activity is aimed at the discovery, evolution and development of novel selective biocatalysts suited for industrial use, and builds on Europe's strong position in enzyme manufacturing and utilisation and will allow Europe to attain leadership in industrial biotechnology.

A range of national projects and centres of excellence exist in various European countries such as Austria, UK, Netherlands, Germany, France, Czech Republic which will benefit from moves towards European integration. The creation of a European Biocatalysis Network (EBN) to provide network information between different European institutions and disciplines, as well as between basic and applied research, is essential for linking the search for new biocatalysts and the optimisation of the biocatalyst with the biocatalytic process design. Existing European Centres of Excellence (CoE) also suggest that focused major projects on bioligation and bioredox would benefit from better integration and collaboration.

# Novel biocatalysts

The top research priority is the search for new biocatalysts by the screening and development of novel enzymes for specific applications in response to the drive towards sustainable chemistry which requires that key catalytic transformations such as those for chiral compounds are shifted to biocatalytic processes. Examples of such applications include enzymes from the Enzyme Commission system like oxidoreductases, isomerases and ligases.

# High research priorities are:

- Screening nature's biodiversity: the search for novel enzymes and microorganisms from a wide range of environments (e.g. marine) including extreme environments. This includes the use of metagenomics and directed evolution in order to discover new enzymes/molecules, which cannot be detected in current hosts, and improvement of the isolation and cultivation of microorganisms.
- Target oriented screening methodologies: the implementation of improved target oriented screening technologies, including applied research to define how to mimic enzymatic processes in small and microscale systems and tests under the desired process conditions.

- New screening tools: the implementation of new tools and technologies to discover functionality and properties of new enzymes.
- Novel biocatalysts for specific applications.

Specific attention has to be given to new products and intermediates derived from biocatalytic processes and to new technologies making more organisms amenable for metabolic engineering.

# Improvement of biocatalysts

High priority must be given to:

- **Understanding biocatalysis:** the top research priority is clearly fundamental research on the understanding of catalytic enzyme / substrate interactions and the search for new biocatalysts.
- Developing methods and technologies for **biocatalyst improvement**:
  - Development of screening methods, directed evolution and rational design for the optimisation of biocatalysts.
  - Development of methodologies to integrate novel transformations into existing enzyme scaffolds, trying new approaches such as designing peptide based enzyme mimetics for use in non aqueous systems and improving catalytic efficiency.
  - Optimisation of biocatalysts for the production of biobased performance materials and nanocomposites (in collaboration with the SusChem Materials Technology section).
  - Development of tools to predict *in silico* the most suitable enzymes with optimised properties.
  - Multidisciplinary research to achieve high performance integrated multiphase bioconversions, which involves different disciplines such as molecular biology, enzyme technology and biochemical engineering to optimise biocatalyst function with respect to compatibility in multistep reactions.



# HR IAP-related Activities Action and timeline Distribution Amount Туре Biocatalytic process design Years +→ gration of biocatalysi SPPD Energy SPPD Energy Health SPPD lationa SPPD Energy SPPD step reactions, cascade/chem Energy

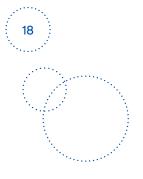
# Biocatalytic process design: expansion of the range of biocatalytic processes for industrial use

The focus here is to solve reaction and process problems of industrial relevance and support the the move to sustainable chemistry by developing systematic process design technology for the quick and reliable selection of new and clean high performance manufacturing process configurations.

The top research priorities are clearly the **integration of biocatalysts into industrial processes** (see *SusChem SRA*, p. 53), and biocatalytic reaction engineering (see *SusChem SRA*, p. 55). This will help to achieve better control of processes, and improve the safety, health and environmental impact through the development of more selective and efficient processes. High research priority must be given to:

- Multiphase bioreactors.
- The development of **multi-step reactions, including cascade reactions** for example featuring natural and nonnatural catalysts working in tandem.
- The integration of chemo- and biocatalysis, either in subsequent steps or in heterogeneous catalysis, for example through catalyst or engineering design.

Specific attention must be given to **biochips and microdevices** for analytical purposes as well as to **modular bioreactors** and to the reduction of the number of unit operations in biocatalytic processes.



# DEVELOPING THE NEXT GENERATION OF HIGH EFFICIENCY FERMENTATION PROCESSES

Fermentation processes are commonly used today for the production of numerous products. However, to meet growing demands in very competitive markets still requires technological improvement. Current bottlenecks include low volumetric productivity and low yield of the organisms under non-optimal fermentation conditions (pH, temperature, substrate concentration, product inhibition) in bioreactors. Reasons for low productivities in fermentation processes include poor sugar uptake, production of side-products, overflow mechanism, redox imbalance, energy (ATP) shortage, and/or product inhibition at high concentrations. Another key issue is the current poor understanding of cellular behaviour in bioreactor surroundings, the improvement of which requires better ways of ways of monitoring the events in the bioreactor (real-time analytical measurements tools) and mathematical models to control processes better and improve understanding for strain optimisation.

New challenges are also emerging including the design and construction of microbioreactors and high-throughput screening needed by industry for novel and improved processes. Future efforts will also concentrate on the development of new technologies that can provide tailormade products (e.g. biopolymers) for industrial and medical applications. The reliable and renewable supply of energy is also of importance, and therefore many bioprocesses will be combined with energy generation.

Another challenge lies in the difficulties of scaling-up processes from laboratories to large-scale fermenters, and the investment needed to develop and implement new bioprocesses which account for a significant part of the total production costs. These new expectations for fermentation processes require the use of highly advanced technologies and the cooperation of experts from various areas of science.

# Goals

This priority is aimed at increasing the efficiency of fermentation processes by:

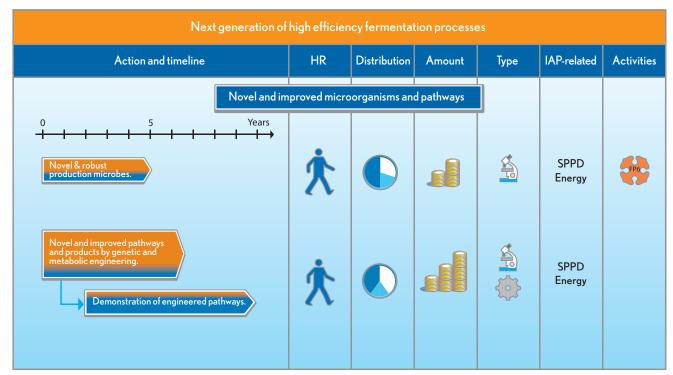
- Enhancing existing or new microorganisms to reach optimum production capacities under industrial conditions.
- Improving fermentation process engineering through better bioreactors and downstream processing.

# **Key** activities

- · Novel and improved microorganisms and pathways
- Improved fermentation and downstream processes



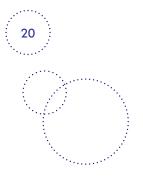
# Novel and improved microorganisms and pathways



## Novel and robust production microorganisms

Industry needs microbial production systems to perform new, innovative and efficient bioprocesses. Such systems will need to withstand high substrate and product concentrations. Since high concentrations can lead to stress conditions like pH extremes or toxicity of substrates, products or adjuvant chemicals, it is necessary to develop robust multipurpose production systems. These developments will be enabled by investigation of the complete genome, proteome, and metabolome of a set of suitable microorganisms, which are compatible with existing industrial practices. In addition, it is important to study flux analysis and energy streams of production microorganisms in order to understand better the economics and chemistry of a microbial production system. A versatile microbial production system can be developed once effective molecular biology systems for the introduction of new genes and metabolic pathways are constructed and guantitative mapping of material and energy fluxes in, out and within the cells is understood.

Complete control of the molecular biology tools will enable the fast deletion or inhibition of genes which disturb the efficient production of the target chemical. Two strong trends can be followed in parallel, on the one hand screening in nature for novel robust production organisms, and on the other hand the improvement of a few "plug bugs" which are highly suitable for industrial production systems. Of particular importance is also the development of microbes that are able to cope with varying feedstock streams (C5/C6 sugar mixes, by-products, etc.). Strong cooperation between industry and academia will promote faster development of novel and robust production microorganisms that are industrially relevant and useful for the production of a variety of industrial products.



To develop **novel and robust production microorganisms**, the following topics must be studied:

- The study, isolation and use of the "moderate" extremophiles (those growing at temperatures of 50 - 60 °C and at relatively low or high pH) from different environments for harvesting the natural potential of useful production organisms. It is very important that these microorganisms are amenable to genetic engineering as they will need to be improved and modified in a later stage.
- The molecular biology toolbox for the organisms in question should allow fast and effective manipulation of the organisms. It must be possible to eliminate/suppress and/or add/over express genes in any part of the genome of an industrial production organism for the synthesis of desired biochemicals.
- The genomes of several microorganisms, which are suitable for industrial production processes, will need to be sequenced. If not done already, and the genes will need to be annotated. The intimate knowledge and understanding of the genome of a microorganism is a prerequisite for optimising it for the production of new biochemicals.
- The study of functional genomics for deciphering the genome of industrial production organisms is very important. Although many industrial microorganisms are completely sequenced, the allocation of genes to function still suffers from a significant lack of understanding: there is an abundance of genes for which no function has been found and the physiological role and importance of many genes remains very poorly understood.
- The effect of stress conditions on the patterns of gene expression will be investigated. The knowledge derived from these studies can be used to adapt the organisms to stress conditions through genetic engineering. The stress conditions in question include extremes in pH and temperature as well as osmotic stress and presence of (slightly) toxic compounds.

- The secretome of the microbial production system will be fully analysed in order to identify possible side products and to complete the flux analysis. The goal of this study is to further increase the yield of the production processes by eliminating the leaking of material streams into unwanted byproducts. In addition, the study of the secretome can be used to identify new biochemical pathways which can be further exploited for chemical synthesis with these organisms.
- The development of zero-growth production processes would significantly improve current production processes that are typically reliant on microbial growth.

A key achievement using the technologies mentioned above will be the design and construction of microorganisms by synthetic biology for a given application.

# Novel and improved pathways and products through genetic and metabolic engineering

Metabolic engineering aims to improve cellular activities by the manipulation of enzymatic transport and regulatory functions of the cell, typically using recombinant DNA technology. Improved bioprocesses can be obtained by optimising the microbial metabolism via the manipulation of enzyme levels to alter or redirect the metabolic flux towards a particular metabolite. Also the mathematical modelling of microbial metabolism is increasingly important, as it permits faster development of production strains and the optimisation of microbial metabolism.

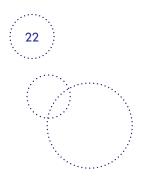
Nowadays, entirely new bioprocesses can be developed by the introduction of novel, non-native enzymes (e.g. from extremophiles, etc.) into an "optimal" microorganism, which has desirable properties with respect to its specific growth rate, genome, stability, process efficiency, growth requirements etc., but which is a non-native producer of a certain metabolite. The product range of a popular production strain can thus be significantly enlarged.



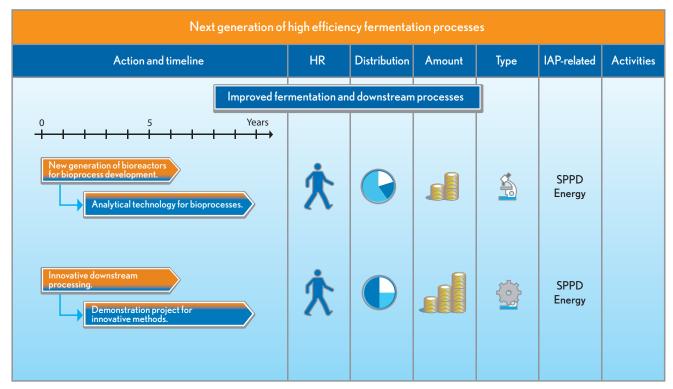
To develop **novel and improved pathways and products through genetic and metabolic engineering**, the following topics need to be studied:

- Metabolic engineering and modelling: metabolic engineering for the improvement of bioprocesses needs urgent attention. The genetic tools for metabolic engineering need to be developed further towards gene fine tuning. The construction of well known knock-out or over-expression mutants, resulting respectively in the massive over-expression or inactivation of genes is now a mature technology and attention should now focus on the fine tuning of genes and metabolism.
- The flux of primary and secondary metabolites will be investigated. This investigation will enable the genetic manipulation of the genome of the production organism towards an optimal yield of the product from its raw materials. The yield of product per mole glucose or a nitrogen source will have to be optimised at the expense of other metabolic pathways. The knowledge to achieve this will be generated by doing flux analysis. RNAi studies can be used in this work to block undesirable pathways in order to understand their effects on the production of chemicals, before pathway enzymes are finally up- or down-regulated.
- Improved mathematical models of microbial metabolism, directed towards both steady state and dynamic models, including the development of methodological tools, particularly for flux analysis and measurement of intracellular metabolites also have to be developed. Special emphasis has to be given to relevant operating conditions.
- Study of microbial physiology: understanding how microorganisms grow and function within a fermentation vessel is crucial for the optimisation of their production potential. Microbial physiology is essential for the understanding of microbial functions, signal transduction, quorum sensing and cell-cell interaction among the microorganisms growing in a fermenter.

• Pathway engineering towards novel products not found in nature: with an enhanced knowledge of microbial metabolism, metabolic engineering and production systems, it will become possible to create completely new pathways to bioproduce new molecules that are not synthesised in nature. To obtain such new synthetic pathways, new enzymes need to be developed using techniques such as directed evolution or rational design. These enzymes then need to become functional to create a new synthetic pathway through the use metabolic engineering. The genesis of such synthetic pathways thus requires the integration of a variety of scientific disciplines.



# Improved fermentation and downstream processes



# New generation of bioreactors for process development

The development of **new generations of bioreactors** for process development is required to speed up process development and for a better understanding of how production microorganisms behave and function in large-scale industrial processes. Microbioreactors are considered very useful in this respect. They can be used for high-throughput screening of production strains, and for process optimisation with a given production strain. The development of new technology for **better analytical monitoring** in bioreactors is also required. This should permit the detection at molecular level of components and nutrients important in fermentation, thus permitting online control and improved quality safeguarding through biomarkers for validation and control. The microscale exploited by the bioreactors would require the monitoring of a single cell, for example, with fluorescent probes.

New types of microbioreactors need to be developed for the study of hydrodynamics, aeration, kinetics, etc. This should allow the collection of useful information for the scale-up from laboratory bioreactors to industrial fermenters. Small analytical monitoring technology that fits within these small microreactors is required to measure and understand what happens.



# Innovative downstream processes

Even though **downstream processing** operations typically incur over half the production costs of a bioprocess, relatively few innovations have occurred in this area. Downstream processing is a rather conservative sector with little innovation to overcome the current technological limitations. New and lower cost downstream processes are needed that are truly innovative and specifically designed for bioprocesses. Also lacking is a systematic approach to the collection of useful data about downstream processing. Whereas the chemical industry has a lot of engineering data to rely on, industrial biotechnology is still in its infancy. It is therefore important to make use of the knowledge and experience of chemists and chemical engineers to develop adequate downstream processing for bioprocesses.

The following actions should therefore be performed:

- Setting up of a large academic network for the systemic collection and elaboration of thermodynamic data and tools box data (this should be realised through a 5-year dedicated project through a joint collaborative academia-industry project).
- Exploring the development of innovative and completely new downstream processing technologies (such as new separation and extraction systems using electrodialysis, membranes, distillation and nanofiltration) and testing them in **demonstration projects**.

# • PROCESS ECO-EFFICIENCY AND INTEGRATION: THE BIOREFINERY CONCEPT

# Element of visionary project "Integrated Biorefinery"

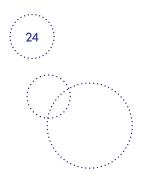
The biorefinery is a concept that has been developed in the food and paper industries and is now being applied in biomass-based energy, materials and chemicals production. By producing multiple products, a biorefinery maximises the value derived from the complex biomass feedstock. It relies on the best use and valorisation of feedstock, optimisation and integration of processes for a better efficiency, optimisation of inputs (water, energy, etc.) and waste recycling/treatment. Integrated production of bioproducts, especially for bulk chemicals, biofuels, biolubricants and polymers, can improve their competitiveness and eco-efficiency. Many improvements are still needed to advance the process: total use of the plant (better fragmentation and fractionation); development of processes to add value to all fractions of the plant and also to valorise by-products of other industrial systems (e.g. black liquor in wood/paper industry, glycerol from biodiesel, whey from cheese production, etc.); downstream processing strategies (low cost recovery and purification); development of closed cycle sustainable systems; etc. It is also necessary to study the whole value chain as well as the "biorefinery value chain" for optimisation of costs, CO<sub>2</sub> reduction, and energy usage. This priority specifically needs joint efforts with other European technology platforms such as Plants for the Future, Sustainable Forestry and Biofuels.

# Goals

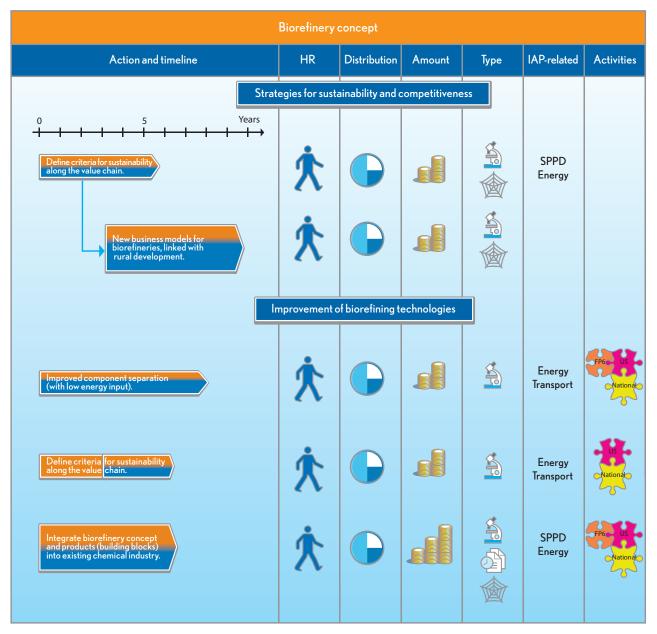
Widespread implementation and use of integrated and diversified biorefineries, to use European agricultural/forestry resources in the most efficient way, and to improve process eco-efficiency through integration.

## Key activities

- Strategies for sustainability and competitiveness
- Improvement of biorefining technologies



The development of biorefineries requires the following activities:





# Strategies for sustainability and competitiveness

This topic focuses on the creation of criteria and the development of tools to help in establishing strategies and business models for the different types of biorefineries to meet sustainability and competitiveness in different markets:

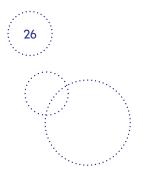
- Industrial research and development, user groups and fora to define and discuss criteria for sustainability, reduction of CO<sub>2</sub> output, economic optimisation strategies, lifecycle assessment of the entire production chain starting from field production up to industrial and/or consumer use.
- Comparative assessment of various biorefinery models in terms of environmental impact, economics and socioeconomic impact, risk-benefit analysis and public perception aspects.
- Critical economic evaluation of different biorefinery processes (production of biofuels and other by-products from sugar beet/oil rape, sugar/ethanol) in respect of EU support distortions and a global market perspective.
- Academic research projects, industrial collaborative research, and stakeholder involvement to develop and validate **new business models** for different kind of biorefineries taking into account individual rural developments.

# Improvement of biorefining technologies

- Academic research with industrial participation for the optimisation of biomass feedstocks for biorefinery systems (plant breeding, harvesting and storage). This theme will be undertaken in cooperation with the European Technology Platforms Plants for the Future and Sustainable Forestry
- Academic research projects, industrial collaborative research projects and industrial research on whole crop and biomass (including by-products and waste) biorefining methods for **separating different components** such as sugar, starches, lignocellulose, fats, proteins, aminoacids, organic acids from seed, leaf, woody and root parts of various crops including the development of process equipment for the disruption of plant materials and subsequent **fractionation with little energy input**.

- Academic research projects, industrial collaborative research projects and industrial research on the utilisation of plant and biomass fractions that are residual after the production of, for example, bioethanol and from other production chains (e.g. production of methane). Valorisation, retreatment or disposal of co-products and wastes from biorefineries is an important consideration in the overall biorefinery system.
- An important aim under this activity will be to develop large scale biogas production from dedicated crops as well as from organic waste (lignocellulosics and current by-products from biorefineries) within 10 years by process intensification of biogas reactors and improved purification as described in *Energy: Alternative Sources*.
- Academic research projects, industrial collaborative research projects, industrial research to produce chemical building blocks for polymers, lubricants and fine chemicals. The development of these chemical building blocks will contribute to **the integration of the biorefinery concept** and products into existing chemical production chains.

In evaluating the technological and economic feasibility of the above technologies, it is crucial to have access to industrial or pilot-scale facilities in order to test new technologies under operational or near operational conditions, and improve them while reducing the development time. An "Integrated Biorefinery" visionary project (see *Strengthening the foundations*) is therefore being developed to create new demonstration/pilot facilities in order to provide support for research consortia, to develop a proof of concept or to scale-up promising laboratory research.



# Energy

Aiming for more eco-efficient and environmentally friendly usage of energy in Europe, the following areas of research have been identified as those of highest priority within SusChem:

- Alternative energy sources.
- Energy conservation.
- Energy storage.

# **○** ALTERNATIVE ENERGY SOURCES

Reliance on a few limited sources of energy is detrimental not only to the environment but also to the future economic stability of Europe. The future lies in a diversification of energy sources, tailored to the requirements and resources of each country. For example the implementation of photovoltaic systems makes more sense in sunnier regions, while biomass resources for fuel production are more appropriate in regions with larger biomass supplies. Portable technologies will also play an important role in future markets. Other new technologies such as the exploration of the application of nanoparticles as a fuel source, the further development of photovoltaic systems and wind power are all necessary to provide new and versatile means of energy generation.

# Goals

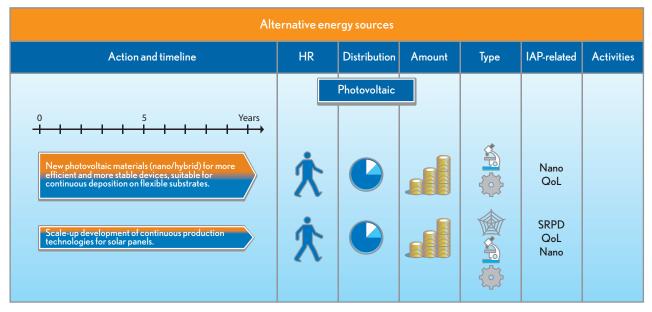
The aim of the actions listed below is to improve current technologies into  $2^{nd}$  generation more efficient energy sources within the next 10 years, and to investigate new technologies to diversify the energy sources portfolio in the mid to long term.

# Key activities

- Photovoltaic
- Fuels production from biomass
- Fuel cells
- (Metal) nanoparticles as fuel
- Wind power



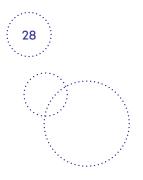
Photovoltaic



If solar cells are to provide an alternative to fossil fuels, significant research needs to be done to develop new routes for crystalline silicon production, in the development of amorphous silicon **hybrid materials** which could result in enhanced efficiencies, in concerted efforts for cheaper and more stable dyes, and in improving the efficiency of the dye sensitised cells. A strong supporting effort is needed in the search for new and efficient metal based sensitizers such as Ru(II) compounds and for achieving molecular control of interfacial charge transfer at wide band-gap **nano**crystalline semiconductors.

Research in **new material systems**, especially in the field of nanotechnology, can lead to low cost solar cells. Progress in organic or hybrid systems promise new **continuous**, roll to roll **production technologies**, i.e. printing. In particular polymeric solar cells, such as those based on electron donor polymers such as polythiophenes, polyfluorenes, etc., and on electron acceptor molecules based on fullerenes, are promising from the point of view of their potential cost-per-watt-peak. However, it is still necessary to perform research in this field to achieve longer lifetimes and higher efficiencies, goals that may be reached by investigating new polymeric and molecular materials able to harvest sunlight better and to transfer photo produced charges more efficiently. Besides research in material systems and cell concepts, a crucial subject for low cost energy from solar cells is process development (new processing paradigms are needed which are able to deliver enhanced device performances whilst ensuring the sustainability of this technology, e.g. through water-based processing of the active materials) and the scale-up of new technologies into the industrial scale by exploiting roll to roll continuous technologies.

Making available cost-efficient photovoltaic systems is one of the key challenges in reducing the dominance of fossil fuel over the coming decades. It has become obvious that the growth of photovoltaics (PV) will be severely hampered by a shortage in polysilicon feedstock material. To alleviate the impact of the shortage, several alternatives need to be developed and brought to market almost overnight: thin film silicon PV, other thin film PV (especially polymeric PV), and also multi-junction III-V solar systems operating under concentration factors of 500 to 1000. The latter solution has the advantage that most elements of the technology have already reached some degree of maturity in photovoltaics on board satellites, a development effort in which the European Space Agency (ESA) has played an important role.



The cost of production of passive systems for the generation of electricity needs to be reduced. In this area, the generation of technologies for the application of solar cells to various **surfaces** (static and **flexible**) is very important.

Synergies are expected between SusChem and the ETP Photovoltaic.

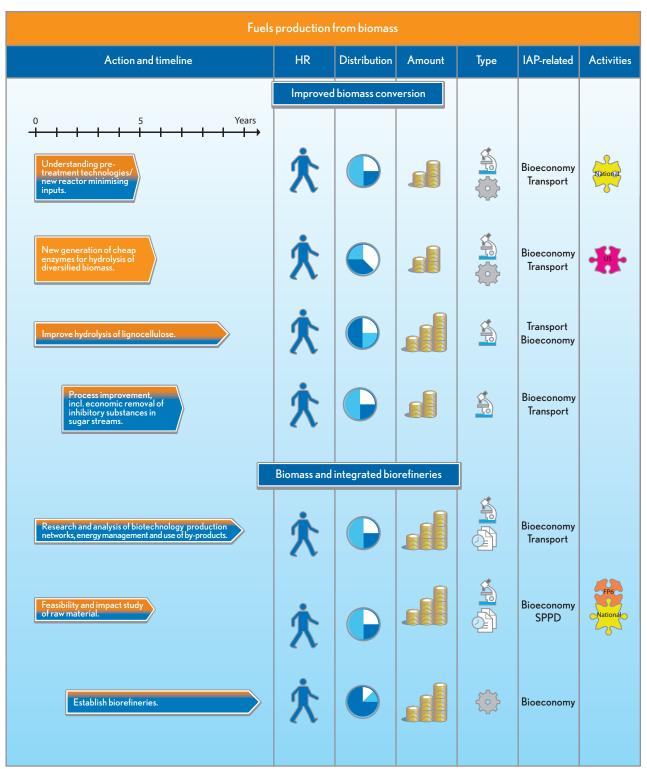
# Fuels production from biomass

To be competitive, production of liquid fuels such as bioethanol, biobutanol, or biodiesel relies on cheap and reliable sources of renewable raw materials and efficient production processes. At the moment, sugar prices in Europe are too high to allow competitive production of bioethanol or butanol, and only a part of the crops are being used. Therefore new technologies need to be developed to convert cellulosic, fibre or woodbased, waste biomass, efficiently into fermentable sugars. Similarly biodiesel is competitive as transport fuel only if subsidised in Europe today, due to the cost of raw materials and the relatively poor efficiency of the process.

Efforts have to be made to diversify raw material use and to improve the process, while making it more economic by using by products such as glycerol. Also, due to the low energy content of biomass, pre-processing technologies have to be developed to enable transportation of biomass to and from biorefineries to have a positive CO<sub>2</sub> balance or to be CO<sub>2</sub> neutral.

Several types of liquid biofuels exist, or are under development, and have the potential to replace fossil fuels, especially in the transportation sector. The focus here is on organic fuels such as ethanol, butanol, methanol and their derivatives ETBE and MTBE, which can be produced by fermentation or gas to liquid technologies, and also on biodiesel and liquid biogas which can provide interesting biomass-based alternatives to diesel and LPG.





# Improved biomass conversion and integration into a biorefinery structure

# Improved biomass conversion

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Biomass conversion by **hydrolysis** technology involves the breakdown of carbohydrates into their component sugars by a range of chemical and/or biological processes. Biomass is first subjected to pretreatment to solubilise the hemicelluloses and expose the cellulose for subsequent enzymatic degradation. The cellulose then undergoes enzymatic hydrolysis to produce glucose, which can be converted to biofuels and chemicals by fermentation.

The following actions are necessary to allow the eco-efficient conversion of diversified biomass and therefore pave the way for the development of commercial 2<sup>nd</sup> generation biochemical processes for liquid biofuels production:

- Developing an understanding of the chemical nature and architecture of cell walls at the nano-, micro- and macrochemical, and physical scales, and their behaviour in pretreatment and fermentation.
- Analytical methods improvement to characterise structural and non-structural products in the biomass and follow them and their reaction products through pretreatment and fermentation.
- Research projects on understanding pretreatment technologies, including improved chemical hydrolysis of lignocellulose, and designing of new more reliable reactors and equipment, and minimising the energy and chemical (acid) input.
- Research in novel promising technologies for the physical/ chemical fractionation of biomass in separate (C5/C6) sugar and lignin fractions. The C6 sugars will be used for the production of bioethanol; whereas the C5 sugars will be converted either to ethanol or to other value-added products and lignin fractions will be converted to valueadded products making the entire integrated process more economically profitable and environmentally friendly.
- R&D frontier projects to create a new generation of cheap enzymes for hydrolysis of cellulose and lignocellulose to fermentable sugars (able to complete the biomass hydrolysis during fermentation). Development of hemicellulases and lignilases to be applied before or after traditional pretreatment to minimise and, eventually, replace thermochemical processes, thus lessening the effects of overall pretreatment severity at the macromolecular level and simplifying processing.

 Industry academia partnerships in process improvement, including: reduction or economic removal of inhibitory substances in sugar streams for fermentation; introduction of novel feedstocks from biomass fragments.

# Biomass evaluation and improved economics via biorefineries

To develop economic industrial processes, it is important to ensure the availability of biomass at low cost. Depending on the environment and the products required, the evaluation and choice of biomass is crucial. Moreover the organisation of the production in biorefineries and the valorisation of coand by-products are important to reduce costs and achieve economies of scale. It is crucial to develop the production of biofuels with added value to the whole biomass (further transformation or energy creation), in conjunction with the production of associated bulk platform chemicals and/or high value compounds:

- Comparative **feasibility and impact analysis** of raw materials such as EU specific biomass and wood, agricultural wastes, and energy crops.
- Comparative assessment of different liquid fuels and production systems such as biobutanol and second generation biofuels (environmental impacts, efficiency of land use, costs and value added).
- Research, feasibility and impact analysis (costs and benefits) to develop biotechnological production networks in biorefineries (including simultaneous production of fuels and chemicals), including energy management and diversion of by-products to parallel processes.
- Integrated production of platform chemicals and high value compounds (such as lubricants, biopolymers, ethylene and nanocomposite materials) together with fuel production from lignocellulosics and other sources.
- Finding applications for low value by-products from biorefineries.
- Assessing potential risks and public perception.

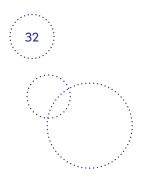


# Action and timeline HR Distribution Amount Type IAP-related Activities Improved biomass fermentation to liquid fuels 
# Improved biomass fermentation to liquid biofuels

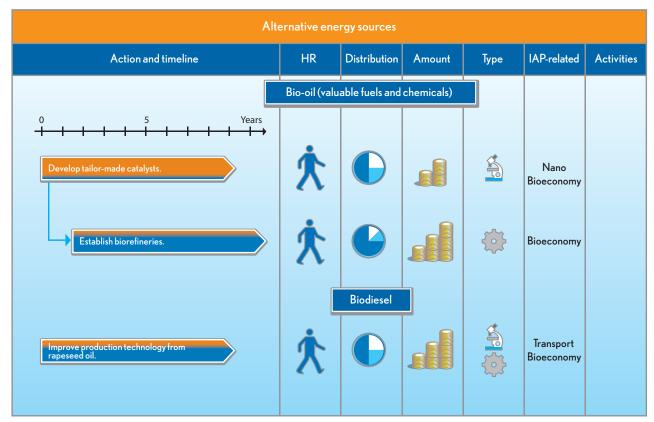
Ethanol is taken here as an example as it is already produced as a 1<sup>st</sup> generation fuel and processes are most advanced. However similar research can be conducted on other organic fuels like butanol and methanol, which have potential in overcoming some of the problems of ethanol transportation and distribution.

The microorganisms should use sugars in biomass efficiently with high yield and complete sugar utilisation, minimal byproduct formation, and minimal loss of carbon into cell mass. Critical aspects to be considered are higher final ethanol titer, higher overall volumetric productivity, especially under high solid conditions, tolerance to inhibitors present in hydrolysates, use of both hexoses and pentoses to produce ethanol at a yield greater than 95 % of theoretical, and the ability to grow and metabolise effectively in minimal media or actual hydrolysates. They must be able to withstand the stress of high ethanol and substrate concentrations, low pH, etc. At present no such strains are available and significant challenges still lie ahead to Developing such strains requires a multidisciplinary approach involving various aspects and research areas:

- Industry-academia partnerships for research in microbial metabolic pathways and metabolic engineering to expand the substrate usage spectrum of microorganisms (e.g. C5 sugars), and to increase tolerance to industrial conditions (e.g. high product tolerance, fast growth, high yield and productivity).
- Effective process control (on-, at-, and inline sensing) and modelling, involving additionally instrument manufacturers.
- Intensification, optimisation, and cost effectiveness of the continuous processes/bioreactor systems in which the activity of the selected/developed strains is exploited and validated (scale-up). The involvement of agroindustries is important in such an activity.
- Improvement, optimisation and/or cost effectiveness of the downstream processing.



# Biodiesel and bio-oil

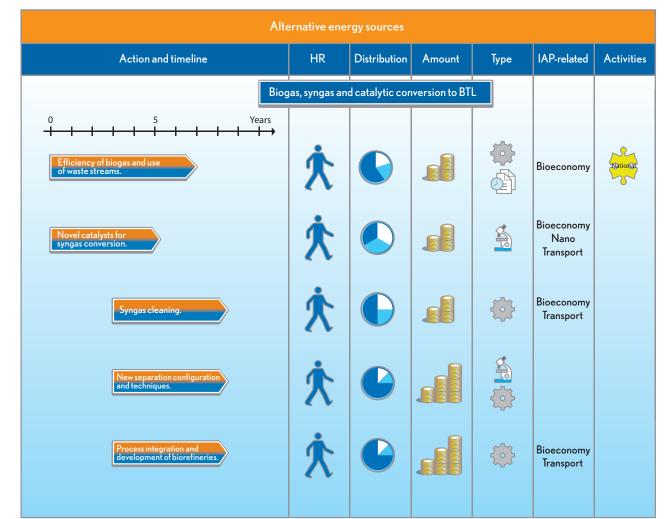


Traditional production of biodiesel could be improved by better transesterification and catalytic technologies. An interesting development could also come from catalytic biomass pyrolysis for the efficient conversion of biomass to produce clean and renewable liquid bio-oil. Such promising technology could help to increase the share (12 %) of biomass in the European energy market, by the year 2010, and have a positive impact on the development of new markets for the non-fuel uses of bio-oil (replacing petrochemicals with biochemicals).

- Improved production technology of biodiesel from biomass (e.g. rapeseed oil and recycled oil from food production and cooking) by highly efficient tailor-made catalysts for transesterification encompassing:
  - Heterogeneous basic catalysts with high stability towards water and impurities and avoiding the presence of catalyst residues in the final product.
  - Biocatalytic transesterification with enzymes displaying high stability towards methanol.

- Catalytic methodologies should enable a cleaner biofuel through a simple product separation from other reaction components while ensuring a cost-effective overall process.
- Finding applications for the **biodiesel** by-products like rapeseed oil cake and crude glycerol constitutes a key research objective. Chemical transformation of glycerol into products of commercial interest is under way. More innovation in this area is needed.
- Developing the production of stable liquid biofuels from biomass flash pyrolysis, in a single stage catalytic process (through mild cracking reactions in the presence of the appropriate catalysts and prior bio-oil condensation, without the use of external hydrogen).



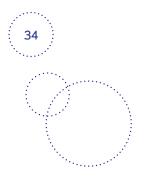


# Biogas, syngas and catalytic conversion to BTL (biomass to liquid)

Gas production from biomass and its further conversion to liquid fuels is of high interest. Two main technologies exist: the production of biogas by anaerobic fermentation and the production of syngas by thermochemical gasification of biomass.

Biogas production technology is already quite well established and is particularly interesting in small-scale applications. However, research could significantly improve the performance of the conversion. Biogas can be produced from dedicated crops (e.g. corn without kernels), lignocellulosics wastes from biorefineries, and from plant and animal wastes from the food industry.

- Improvements in the efficiency of biogas production and use of varied waste streams as feedstock (such as waste from olive oil or dairy production). A demonstration project in Europe which includes cost-benefit analysis and screening for optimal substrates would be useful.
- Biohydrogen could also be an interesting output of biogas production increasing the overall efficiency of the process through efficient catalysts and improving the stability of the catalyst towards the main contaminants.



Biofuels can also be produced from biomass by means of thermochemical processes. In an initial step biomass is transformed into syngas by gasification. The syngas is then cleaned and conditioned and further transformed into ethanol and higher alcohols in a catalytic conversion process.

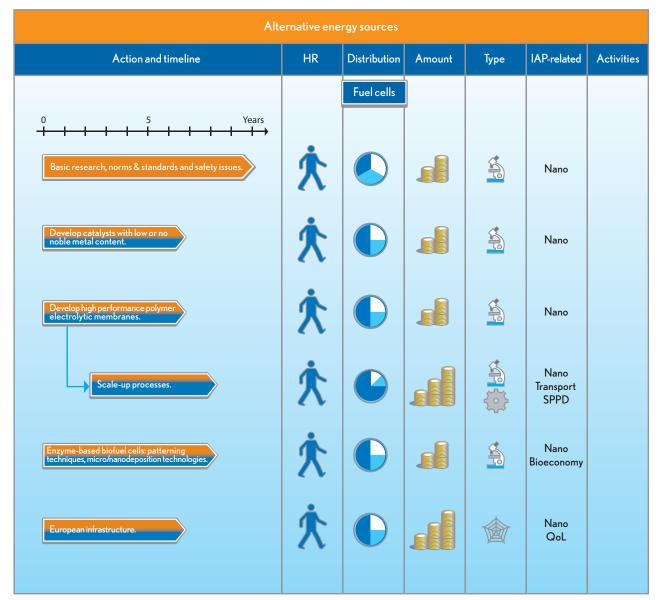
This process is potentially highly integrated and could be even combined with biological production of ethanol. The technology is already applied commercially for diesel and methane but has yet to be developed for alcohols.

In the conversion of syngas to fuels, the major research priorities are:

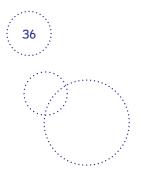
- The transformation of straw and agrofood residues which contain high sulfur and ash levels can be improved by the development of catalysts for syngas cleaning (e.g. materials for S abatement at high temperature and for tar cracking). Of specific interest are catalysts supported on high thermal conductivity materials for syngas production by exothermic or autothermal processes.
- The development of **novel catalysts** to produce ethanol and alcohols from biomass-based syngas in an efficient manner, and to increase their selectivity, conversion and reliability.
- The development of new separation configurations and techniques to achieve high value products from the reactions effluents.
- **Process integration** of the different steps like gasification, gas cleaning and conditioning, chemical synthesis and product separation, and energy integration of the process to combine heat and power with liquid fuels production.
- The development of the biorefinery concept based on the combination of biological and thermochemical pathways; reinforce the study of the synergies arising.



# **Fuel cells**



An essential part of a deployment strategy for transport, stationary and portable applications of **fuel cells**, advances in catalysis and materials science aiming at efficient **catalytic membranes** are a prerequisite for a strong technological foundation for building a competitive EU fuel cell, hydrogen supply and equipment industry. In the future, fuel cells will play an important role in assuring the mobility of vehicles and electrical devices (laptops, mobile phones, etc.). One of the largest hurdles encountered in the development and production of fuel cells is their relatively low efficiencies. Naturally the catalyst used plays a significant role in determining the efficiency of the cell, but the inability of the membranes used to transport selectively protons between segments of the cell also impacts on the performance. Membranes, that are developed or produced through a biological process or through the application of nanotechnology, and that can selectively and efficiently promote the transport of protons from one cell segment to another, can be beneficial.



Variation of fuel sources such as solid oxide fuel cells, also need to be considered. The development of the fuel cell, from prototype via **small-scale production to a mass product**, can only happen if significant improvements are made to individual key components, and the corresponding contributions from the world of chemistry are absolutely vital. Material science needs to provide new proton exchange membranes (e.g. **polymer**, ceramic, etc.) that work at higher temperatures and new **ecological catalysts** for the reforming reaction.

Nanomaterials science offers a great opportunity that should be adequately exploited for the development of new, alternative proton exchange membranes. The three main targets that should be addressed are:

- Overall cost reduction.
- Durability improvement.
- Achievement of high proton conductivity at low water content within the membrane.

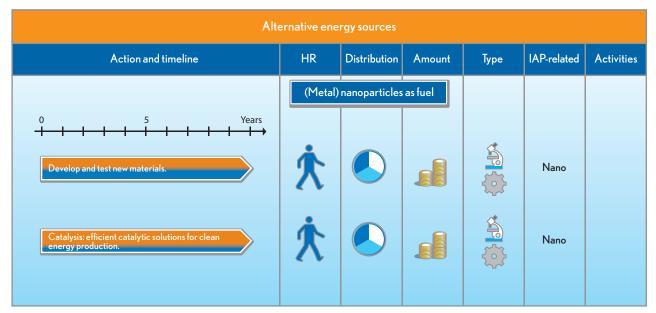
For these purposes, several strategies can be followed:

- The introduction of inorganic nanoparticles with different functionalities could improve water retention in the membrane and simultaneously contribute to cost reduction.
- Heteroaromatic condensation polymer related chemistries need to be investigated in more depth.
- Nanostructured copolymers with novel functionalities such as ionic liquid related chemistries are one of the fields that needs to be explored more fully.

Synergies are expected between SusChem and the European Hydrogen and Fuel Cell Technology Platform.



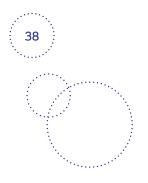
## (Metal) nanoparticles as fuel



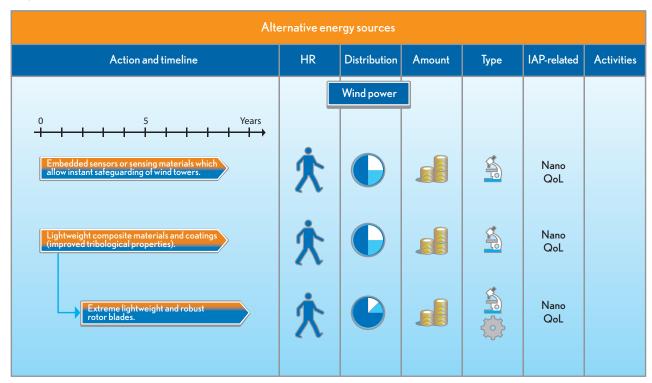
Metal nanoparticles not only have a great potential in providing interesting properties for new material hybrids and composites and as **catalysts**, but also as a source of energy in the form of solid fuels (by making use of high oxidation and redox processes). For example, relative to hydrogen, iron has a seven-fold energy release per unit volume, aluminium nine-fold and boron sixteen-fold (70 000 kJ/l (Fe), 90 000 kJ/l (AI), 160 000 kJ/I (B) vs. 10 000 kJ/I (H<sub>2</sub>)), though these are countered by lower energy released per unit weight. At present this idea is theoretical, therefore preliminary research into the viability is necessary, which will hopefully lead to a first generation of solid fuels for the mass market. Topics that need to be addressed include: a) how to control the burn rate; b) production of the ideal nanometal clusters; c) waste oxide recycling; and d) weight reduction. Prototype Stirling engines running on metal nanoparticles are being developed at Oak Ridge National Lab (by David Beach, Solomon Labinov and others including the Ford Motor Corporation - see http://www.ornl.gov/info/ornlreview/v39\_1\_06/article18.shtml).

#### Nanoparticles as catalysts for fuels

**Metal oxides have been explored as combustion catalysts** in the automotive field, but are likely to have further application in increasing the efficiency of combustion of solid and liquid fuels in power generation as well as in other fields of transportation. Optimisation of the catalyst in line with the specific fuel feedstock and the range of combustion processes will enhance the utilisation of the existing fossil fuel stocks.



## Wind power



Wind power has made a significant impact in many European countries as a sustainable source of electrical energy. Yet industry is faced with two factors which inhibit the efficient exploitation of wind, namely finding the right **lightweight materials** which can stay the stresses that wind towers are subjected to, particularly offshore installations (corrosion, wind, etc.), and sensors which can monitor the stability of the wind tower around the clock to give fair warning when the stability of the **tower** is endangered or servicing is necessary. These two factors affect the efficiency of wind towers and the durability/sustainability of the energy generation. Therefore there is a need to explore new material combinations (nanotechnologies), production and construction methodologies, particularly for the **rotor blades** and **embedded sensors**.



## O ENERGY CONSERVATION

Significant energy savings can be achieved through the adoption of energy efficient processes and technologies, thereby effectively saving money and benefiting the environment.

#### Goals

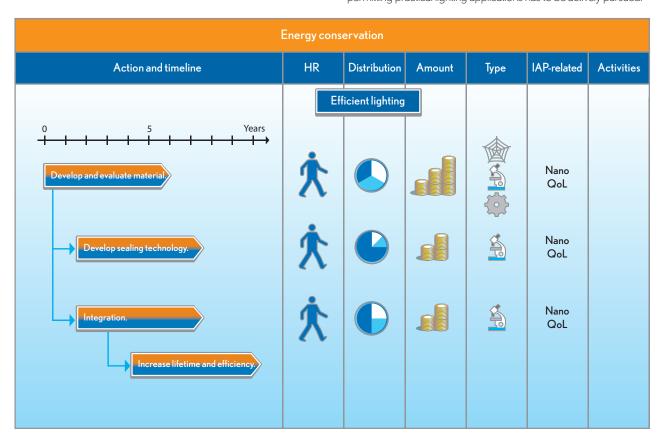
Achieve significant savings (even with current technologies savings of up to 30 % are already possible) in energy usage through the application of new technologies, such as nanotechnology and novel materials.

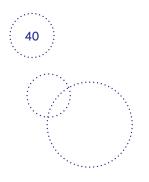
#### Key activities

- Efficient lighting
- Insulation

## **Efficient lighting**

LEDs and similar devices in the future will provide efficient lighting. To realise this, a number of hurdles need to be overcome, namely the identification of suitable materials and composites which yield increased lifetime and efficiency, and the successful development of a new generation of lights. For example, organic semiconductive materials have proved to be promising candidates, and investigations on the physical processes controlling the charge carrier transport and trapping, on the charge-light conversion process, and on the enhancement of the radiative re-emission process, will lead to an optimisation of the material's light emission efficiency. Support is needed for development of new classes of metal based luminophores, such as cyclometalated iridium (III) complexes, which are capable of very efficient luminescence and electroluminescence, coupled with a remarkable colour tuneability of the emission, by selecting appropriate ligands in the iridium coordination sphere to augment, or as replacements for, indium tin oxide (ITO). Moreover, research on polymeric materials with molecular architectures able to deliver enhanced electroluminescence at low threshold voltages and to ensure suitable operating lifetimes for permitting practical lighting applications has to be actively pursued.





## Insulation

Energy conservation									
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities			
0 5 Years		Insulation							
Polymer design (flexible, cheap).	X				Nano QoL				
Better properties for use in new buildings and in the renovation of old buildings (passive usage of solar energy).	Ŕ				Nano QoL				

Nanostructured materials have the potential to revolutionise the insulation technology sector. These have a significant advantage over current foams (from **polymers**) in that they have a lower thermal conductivity even at reduced thickness.

Over 60 % of thermal conductivity can be attributed to gas diffusion. By shrinking the cell dimensions within the foam to less than 100 nm, the gas-based thermal conductivity becomes negligible. This leads to significant savings in energy by making applications such as refrigerators or houses more efficient, as they will require less energy to maintain their internal temperatures. It is still necessary to scale-up the manufacture of these nanostructured materials to large production volumes and to incorporate them into industrial and commercial applications.

These materials will be important for the **insulation** of **new buildings** and for the **renovation** of **old buildings**. Applications in the automotive industry also exist.



## ••• • ENERGY STORAGE

With the burgeoning demand for consumer products, particularly in the mobile technologies sector, there is a greater demand for solutions to providing the energy for these products. Through the development of storage technologies, benefits for the consumer and for the environment will flourish. Furthermore, the increasing use of renewable but non-permanent energy sources such as wind and photovoltaics also require smart storage solutions to make the generated energy constantly available.

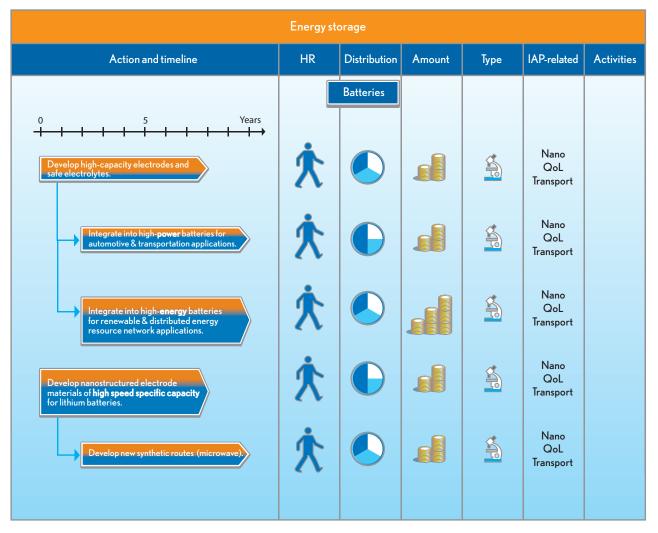
## Goals

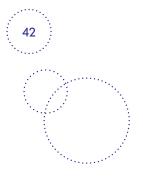
Explore new technology processes to enhance and improve the storage capabilities of mature products and those in development.

#### Key activities

- Batteries
- Gas storage
- Supercapacitors

## **Batteries**





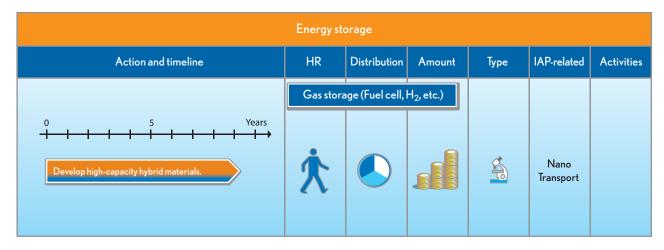
**Higher specific energy**, shorter charging times and long-cycle lives need to be attained to keep pace with the increasingly demanding needs of personal electronic equipment. This can be achieved through the development of new chemistries for cathodic **nanostructured** materials avoiding the use of environmentally unfriendly cobalt. Research into new alternatives to graphite as the anodic material is also needed.

One alternative is new nanostructured metal compounds which can potentially produce a tenfold increase in capacity of the battery. This is a field of special importance to the European battery industry (including research on new electrolytes and membranes). **Lithium ion technology** is currently more promising for secondary (rechargeable) batteries mainly due to its high cell voltage and possibility of short charge times. However, safety is a major drawback. Progress in these areas is key for the development of new transport systems (hybrid vehicles), new energy networks (based on renewable sources such as photovoltaic systems) and new electronic devices. These technical challenges required to study and to implement breakthroughs in active material design whatever the electrochemical system used (lead-acid, Li-ion or Ni-MH): nanomaterials use is expected to solve these issues due to a better resistance to structural stains and improved kinetics.

The research on these new materials will depend on the electrochemical system:

- Li-ion: research on new alternatives to graphite as the anodic material (new nanostructured silicon compounds), new cathodic materials related to 5 V systems, new electrolytes.
- Lead-acid: research on nanostructured, for example, PbO<sub>2</sub> as the positive **electrodes**.
- Ni-MH: nanostructured Ni(OH)<sub>2</sub> (active cathode material of Ni-MH) or precursor of nickel based **cathodes** for Li-ion batteries, nanodispersed coatings for separators.

Furthermore, new lithium batteries based on novel nanostructured electrode materials will be fabricated by means of the development of **new synthetic routes**, eventually assisted by **microwaves**.



## Gas storage

The use of (bio)processes to generate hydrogen from appropriate biomasses, and technologies which enable the production of hydrogen in a clean form, such as new (bio)catalysts, require an efficient and safe hydrogen storage system.

**Hybrid organic-inorganic materials** are increasingly filling the space left between inorganic, polymer and organic chemistry. The driving forces behind these developments are the

requirements for a variety of applications including catalysis, selective separation and purification, chemical and biological sensing and optical communications. This family of materials includes dispersions of inorganic nanoparticles in organic (polymer) matrices and the converse. Also included are porous metal organic framework materials and the inclusion of organic macromolecules into mesoporous oxides such as silicas. A class of pure polymer materials which are relevant are nanoporous polymers.



## **Supercapacitators**



Supercapacitors containing electronically conducting polymer electrodes are of great interest as they provide the potential for storing large amounts of energy in a small volume. This is of great interest for the automotive industry, particularly with regard to hybrid and electric vehicles. The largest hurdles facing the products in reaching the market are **material development, production** scale-up and quality control.

## Healthcare

The health sector will benefit greatly from new products and technologies provided by material science. The scope covers new treatments through to medical devices to new delivery systems.

The challenges for the next century in healthcare are: an ever-increasing number of patients with allergic, inheritable or contagious diseases; cancers; the demographic trend to an older society; and the exploding costs of healthcare. Nanotechnology has the potential to revolutionise medical technologies and therapies, by providing the tools to cope with the challenges, to such an extent that its contribution will be crucial for future human health.

Nanoparticulate formulations will be one of the most important technological and scientific challenges in the fields of advanced food and drug technologies. Exploitation of these nanoscale functionalities for new applications promises to have an immense impact in improved healthcare and quality of life, not only for the European Community, but also for the rest of the world, and in particular for the third world. This will be achieved through effective drug applications, faster and non-invasive medical diagnostics and treatments. One important role is the establishment of the appropriate safety standards for these new products and formulations. Irrespective of the broad nature of these applications, the technologies needed here encompass similar and complementary generic knowledge and expertise.

The following areas of research have been identified as those of highest priority:

- Material development for drug delivery and therapies.
- Diagnostics.

## MATERIAL DEVELOPMENT FOR DRUG DELIVERY AND THERAPIES

Therapeutic systems are larger than classical drugs (e.g. aspirin) and therefore there is more scope for diversity and complexity, which makes their description much more challenging and their delivery more difficult. The increased complexity, however, gives these systems the power to tackle more challenging diseases. These drugs, diagnostic agents and regenerative medicines are capable of multitasking and can even combine roles such as diagnosis and therapy – so called theranostics.

Having multiple functional delivery systems, the key function is the targeting or ability to recognise molecules/cells implicated in disease. Research efforts to enhance these functional materials and in particular to reduce their production costs are essential. Furthermore the identification of such materials needs to be done by a combination of rational design and high throughput screening.

## Goals

The main goals are to develop innovative materials, hybrids and formulations for the efficient and targeted delivery of drug active ingredients or therapies. The goals can be achieved with synthetic nanometre-sized delivery systems for therapeutic agents and biologically active drug products, consisting of at least two components, one of which is the active component.

#### Key activities

- Targeted drug delivery
- Smart drug delivery systems



## Targeted drug delivery

Material development for drug delivery and therapies								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
0 5 Years	Targe	eted drug deliv	/ery					
<u>+ + + + + + + + + + + + + + + + + + + </u>	•		9		Nano			
Functionalise metal nanoparticles with polyfunctional organic molecules.	X				QoL Bioeconomy			
Develop new protocols for the	*			4	Nano			
Develop new protocols for the assembly of the nanobioreactor.	Χ				QoL Bioeconomy			

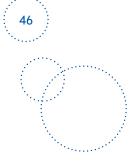
## Functionalised (magnetic) metal nanoparticles having

suitable polyfunctional organic groups or polymer chains able to link to specific biomolecules or receptor sites are needed, e.g. for cancer therapy and drug delivery. Different nanostructured inorganic matrices are suitable as bone tissue substitutes. Furthermore they have the potential for controlled drug delivery, specific to bone pathologies. Biomaterials have the ability to control the release of biologically active molecules both in space and time: embodying both the control of drug release rate, and the delivery of this drug to a specific body organ, tissue or receptor. Electronically conducting polymers are attracting a great interest in that they can be used as drug delivery systems in the form of drug eluting coatings of STENTs, which are used in heart surgery, thereby assisting in treating coronary diseases.

Activities which should be pursued are:

• Synthesis of functional composite hybrid materials, polymers or biopolymers (through, for example, inverse microemulsions or electrochemical synthesis), their analysis (high-throughput screening) and their processing.

- Generating metal nanoparticles of well defined size and the self-assembly of nanostructured surfaces.
- Development of microreactors and continuous synthesis. Microreactors are units with small channels in the range of 10 - 500 micrometres, where chemical reactions can take place under flow conditions. Compared with classical batch reactors microreactors have the following advantages. The small channel dimensions guarantee a fast mixture of the reactants via diffusion. For diffusion limited reactions this results in a reduction of the reaction time. Furthermore, the high surface to volume ratio in the channels guarantees a high heat transfer capacity, resulting in isothermal conditions that are close to room temperature - which again facilitates fast reactions. Because the reactions are carried out via continuous flow of the reactants, the products can be used immediately, independent of the scale applied. The resulting yields can be increased since unstable intermediates do not have the time to decompose. In addition, the formation and use of risk compounds can be managed within acceptable safety regulations since no large amounts are formed or used.



## Nanobioreactor

- Docking and virtual screening software and workstations; parallel synthesis machines; in vitro screening systems.
- *In silico* design, combinatorial organic synthesis, and *in vitro* profiling of new biologically active small molecules.
- A European G-protein-coupled receptors (GPCRs) Crystallography Platform.

While ca. 30 % of all target drug delivery projects in the industry are GPCRs, they suffer from the lack of structural information which would make structure-based design accessible. To date the only crystal structure of a mammalian GPCR, that has been resolved, is that of bovine rhodopsin. Bovine alone rhodopsin is of little use as it has little structural resemblance with other GPCRs.

A European Crystallography Platform needs to be established to work out general solutions to crystallising and solving the structures of GPCRs, which undoubtedly give a competitive edge in achieving targeted drug daelivery.



## Smart drug delivery systems

Material development for drug delivery and therapies									
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities			
	Smart c	lrug delivery s	ystems						
0 5 Years									
Study and apply biocompatible polymeric structures.	Ń				Nano				
	~ ~			<b><u></u><u></u></b>					
Scale-up, cooperation (medical schools, chemical industry, pharmaceutical industry, biotech).	, in the second				Nano				
				503					

There are problems facing the application of nanoparticles in delivery systems, e.g. the tendency to aggregate during storage or under physiological conditions. Understanding and preventing aggregation is a top research priority. Complex delivery systems must be chemically analysable and stable over extended periods, but most importantly they must be producible.

Core-shell systems, such as carbon nanotubes, dendritic polymers or Janus particles (left/right, top/bottom), which have functionalised outer layers and inner core pockets for the storage of active ingredients, present a new means of tailoring drug delivery for a wide spectrum of applications and disease therapies (D.A. Tomalia, Prog. Polym. Sci., 30 (2005) 294-324). By fine-tuning dendrimers' properties, the timed release of medications could be allowed for at the desired reaction site. Beyond this is the potential of medications, which respond in situ to local factors (hormone levels, presence of antibodies, etc.) and release the active agent, thereby becoming truly a smart drug. Present work is in the preliminary phase, but to realise the full potential, production **scale-up** of the dendrimers needs to be explored in conjunction with **cooperation** between medical schools, and the chemical, pharmaceutical and the biotechnology sectors.

Synthetic nanostructured silica based systems may act as smart drug carriers: the sol-gel process used to synthesise nanoporous silica xerogels matrices allows entrapping of bioactive molecules at room temperature during the formation of the inorganic backbone. Silica xerogels' release behaviour can be tailored by controlling the sol-gel synthesis conditions, gelation rate and wet aging time, which determines their physical characteristics including pore size and distribution, surface area and bioresorbibility. These materials with a high surface area can be synthesised with tailored surface chemicalphysical properties, and stoichiometry which can be utilised to surface-link bioactive molecules using an innovative approach to modulate and drive their release, stimulating specific cellular responses at the molecular level.

For smart drug delivery the synthesis of new chiral **biocompatible** (enantiomerically pure) **polymeric** and dendrimeric materials with controlled composition and structure bearing active agents is also a very promising option. Moreover, biomimetic apatites loaded with an opportune antibiotic, which acts as synthetic bone substitutes and drug controlled release systems, will be able to act as an osteoconductive-inductive device for "one stage surgery".

## • DIAGNOSTICS

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Diagnostic imaging procedures provide crucial input for clinical decision making and therapy planning. Imaging has advanced to become an essential tool in diagnostics over the last 25 years. The use of specific targeted agents plays a crucial role for localisation and staging of a disease. Imaging tools and marker/ contrast agents are being dramatically refined towards the end goals of detecting disease as early as possible, eventually at the level of a single cell, and monitoring the effectiveness of therapy.

Nanotechnology could help to design a plethora of very specific imaging agents. Analytical devices, which require smaller samples, will deliver more complete and more accurate biological data from a single measurement. Nanotechnology enables further refinement of diagnostic techniques, leading to high throughput screening (to test one sample for numerous diseases, or screen large numbers of samples for one disease) and ultimately point of care diagnostics. Miniaturising the imaging system will make it possible to perform image-based diagnostics everywhere, and not only in advanced hospitals.

This could lead to personalised treatment and medication tailored to the specific needs of a patient.

## Goals

Technological advancement to pave the way towards major changes in the way drugs can be prescribed in future, by enabling "personalised" medicine tailored to individual needs.

#### Key activities

- Lab on a chip or instant diagnostics: sensors
- Imaging materials
- Implantable biomedical devices



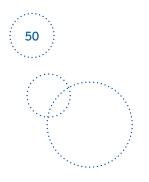
## Lab on a chip or instant diagnostics: sensors

Diagnostics								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
L	s							
0 5 Years								
Understand charge transport, ion transport in nanoporous systems and tubes.	X				Nano			
Develop methodologies.	Ŕ			<b>1</b>	Nano			

A diagnostic tool can be a single chemo- or biosensor, or an integrated device containing many sensors. The sensor contains an element, capable of recognising and 'signalling' through some biochemical change, the presence, activity or concentration of a specific molecule of biological importance in solution. A transducer is used to convert the biochemical signal into a quantifiable signal. Key attributes of theses types of sensors are their specificity, sensitivity, and robustness.

Nanosensors will be able to provide live online data to physicians during surgery, thereby increasing safety, lowering radiation doses and improving patient outcomes. In addition, these sensors would be able to continue to monitor important parameters such as blood pressure after surgery. Nanoscale entities could identify pathology/defects, and the subsequent removal or correction of lesions through nanomanipulation. Some potential avenues to pursue are:

- Synthesis of composite materials (polymers, hybrid materials) with functionalities, and the analysis (quality and suitability) and production of these materials.
- Connecting biomolecules with metals.
- Recognising materials (composite materials (biopolymermetal), doped materials, membranes, tubes, conductive materials, biomarker detection).
- The combination of nano-biotechnological methodologies for the construction of sensor surfaces and micro-electronic technologies for the read out of biomolecular interactions.
- New bioelectronic devices (biochips) for the recognition of nucleic acids and proteins.
- Biocompatible coatings for microsized batteries (lithium ion batteries and primary lithium) for implanted biomedical devices (see further, *Implantable biomedical devices*).
- Detectors based on synthetic biological sensors for early cancer diagnosis, and/or for anti-bioterrorism protection.



#### **Imaging materials**

Diagnostics								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
0 5 Years	۳ ۲	aging materia	Is		Nano			

The main benefits of molecular imaging for *in vivo* diagnostics are the early detection of diseases, the monitoring of disease stages (e.g. in cancer metastasis), in patient selection leading to individualised medicine, and in the real time assessment of therapeutic and surgical efficacy.

A wide range of particles and molecules are currently used for medical **imaging**, but there remains significant room for **material development**. Some recent developments in optical imaging focus on using nanoparticles as tracers or contrast agents. Fluorescent nanoparticles such as quantum dots and dye-doped silica nanoparticles are systems, which depending on their coatings and their physical and chemical properties, can target a specific tissue or cell. Their fluorescence can easily be tuned for specific imaging purposes. They offer a more intense fluorescent light emission, longer fluorescence lifetimes and a much broader spectrum of colours than conventional fluorophores. They are expected to be particularly useful for imaging in living tissues, where signals can be obscured due to scattering. Toxicological studies need to be undertaken to precisely study their impact on humans, animals and the environment.

New developments are focusing on nanoparticle coatings and formulations, to improve efficiency in targeting, treatment and biocompatibility. These are called theranostics. Similar agents are based on liposomes, emulsions, dendrimers or other macromolecular constructs

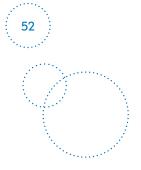


## Implantable biomedical devices

	Diagnos	stics				
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities
	Implanta	ble biomedica	al devices			
0 5 Years	Ŕ				Nano Energy	

Nanotechnology has application in devices for therapeutic uses such as in new endoscopic instruments. Continuous, smart measurement of glucose or blood markers of infections constitutes a substantial market for implantable devices. Miniaturisation for lower invasiveness, combined with surface functionalisation and the 'biologicalisation' of instruments will help increase their acceptance in the body. Self-diagnosis, remote control and external transmission of data are other considerations in the development of these devices. Of great importance is autonomous power (see also *Energy: Batteries*):

- Biocompatible materials for **microsized** batteries for implanted biomedical devices.
- Active materials (electrodes, electrolytes) suitable for *in vivo* use of microbatteries.
- Lithium batteries specifically designed for *in vivo* implantation. Lithium batteries, and particularly primary lithium batteries, contribute to a high quality of life by permitting miniaturisation and multifunctionality of biomedical devices for healthcare. implantation. Lithium batteries, and particularly primary lithium batteries, contribute to a high quality of life by permitting miniaturisation and multifunctionality of biomedical devices for healthcare.



## Information and communication technologies

The overall aim is to improve the competitiveness of European industry and enable Europe to master and shape the future developments of Information and Communication Technologies (ICT) so that the demands of its society and economy are met. Activities will strengthen Europe's scientific and technology base and ensure its global leadership in ICT, help drive and stimulate innovation through ICT use and ensure that ICT progress is rapidly transformed into benefits for Europe's citizens, businesses, industry and governments.

The following areas of research have been identified as those of highest priority:

- Application and introduction.
- Interface engineering.
- Self-assembly and patterning.
- Semiconductors.
- Information storage.

## O APPLICATION AND INTRODUCTION

The adoption of new architectures and materials will eventually lead to fundamental changes in the concepts and design paradigms of integrated circuits. In other words, there is an open field for scientific investigation and industrial research. Early successes in such a field will provide a leading edge, thus improving the market position of European industry with respect to that of the US and Japan, which are presently dominant in the more consolidated fields of standard CMOS technology.

In the coming decade, the semiconductor industry's process geometries will approach the physical limits of atomic structure. At atomic limits, thermal effects will eventually limit how far the industry can scale silicon-based transistors. At that point, it will still be possible to build electronic devices smaller than CMOS, but those devices would not operate faster or be cheaper to produce. It is unlikely that any charge-based device will be able to beat scaled CMOS. Instead, to go beyond CMOS, the industry will have to move to alternative logic devices based on alternative state variables to charge (e.g. spin, mechanical, etc.).

Already, the semiconductor industry is investigating some very interesting areas such as spintronics, quantum computing, and optical computing. These alternative logic devices are highly speculative and require new and novel materials. In order to understand whether any of these non-charge-based alternatives could be potential future technologies, fundamental research, particularly into the materials which will be needed to build these devices, is required. It is important to start this research as soon as possible as it is likely to take 5 years or more to understand the technological viability of these 'beyond CMOS' alternatives. The EU's support will help to achieve the goals which, due to the large amount of basic research involved and the scale of the challenges, call for a coordinated effort from industry and academia.

Besides the immediate application to the design of novel devices and integrated circuits based on standard logic concepts, an example of a far reaching by-product of these investigations will be the study of single electron coherent propagation in quantum computing gates based on quantum wires. Results have already been shown for a single qubit rotation gate implementing a quantum NOT transformation, as a part of feasibility studies on a solid state realisation of a universal set of quantum gates. In this respect, recent progress in fabrication processes makes the solid state implementation of quantum computing devices achievable for the first time.

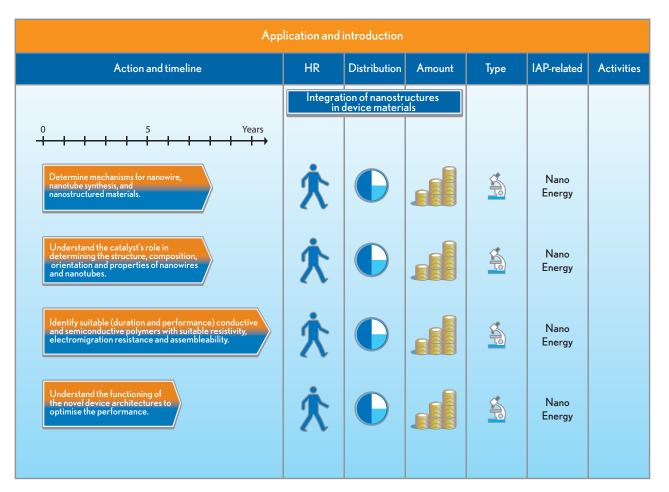
#### Goals

- To focus on the most promising architectures and materials for future generations of semiconductor devices indicated by the ITRS 2005 (*International technology roadmap for semiconductors*, 2005 edition, http://public.itrs.net), namely, those devices covered in the 'Emerging Research Devices' chapter.
- To perform the investigations necessary for the understanding of the physical and electrical properties of such devices and any of their associated materials.
- To implement the tools necessary for their analysis, design and optimisation in accordance with expected developments in fabrication processes.

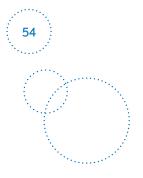
## Key activities

- Integration of nanostructures in device materials
- Low-k and high-k dielectrics
- Polymers for high density fabrication
- Microsized batteries for ICT applications
- Interconnects
- Polymer conductors
- Printed electronics
- Nanomaterials for power management

## Integration of nanostructures in device materials



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A number of new **nanostructured** materials including carbon **nanotubes**, silicon and germanium **nanowires**, and other semiconductor nanostructured materials are of potential interest for use in future device applications, but the **mechanisms** to control the nanostructure, composition and size are not understood or controlled.

The role of **catalyst** aspect composition and structure, in conjunction with temperature and gas composition (and other factors), in the production of, for example, carbon nanotubes, is not understood in determining the structure of the nanotube. Furthermore, understanding the mechanisms of how to control growth, structure, composition and orientation on predefined templates will be vital. Research is needed to obtain nanotubes using catalysts compatible with silicon to allow technology transfer from laboratory to industrial production, and with CMOS compatibility.

Organic semiconductors are a very promising class of materials for nanostructured devices, which may be patterned into regular nanostructures through a wide variety of methods. Organic semiconductors have interesting properties suitable for application in a wide range of devices (OLEDs, OTFTs, etc.) and this would provide a facile pathway for realising nanostructured functional devices, but a complete characterisation of their electronic transport properties is still a long way from being achieved. A better knowledge of the major transport parameters, such as the charge carrier mobility and lifetime, and their trapping processes, is highly desirable to achieve full control of the material. The degradation of novel organic semiconductors is another issue that needs to be addressed in order to enhance their lifetime and increase the potential applicability. The self-assembly of molecular systems makes it possible to generate a variety of nanostructured materials allowing one to develop nano- and micro-architectures with predetermined physical properties through their chemical functionalisation and their structural arrangement.

Inorganics are being used increasingly to prepare nanotubes and certain new types of inorganic nanotubes are expected to play a role in ICT in the near future. Chrysotile is a mineral which is eminently suitable for nanowire preparation, and can be easily engineered to fill the inner nanometre-sized cavity of densely packed bundles of multiwalled hollow tubular fibres. These new geo-inspired inorganic nanotubes can open innovative applications in photonic, electronic, biomaterials and environmental fields.

Inorganic nanocrystals or nanoporous materials can be synthesised in order to prepare innovative biomaterials. Their nanostructure allows them to be linked to biologically active molecules at the surface of crystals or porous cavities which can be released with controlled kinetics as a function of chemical conditions (see also *Healthcare: Targeted Drug Delivery*).

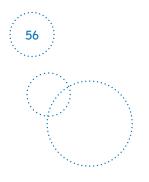


## ${\sf Low-k} \text{ and high-k} \text{ dielectrics}$

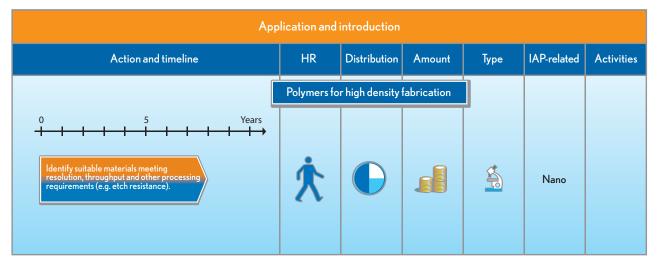
Application and introduction								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
	Low-k a	nd high-k diel	ectrics					
0 5 Years	Ŕ				Nano			

Electrical interconnects are separated by an inter-level dielectric (ILD) and as dimensions continue to get smaller the capacitive coupling between interconnects becomes larger and this slows signals and increases power consumption, therefore the semiconductor industry will need a lower **dielectric constant** ILD material.

Nanoporous films self-assembled from surfactants show potential, but they often have low mechanical strength and adhesive properties and crucially they absorb water during processing. Research is needed into the basic mechanisms of self-assembly to determine how to control the nanostructure, composition and internal bonding of nanoporous materials. A fundamental study of the chemical processes that occur during and which drive self-assembly is needed to determine how they can be controlled to give the resulting nanostructure and surface formation. This has implications for a broad range of applications such as the fabrication of nanoporous catalysts, elements of fuel cells, etc.



#### Polymers for high density fabrication



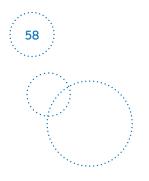
**Polymers** are widely used in the electronics industry and they are fundamental components of both manufacturing processes and final products. Their electronic applications include use as conductive and intrinsically conducting polymers, new dielectrics and electro-active polymers, photoresists, encapsulants, underfills and adhesives. **High density fabrication** utilises the direct imprinting of polymers to enable the creation of nanoscale features in the size range 1 to 200 nm. Material selection for high density fabrication is becoming more and more important as the applications for polymers become ever more stretched. With their widely varying electrical and mechanical properties, polymers have traditionally been employed as insulators and dielectrics but, increasingly, the development of new materials has broadened their utilisation into areas where their semiconducting and conducting properties have encouraged their use in many novel applications such as in displays, corrosion resistant coatings, sensors, solar cells, textiles and capacitors. Their selfassembling properties show promise for their use as materials for 'bottom-up' templating and patterning applications. The **identification of suitable materials** and their formulation, properties, and selection criteria, **to meet resolution**, **throughput, and other processing requirements** (e.g. etch resistance) is a key research requirement in this area. A special note: although the end users of these processes may be located outside Europe, many of the tool makers are European.



## Microsized batteries for ICT applications

Application and introduction								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
	Microsized ba	tteries for IC1	applications					
0 5 Years	Ŕ				Nano Energy			

Solid-state **microsized batteries** are in demand by the ICT industry for mobile and portable electronic device applications. Lithium batteries are a system of choice offering high energy density, flexible and lightweight design, and an all important longer lifespan than comparable battery technologies. Many challenges are associated with the research and development of these batteries towards commercial applications, for example, in synthesis, characterisation, electrochemical performance and safety. Development of **design concepts** (towards improvements in energy density) and **new materials for microsized lithium batteries** is a key requirement in future research efforts in this field. The design of new materials will be a critical research requirement, and focus should be on coupling the efforts of theorists, who are able to perform band-structure calculations on potential new compounds, and experimental chemists. Of equal importance is a better understanding of the electrode-electrolyte interface to facilitate design of new interfaces. *In situ* characterisation will yield important information here (see also *Energy: Batteries* and *Sustainable quality of life: Home as a self-sufficient energy provider*).



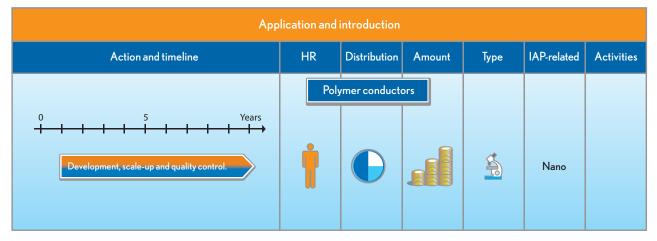
#### Interconnects

Application and introduction									
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities			
		Interconnects							
0 5 Years			_						
Identify suitable metallic nanowire and nanotube materials with suitable resistivity, electromigration resistance and assembleability.	X				Nano				
Identify suitable nanostructured barrier layers.	Ŕ				Nano				

High density, low electrical resistance interconnect materials are critical to enable ultra high speed, low power communication in future technology generations. Currently there are two major challenges to producing low resistance interconnects in future generations of technology: 1) currently a copper interconnect must be clad with a 20 nm thick diffusion barrier to confine it and as interconnect dimensions continue to decrease, the resistive barrier layer becomes a larger percentage of the interconnect and increases the effective resistance; and 2) as the copper dimensions are decreased, the grain size becomes much smaller and scattering at the grains and interfaces increases the electrical resistance. To enable low resistivity in copper interconnects would require identifying a nanometre scale diffusion barrier and assembly techniques to grow large grain smooth copper interconnects. Potential materials with this level of control are metallic nanowires which are single crystals with smooth surfaces. Other promising alternatives include metallic carbon nanotubes. Research should be conducted on novel synthesis techniques to fabricate nanostructured barrier layers and interconnect metals, or other nanostructured materials, with controlled properties.

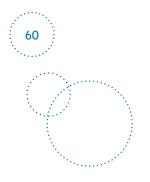


## Polymer conductors

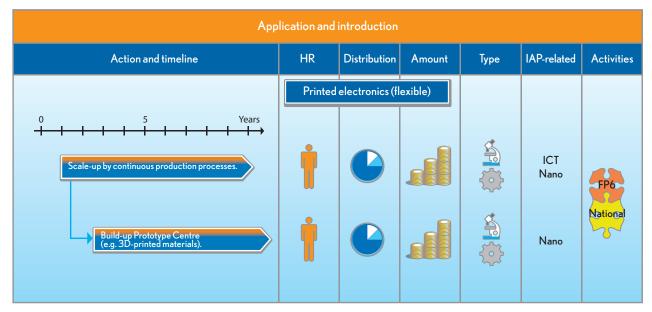


**Electrically conducting polymers** will play a crucial role in the future transport of energy, whether in the form of a component in supercapacitors or in microelectronics. The largest hurdles to date are the **large scale production** and **quality control** (analysis) of these polymers, as well as proper macromolecular design for ensuring good electric properties and prolonged operating lifetime. Also new and low-cost processing technologies which are able to fully exploit the properties of these materials have to be designed and implemented.

Finally, a better understanding is needed of the electronic transport properties of conductive polymers. Specific research activity should be carried out to determine and model the main parameters controlling the material's electronic transport processes. A correlation of these parameters with the material's morphology and structure is highly desirable to fully control the growth and the final performance of the material.



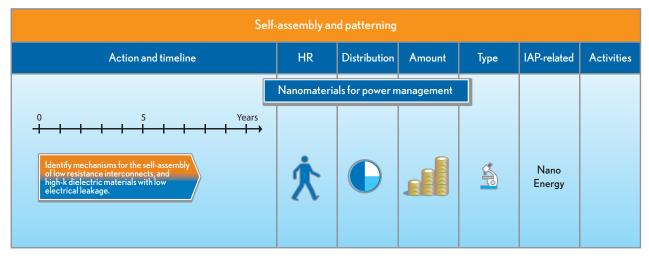
## **Printed electronics**



Printed electronics have already found their way into the market, yet the challenge remains to make cheap and **flexible** printable electronics. A major development impulse would be initiated through the creation of a **Prototype Development Centre**, where the major focus would be on the **scale-up through continuous production**. To ensure proper exploitation of this technology, printing technologies and machinery (e.g. inkjet, microcontact printing, etc.) able to process organic electronic materials into complex nanopatterns need to be realised. In parallel, new materials specially designed for optimal operation with the new machines have to be developed with a strong emphasis on water-based processing, which will ensure higher sustainability for this technology, and furthermore will lead to the realisation of nanostructures on large areas using simple and low-cost methods.

# 61

## Nanomaterials for power management



As computing speeds and power consumption continue to increase, increased focus will be placed on reducing power consumption by switching off components that are not being used, and rapidly activating the same components when necessary. Since batteries and power supplies are very slow, ultrafast capacitors will be needed to store charge and quickly restore component power when demand occurs. This will require high dielectric constant materials with **low resistance interconnects**, but these must be very low cost, and **directed self-assembly** is an option for fabricating such devices. Research will be needed into self-assembly of low resistance interconnects and **high dielectric constant materials** with **low electrical leakage**. These fabrication techniques may be applicable to fabrication of higher density battery technology for use in a wide range of applications (see also *Energy: Supercapacitors*).

## **○** INTERFACE ENGINEERING

62

Controlling the effects or events taking place at boundaries between two or more materials is crucial in the construction of semi-conducting components. The interaction (contacting) between nanostructured materials, e.g. organics and molecules, is a very important issue. This requires significant effort between experimentalists and modellers to develop an understanding of the issues before technological solutions can be found. There are several key questions which need to be addressed:

- Understanding metal-carbon bonding is critical including the kinetics of formation. A variety of techniques will be required (spectroscopic, electron tunnelling microscopy, FTIR, etc.) to understand whether the bond formation changed the metal or the organic, i.e. whether the organic is deposited on metal or metal deposited on the organic.
- The stability of the metal-organic contact when electronic conduction is occurring and metal migration needs to be understood as well.

## Goals

- Provide information through the development of new metrology techniques which can resolve materials and events at the nanometre scale.
- Investigate the effects of various deposition materials and techniques on the electrical and chemical properties of organic and conductor interfaces.

## Key activities

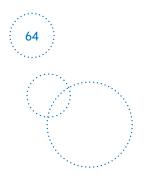
- Understanding of interfaces
- Understanding of organic-conductor interfaces



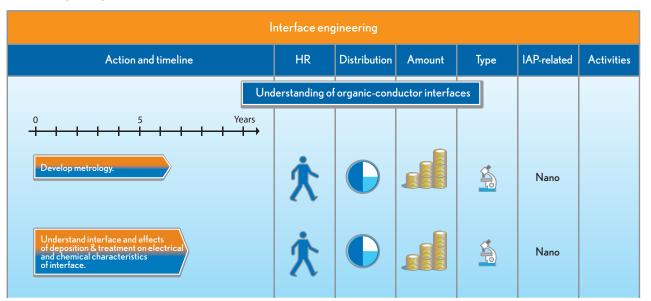
## •• Understanding of interfaces

Interface engineering								
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities		
0 5 Years	Unders	tanding of inte	erfaces		Nano			

The need to characterise full interfaces of nanomaterials integrated together to make up an IC chip is of critical importance to the introduction of new and novel nanomaterials for ICT device applications. Here, novel metrology techniques will be required to **characterise the electronic and structural interactions at nanometre scale interfaces**. The study of the interaction forces between molecules and interfaces by means of atomic force microscopy and fluorescence based technologies on the nanometre scale will provide valuable information on interfaces. Investigation of surface functionalisation processes with organic and biomolecular moieties, as well as self-assembly at surfaces (e.g. SAM of thiols, oligodeoxynucleotides and analogues, peptides and analogues), will enable insights to be gained into the basic properties of interfaces.



## Understanding of organic-conductor interfaces



Here the **development of metrology** to enable the understanding of organic-conductor interfaces is critical. Metrology techniques will enable the **effects of material deposition** processes and post-deposition **treatments on the electrical and chemical characteristics of this interface** to be studied. As a start it is necessary to develop metrology tools to characterise the interface between the metal and organic components so that devices can be fabricated and contacted to, and their performance evaluated and compared with, conventional electronics. With the proper characterisation toolkit at hand, the correlation between device performance and the structure, properties, and chemistry of critical materials and interfaces can then be adequately determined so that organic electronics can move forward. Organic-conductor interfaces play a major role in the performance of novel organic based devices (OLEDs, OTFTs, etc.). As mentioned already, a deeper understanding is needed of the charge carrier injection properties of the interfaces that may act as blocking barriers or as charge injectors. The charge carrier trapping processes are crucial at interfaces where defective states may be present in high densities and may be highly reactive. The basic understanding of the interfaces involved in organic/conductor and organic/semiconductor components will be pursued both experimentally and using molecular modelling. In particular, the grafting of organic conjugated molecules to metallic surfaces will be a key step for understanding the complex charge transfer process occurring between the organic/conductor interface.

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## **○** SELF-ASSEMBLY AND PATTERNING

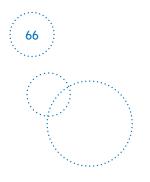
Physics and electrical engineering now depend on the fabrication of structures with dimensions less than 100 nm to generate tools and devices for many areas of research, development, and manufacturing. The future lies in materials which may be manipulated, and technologies which can manipulate, at the atomic level.

## Goals

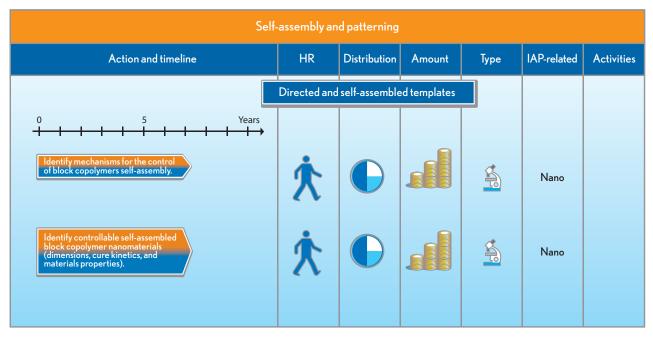
Pursue the development of directed self-assembly templates, patterning technologies, such as printing methods, and the processing of materials in 3D.

## Key activities

- Directed and self-assembly templates
- Advanced patterning techniques



## Directed and self-assembly templates



As dimensions approach 10 nm, the ability to generate controllably patterns with lithography is becoming more challenging, so research is needed into the mechanisms required to self-assemble templates that are aligned to lithographically generated features or to assemble prefabricated nanostructured materials in pre-defined locations. The use of **block copolymers** or surfactants to self-assemble into locally ordered materials has been known for several years, but **mechanisms** are also starting to emerge to enable assembly into pre-defined locations. Significant research is needed to understand self-assembly mechanisms' dependence on molecular size, shape and interactions with other molecules, surfaces, confining geometries, and fields (electromagnetic, stress, thermal, etc.). This research will enable an understanding to be developed of how to control feature shape, size, separation and alignment. This may enable new lithographic techniques, but could also enable the construction of new **nanostructured materials** for a wide range of other applications.



## Advanced patterning techniques

Self-assembly and patterning									
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities			
	Advanced	patterning te	echniques						
0 5 Years									
Identify conductive and semiconductive polymers/molecules suitable for controlled microdeposition through inkjet printing.	Ŕ				Nano				
Suitable for microcontact printing.	Ŕ		Contract in the second se		Nano				
Identify viable nanosized objects to be used as disposable templates for well-defined and reproducible patterns (e.g. DNA strands).	Ŕ				Nano				

Here the identification and characterisation of new materials for various applications is key:

- Identification of conductive and semiconductive polymers/ molecules suitable for controlled microdeposition through inkjet printing.
- Identification of conductive and **semiconductive polymers/ molecules** suitable for **micro-contact printing**.
- Identification of **viable nanosized objects** to be used as **disposable templates** for well defined and reproducible patterns (e.g. DNA strands).

In all cases, materials and techniques must be identified to satisfy particular criteria, for example, rapid and reliable replication of features near or below approximately 100 nm, low operating and capital cost, flexibility in the materials that can be used, fidelity in the replication, ability to pattern on nonplanar surfaces, low density of defects, high speed and parallel operation, and capability for fabrication in three dimensions. Self-assembled DNA patterns as templates for the controlled localisation of functional units (devices, such as organic molecules, nanotubes, redox proteins, etc.) may be used to control the nanometre localisation of nanocircuitry elements of complex arrays in a bottom-up approach. 1D, 2D and 3D templates generated by the self-assembly of DNA strands may also generate micrometre-sized (and above) structures that can be in turn exploited to arrange and confine matter. The self-assembly process of DNA, once fully understood, will enable the controlled creation of a virtually limitless range of nanometric structures of the desired geometry.

Looking at additive patterning methods, inkjet technology, coupled to surface wetting/dewetting control, may well perform the function of guaranteeing the controlled deposition of organic semiconductors/conductors, as well as of metallic nanoparticles, thus allowing the creation of even 3D circuits and tracks.

## **O** SEMICONDUCTORS

Carbon nanotubes present an alternative to current silicon based semiconductors, but the research is in its infancy.

#### Goals

68

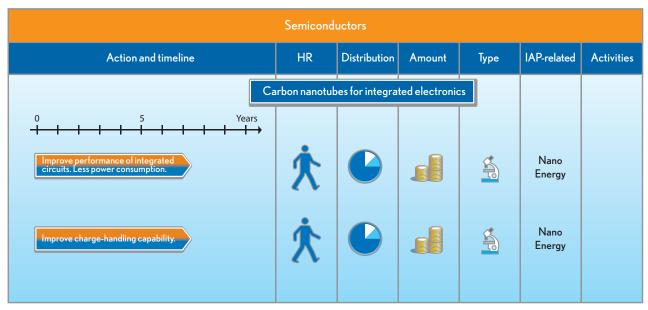
In the case of carbon nanotubes, it will be critical to characterise the structure and properties of these materials very carefully. This is important as it provides a means to ascertain a high level of quality control during production processes whilst maintaining the desired properties. In addition, it will be critical to determine the bonding and defect levels, and then understand how these in turn affect the material properties as this has an important impact on the handling methodologies of carbon nanotubes during production processes.

#### Key activities

• Carbon nanotubes for integrated electronics

# 69

## Carbon nanotubes for integrated electronics



There is a large body of research in the area of carbon nanotube synthesis, characterisation, and application. However, there are significant challenges in the use of these materials for nanoelectronic applications. The measurement of the properties of a material, particularly the electrical properties, is hampered by contact resistance issues. Improved metrology techniques require an understanding of how to probe contacts at lower resistances. Controlling the synthesis of these materials is a challenge; control of the chirality (chirality determines whether the carbon nanotube is metallic or semiconducting in nature) and yield of these materials is necessary. Studies have shown that these materials could yield improved performance of **integrated circuits**, at both the device and interconnect level due to the ballistic electrical transport through these materials which might be possible under certain conditions There is a need for:

- The determination of the band structure based on *ab initio* methods.
- The calculation of the electrostatic properties basing on quantum mechanical methods. This is also linked with the key action "low-k and high-k dielectrics".
- The determination of the transport properties in the ballistic case using, for example, the quantum transmitting boundary method or a Boltzmann-like equation.
- The determination of the transport properties including scattering using, for example, the formalism of the Non-Equilibrium Green Function.
- The implementation of numerical tools for the analysis of the physical and electrical properties listed above, and for the design and optimisation of efficient field effect transistors considering the effect of the device size and of the gate material on the overall performance.
- The analysis of the coherence properties of a wave function propagating along a nanotube, in view of the application of such a device as the fundamental unit of a quantum gate.

## • INFORMATION STORAGE

70

In the future the ICT sector will require that the amount of information that can be stored increases from Gigabits to Terabits; density increases will continue to be a demand as consumers invest in new applications such as digital video and digital music. Cost per byte will continue to be a market concern as well as the provision of low power solutions. In a society where information is one of the most valuable assets, materials and technologies which are able to deliver this ultrahigh density and ultrafast data storage are the key for ensuring Europe takes a leading position in tomorrow's knowledge society.

The ability and requirement to combine both the low cost manufacture and the high performance can only be realised if strong cooperation between industry and academia is established throughout the duration of this research.

## Goals

The goal of this research is to provide the market with solutions to these requirements for highly innovative storage options, and to investigate the key technological concerns associated with these novel approaches (materials and characterisation related), through a close collaboration between chemistry, physics, biology and engineering. In this sense, the most promising fields of investigation are:

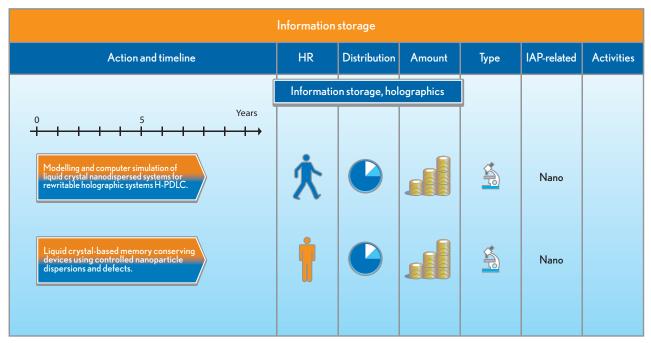
- Holographic storage, by means of new molecular and polymeric materials.
- Biological-based storage and switching, where biological molecules (DNA- or protein-based) will perform multiple roles (for example, storing information and/or performing conformational switching in molecular circuits).
- Ultrafast photo-switching by means of molecular or polymeric materials.

#### Key activities

- Information storage, holographics
- DNA-based and protein-based biological switches
- Molecular switches and photoresponsive devices



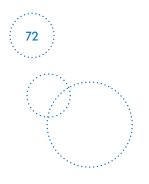
## Information storage, holographics



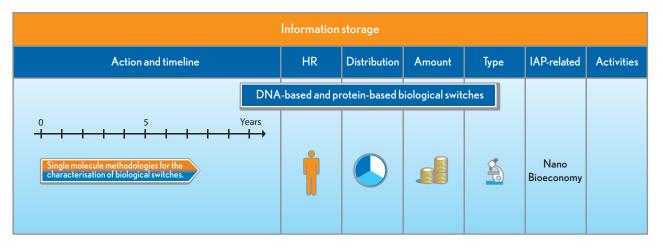
The major challenge to implementing holographic storage has been the development of a suitable storage medium. The criteria for a viable storage material include high dynamic range, high photosensitivity, dimensional stability, optical clarity, manufacturability, non-destructive readout, thickness, and environmental and thermal stability. **Modelling and computer simulations of liquid crystal nanodispersed systems for rewritable holographic systems** are a key research requirement.

A family of **memory conserving devices** may rely on the dispersion of **liquid crystalline** nanodroplets for the realisation of rewritable, memory conserving displays. Also photo-induced switching of molecular or supramolecular structures can find useful applications in all-optical manipulations of information,

informational storage and holographics. Azobenzene sidechain polymers are currently intensively studied for the variety of their photochromic properties. By irradiating with light of appropriate intensity, frequency and polarisation, it is possible to modulate reversibly their bulk optical properties and inscribe relief gratings on the surfaces. In general, the light-driven reversible isomerisation of photochromic molecules makes them excellent candidates for new molecular devices to be used for information storage.



## DNA-based and protein-based biological switches



Controlled conformational changes and architectural transitions in DNA-based nanostructures can be used to set objects near or far apart in space and on a surface, thus serving as a switch in a molecular arrangement of circuit nanoelements.

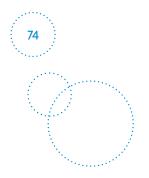
Research methodologies invented and attuned to **single molecular** levels (e.g. molecular switches) need to be adapted for the synthesis and **characterisation of biological switches**  based on DNA or proteins. As with any molecular switch there are fundamental challenges in selecting materials (or molecules) which achieve the right balance between the temperature stability and switchability of the molecule. There is a narrow window between keeping the energy required to flip the switch low enough to work in practical devices but high enough to remain stable at ambient temperatures.

# 73

# Information storage Action and timeline HR Distribution Amount Type IAP-related Activities Molecular switches and photoresponsive devices Molecular switches and photoresponsive devices Mano Mano Undamental understanding of structure deformability, magnitude, for nanoactuators, nhoresponsive devices. Mano Mano Mano Mano Mano Mano Mano Mano Mano

#### Molecular switches and photoresponsive devices

Binary code, which is inherent in current computer chip information storage technology, could potentially be replaced with a molecular binary code. A molecular switch has the potential to act as a molecular binary code. This might reduce the size of information storage by a factor of 100,000 and increase the speed of information storage by 1,000,000. Research is at a very fundamental level in this area and a **fundamental understanding of structure deformability** is a requirement. The optimisation of **response time and magnitude** for application in **nanoactuators and photoresponsive devices** is also of key importance. Smart molecular and polymeric multifunctional and hybrid materials based on photoactive molecules and polymers able to change shape and properties reversibly upon irradiation will be a key component of future industrial applications. These applications will require lightweight and specific properties to provide embedded sensing and photo switchable behaviour for information storage and transmission.



#### Nanotechnology

Nanotechnology is enabling new developments in material science, providing innovations for industries ranging from construction, information & communications, healthcare, energy, transportation through to security. Sustainable development of nanomaterials, including an appropriate assessment of possible risks and their potential for environmental protection will contribute to sustainable economic growth (see also *Sustainable product and process design* and SRA).

The discovery of new materials with tailored properties, and developing the ability to process them, are the rate-limiting steps in new business development for many industries. The demands of tomorrow's technology translate directly into increasingly stringent demands on the chemicals and materials involved, for example, their intrinsic properties, costs, processing and fabrication, benign health and environmental attributes and recyclability with a focus on eco-efficiency.

The corner stones needed are an understanding of the phenomena at the nanometre scale and the tools to make use of these properties by controlling the size and the structure of the materials, and developing the industrial production of nanomaterials, by bridging the gap between the laboratory and the market.

Thus, the research areas of highest priority are:

- Materials.
- Novel production technologies.
- O Development of analytical techniques.
- Computational material science.

#### • MATERIALS

Materials science deals with the design and manufacture of materials, an area in which chemistry plays the central role; there is also considerable overlap with the fields of chemical engineering, biotechnology and physics. Substantial contributions include: modern plastics, paints, textiles and electronic materials, but there are greater opportunities and challenges for the future.

To understand the phenomena that arise at the nanometre scale and to gain the ability to structure, control and integrate new properties that are related to a reduction of the material size, a fundamental understanding of structure property relationships is necessary. Associated with this is the need for new computational modelling methods, analytical techniques and production processes. Developments need to focus on:

- The synthesis and function of nanoparticles.
- Nanostructured surfaces.
- Nanostructured materials (porous materials).

The rigorous development of these fields will help to increase the function, effect and the value of nanomaterials. Sustainable development of nanomaterials will support innovation in the chemical sector and related industries, leading to the application of nanomaterials and biomaterials in:

- Controlled release of drugs and nutrients.
- Healing dressings and/or scaffolds in tissue engineering.
- Artificial hybrid organs.
- Smart packaging materials.
- Eco-friendly antifouling coatings.
- Smart materials (e.g. membranes, adsorbents) for separation of biomolecules.
- Smart surfaces and matrices for the immobilisation of enzymes and receptors.
- Self-cleaning surfaces.
- Self-organising polymers.
- Molecular recognition as an interface between the personal computer and biological activity.
- New biomaterials with properties that were considered 'impossible' in the past.

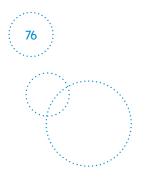


#### Goals

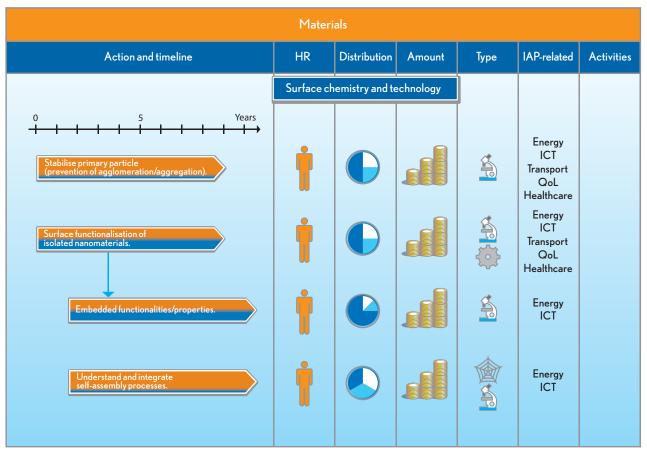
For the realisation and market implementation of novel products with enhanced and new functionalities, new concepts for breakthrough synthetic methods accompanied by cost efficient production technologies have to be developed. These concepts have to include the controlled production of nanostructured functional surfaces through self-assembly, the fabrication of nanostructured (porous) materials and the integration of nanomaterials into high performance products.

A key issue to generate the maximum added value in the future will be complex formulations and the embedding of nanoparticles into a matrix.

- Surface chemistry and technology
- Synthesis and processing
- Nanostructured polymers, hybrid and mesoporous hybrid materials
- Materials for nanostructured sensors
- Nanomaterials for packaging applications



#### Surface chemistry and technology



A crucial factor in the production of nanoparticles, is the prevention of the **agglomeration/aggregation** during their synthesis. Methods and techniques which stabilise freshly produced nanoparticles (**primary particles**) without influencing their surface functionality or properties need to be investigated.

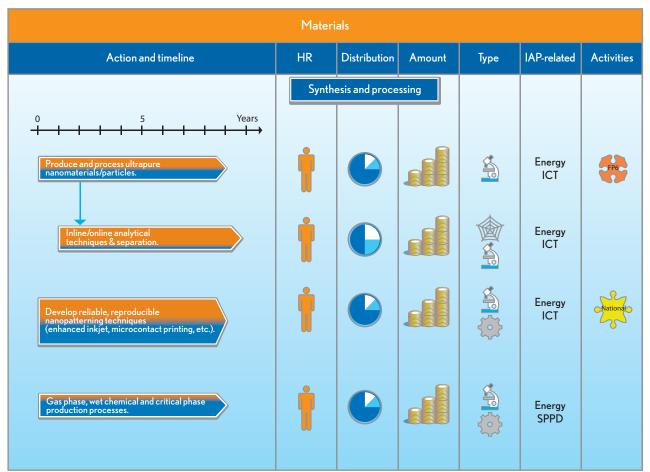
The exploration of the impact of **surface** chemical state and **functionalisation** on the properties of **isolated nanomaterials** 

will open new avenues of controlled synthesis. This will lead to the ability to create **embedded functionalities/properties** in materials and product lines during production processes.

The **understanding and integration of self-assembly processes** in current production process and the development of new production methods will open up new ways for bioinspired innovative products.



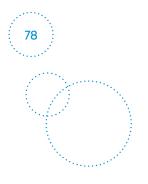
#### ••• Synthesis and processing



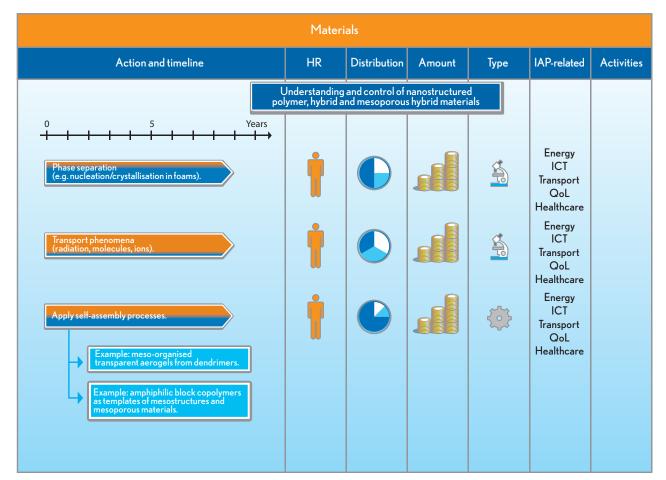
The production and processing of **ultrapure nanomaterials/ particles**, the development of **inline/online analytical techniques** and **separation** technologies are a prerequisite for the transformation of materials into products.

The **development of reliable**, reproducible **nanopatterning techniques** (enhanced inkjet, micro-contact printing, etc.) and the use and integration of these techniques will allow the production of high performance low cost products with enhanced properties. One example is the Plastic Electronics Technology Centre (PETeC) in County Durham, UK.

The development, implementation and scale-up of nanomaterial synthetic methodologies such as **gas phase, wet chemical or critical phase**, into production processes is a challenge which needs to be addressed in order to bridge the gap between the laboratory and the market.



#### Nanostructured polymers, hybrid and mesoporous hybrid materials



Target applications are catalysis, selective separation and purification, chemical and biological sensing and optical communications.

Porous materials are typically made by hydrothermal methods. This type of synthesis is not well understood. The understanding of all stages of the synthesis, from **nucleation** via nanoparticles and low dimensional intermediates to products is essential for controlling size and structure and the nanometre scale.

#### Nanostructured hybrid and polymer materials

Hybrid organic-inorganic materials are increasingly taking place in the free space left between inorganic, polymer and organic chemistry. The driving forces behind this development are the requirements for a variety of applications from catalysis, selective separation and purification, chemical and biological sensing and optical communications. This family of materials includes dispersions of inorganic nanoparticles in organic (polymer) matrices and the converse. Also included are porous metal organic framework materials and the inclusion of organic macromolecules into mesoporous oxides such as silicas. A class of pure polymer materials relevant for the present section is particular nanoporous polymers.

#### Metal organic frameworks (MOFs)

Coordination polymers are ordered materials with one-, twoor three-dimensional networks formed from metal atoms linked together by multidentate organic ligands.



The international attention on coordination polymers has increased dramatically during the last decade as described in recent reviews. The attractive feature of the coordination polymers is that they link the tremendous richness of organic chemistry with inorganic chemistry on the molecular level. This coupling of the two disciplines makes the field extremely large with a tremendous number of possible materials that can be constructed. The materials formed are in most cases crystalline solids with one-, two- or three-dimensional porous networks with pore dimensions from 1-5 nm. The materials show high thermal stability (up to 500 °C). The main focus within the field so far has been on synthesis and characterisation of new structures: The materials have potential applications as adsorbents, molecular sieves, catalysts, etc.

#### Mesoporous hybrid materials

The focus on mesoporous hybrid materials is due to the need for the processing of larger molecules not able to enter the framework of microporous materials. A number of examples are given in the following:

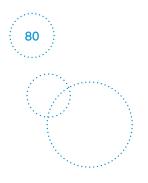
- Meso-organised transparent glassy xerogels can be obtained upon drying of first generation dendrimers: bicontinuous phases are obtained.
- Amphiphilic block copolymers, consisting of hydrophilic and hydrophobic blocks are widely used as templates for mesostructured and mesoporous materials, particularly those based on polyethylene oxide (PEO) and polypropylene oxide (PPO).
- An important part of this subfield is the templated growth of textured inorganic or hybrid materials with tailored porosity. The best known mesoporous materials (MCM and SBAseries) have been prepared by precipitation methods.
- The surfactant template approach can also be used to functionalise materials with a selected active group or to homogeneously incorporate functions of nano-objects within the framework through post synthesis impregnation.

#### Tailored polymer copolymers

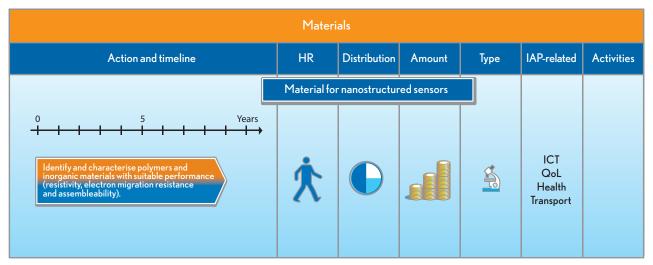
In between nanotechnology and macromolecular science is the preparation of tailored block copolymers. One example is the stepwise polymerisation of polyethylene-co-methacrylate polymers where functionalised side chains can be introduced onto branched polyethylene chains giving polymers with new properties with respect to adhesion and compatibility. This field requires both organometallic catalytic expertise and expertise from advanced polymer characterisation.

#### Nanosized materials

When particles become very small, external surface properties become more dominant. There is a need to take such aspects into account. Recent advances in hydrothermal synthesis allow morphology and size control of oxide nanoparticles. The surfaces of such nanocrystals can be modified by sub-monolayer chemical depositions, uniform nanometre thick coatings or by post-functionalisation. Such designed nanoparticles bring a new dimension into experimental and theoretical investigations of catalytic and surface properties. Of particular interest is the drive to learn and understand how bulk and surface properties change when the particle size reaches critical dimensions. A combinatorial approach will help in identifying the means to optimise conditions leading to narrow size distributions and selected morphologies. The main objective here is to study size dependent properties experimentally and theoretically, and to use that knowledge to understand real catalysts.



#### Materials for nanostructured sensors



Molecular and polymeric semiconductors and conductors have recently been the subject of impressive research efforts, with the aim of breaking the dominance of silicon, and of inorganic materials in general. Such an activity is driven by a number of properties exhibited by organic materials:

- Structural flexibility and lightweight.
- Potential low cost.
- Low temperature processing.
- Compatibility with low-cost fabrication over large areas, such as roll to roll manufacturing.
- Compatibility with several processing techniques.
- Nanomorphology control over large areas, such as with inkjet printing.

In this context the synthesis and the characterisation of main chain conjugated polymers, in particular regio-regular polythiophenes bearing suitable functional groups in the side chain appear of great interest. A key area of research is to be able to identify and characterise **polymers and inorganic materials with suitable performance (resistivity, electromigration resistance and assembleability)** for use as sensors. Nanostructured materials for sensor applications are recognised as having advantages in achieving sensitivity and selectivity for detection in minute sample quantities – however, achievement of the levels of sensitivity and selectivity which might be possible requires significant research effort. For example, the ability to analyse and detect a multiple number of species (inorganic or organic) in one sensor would be hugely advantageous.

Processing techniques should be able to provide the desired material composition, for example adding specific dopants to achieve the desired sensitivity and selectivity, and requiring the least number of processing steps. Vapour-based processes including atomic layer deposition seems to be a promising approach, however, new precursors will be required. Future trends in sensor miniaturisation and integration with electronics will require processing compatibility with silicon-based technologies.

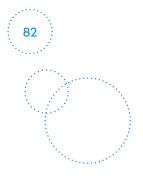


#### Materials Action and timeline HR Distribution Amount Туре IAP-related Activities Nanomaterials for packaging applications Years ICT QoL ¥2 Energy Health Transport

#### Nanomaterials for packaging applications

Future integrated circuit technologies will need to be placed in packages that not only impose very low stress on the silicon, but also connect the device to a printed wiring board. Current package technologies have coefficients of thermal expansion larger than the devices and often cause stress in the device. As dimensions continue to decrease and new devices are integrated, **reduction of stress and electrical losses** in the package will be critical. Some nanomaterials have unique

mechanical properties that may enable low stress packages, but significant work must be done to make these materials compatible with the polymer package materials. Some materials in small concentration, such as nanoclays, have been shown to reduce moisture diffusion through polymers, so integration of nanomaterials with novel combinations of electrical and mechanical properties may enable integrated circuit packages with high reliability.



#### O NOVEL PRODUCTION TECHNOLOGIES

The crucial step for the development of innovative products at the nanometre scale is the integration of known production processes and their adaptation to nanometre scale materials. To meet market demands, both conventional and step out technologies will have to have a scalable design for manufacturing. These new modular technologies can be categorised into:

- Bottom-up and in situ technologies.
- Subtractive direct write technologies.
- Additive direct write technologies.
- Self- and direct-assembly technologies.

Crucial aspects beyond the scalable production processes are the synthesis and processing of ultrapure materials. Here it is important to glean an understanding of, and enable the manipulation of, reactions, nucleation processes, and the formation of materials through the dispersion, modification, and functionalisation of nanomaterials at the large scale. Furthermore, the reproducibility, accuracy, and reliability of these processes should be at the level of, or better than, today's electronic manufacturing standards.

#### Goals

Of particularly importance for the integration of nanotechnology and nanomaterials into high performance products is the development of cost efficient production processes. New manufacturing technologies and synthetic concepts have to be adopted and combined with fast evaluation and testing technologies to reduce development time. Step out technologies include, for example, the integration of high-throughput analysis and reel to reel manufacturing. Other disciplines and methods like formulation engineering, computer-aided multiscale model-based techniques, and methods for microencapsulation, nanoformulation and miniemulsions have to be further advanced.

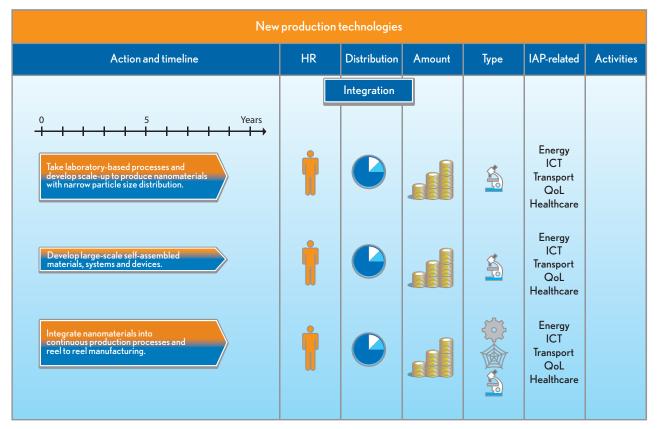
For the exact control of size and shape of nanoparticles, methods like high gravity controlled precipitation and co-/jetprecipitation as well as flame, plasma and sol-gel synthesis and also hydrothermal methods and hot wall reactor technology have to be developed.

Key activities

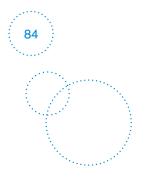
Integration



#### Integration

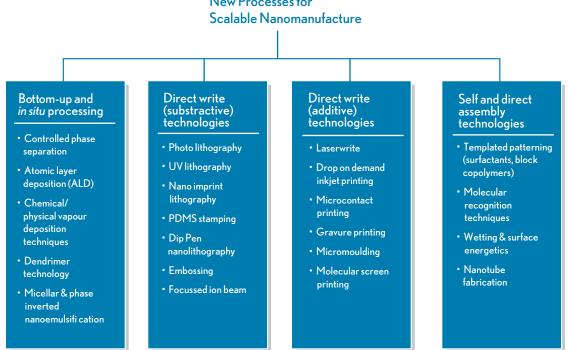


- Take laboratory-based processes and **scale-up** to produce nanomaterials with **narrow particle size distribution**.
- Development of large-scale self-assembled materials, systems and devices.
- Integration of nanomaterial synthesis into continuous production processes and reel to reel manufacturing.
- High-throughput tools for formulation engineering are required for the rapid design, synthesis and testing of formulations, including computer-aided multiscale modelbased techniques combined with experimental techniques to identify the optimal formulation (also includes aspects of manufacturing of the formulated product). The ongoing development and use of Dynamic Combinatorial Libraries for studies of receptors, catalysts, enzyme inhibitors and new materials, like multifunctional nanoparticles will help to reach the goals identified. The results can also be used in related applications, like (gas-) sensors, biomarkers and receptive/ reacting materials (e.g. targeted drug delivery) - see also *Sustainable product and process design*.
- A critical step is the scale-up from laboratory scale to pilot/demo scale, especially for microencapsulation, and production of fine particles and nanoformulations. Cost/risk sharing programs are required to accelerate this essential step in developing new products; strategies are required for micro-encapsulation, concepts, design methodologies and fast scale-up. The demand for tailored nanoparticles and multifunctional materials, like core-shell particles, can only be satisfied by the development of new synthesis routes. Gas phase, wet chemical and critical phase production processes are being focussed on. Examples include studies on precipitation processes (e.g. miniemulsion, high gravity controlled precipitation, co- and jet-precipitation), sol-gel synthesis, hydrothermal methods, flame synthesis, plasma synthesis, hot wall reactors, desublimation and expensive processes like rapid expansion of supercritical solutions (RESS), supercritical antisolvent precipitation (SAS), particle from gas saturated solutions (PGSS) and depressurisation of an expanded liquid organic solution (DELOS).



Furthermore the adaptation of step out and unconventional process technologies can be pursued, as seen in the figure below.

New processes for the manufacturing of nanomaterials (see SRA Appendix p. 63)



The production of quantum and hybrid materials poses a challenging guestion. Here, the development of an 'innovation toolkit' based on quantum scale phenomena, for example transport, optical, electronic and biocompatible properties, is essential. Ensuring that these unique properties of quantum materials are maintained from the synthesis through to the final integrated system is a demanding activity. Furthermore, molecular engineering of complex hybrid materials and their fabrication needs to be developed.

### New Processes for



#### O DEVELOPMENT OF ANALYTICAL TECHNIQUES

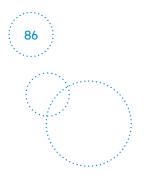
The appropriate analytical tools will play a mayor role in the determination of structure property relationships at the nanometre scale, including the control of materials' shape and size. In addition to the improvement of existing analysis tools such as tomography in 3D, solid state 3D NMR and microscopy/spectroscopy (see also SRA Appendix), other (online) analytical methods need to be developed further.

In the field of nanomaterials, not only is there a need to be able to analyse individual components, but also the properties of the whole system at the macroscopic level, which is built upon the inherent properties of the nanoscale components. Therefore a correlation between the spatial organisation and fundamental property information at the nanoscale (e.g. mechanical, chemical, thermal, etc.) needs to be discerned by the analytical method. There is, however, a lack of analytical standards for nanomaterials; and the environmental, health and safety (EH&S) issues have yet to be resolved. Programmes addressing these issues running in FP6 and in national programs include NanoSafe2 (FP6) and Nanocare in Germany (BMBF).

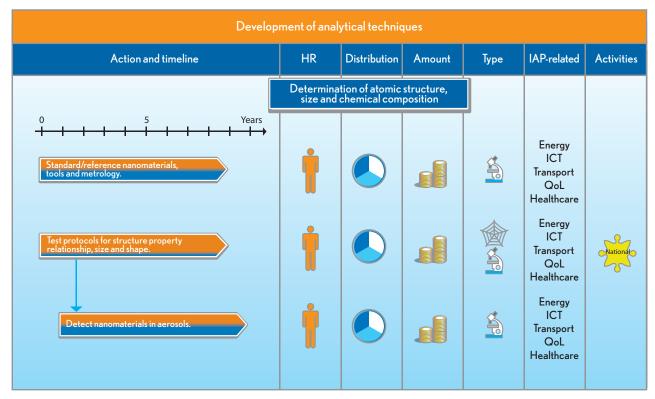
#### Goals

For research and industrial processes, there are a number of expensive analytical techniques dedicated to the analysis of nanomaterials which have to be progressed to gain a better understanding of the structure property relationship. To increase the availability of these methods for smaller companies and research groups, new cost and time effective methodologies and imaging tools have to be developed. Furthermore standards have to be evolved to enhance the quality and impact of these methods. The related analytical techniques are listed in the SusChem SRA Appendix.

- Determination of atomic structure, size and chemical composition
- Environment, health and safety issues
- Detection of nanomaterials in biological tissue



#### Determination of atomic structure, size and chemical composition

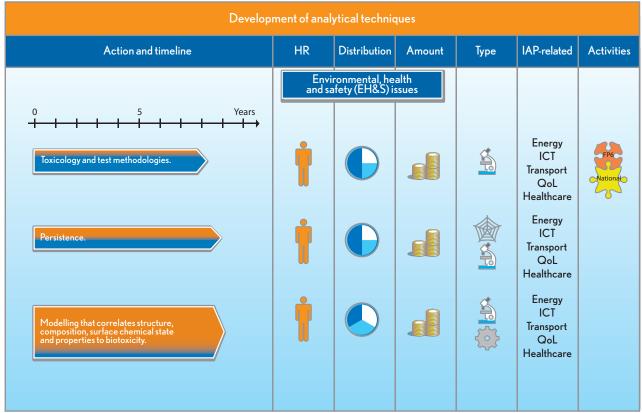


Fundamental conditions and components providing the basic information necessary for the investigations mentioned above such as the environment, health and safety aspects of the production and use of nanomaterials, and enabling adequate quality control are needed:

- **Standard/reference nanomaterials** for characterising size and shape, especially of plate-like and rod-like particles (spherical standards have already been developed).
- Test protocols for a better understanding of the structure property relationship and to be able to compare raw materials with the final composites or products.
- Methods for the **detection of nanoparticles in aerosols**.



#### Environment, health and safety issues

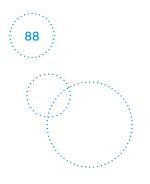


To realise the great potential of nanotechnology and to ensure sustainable development, the possible risks of new technologies, like nanotechnology, have to be taken into account and responsibly investigated (see also *Risk Assessment and Management Strategies*). Experience has shown that nanomaterials do not necessarily demonstrate the same properties as the bulk materials from which they are derived, and consequently there is a need to:

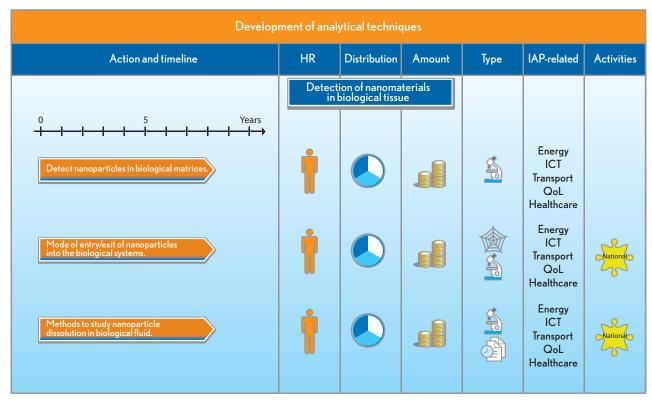
- Establish exposure routes and mechanisms of action of nanoparticles on humans, and the fate and effects of nanoparticles in the environment (**persistence**).
- Develop health, safety and environmental standardised criteria for the classification of nanoparticles that complements the work being carried out by the ISO/TC 229.

- Develop internationally validated **toxicological** and environmental **methodologies**.
- Identify specific candidates for further investigation and characterisation.
- Create models which correlate structure, composition, surface chemistry and properties to biotoxicity.

Some of this work is currently underway internationally as well at the European Union level and at national level. The proposed work will add to these projects. Industry and academia are working together to develop analytical standards, etc. Work will build on existing methods to develop them further and in doing so will support the introduction of nanomaterials.



#### Detection of nanomaterials in biological tissue



To study the effects of industrially produced nanoparticles on human health validated test methods have to be developed. The interactions with biological systems as well as exposure routes have to be fully understood. Various testing methods are currently used to investigate possible effects of nanoscaled materials in the lung, i.e. inhalation, intra-tracheal instillation and various cell culture systems. To systematically study the effects of nanoparticles and the dependency on their physical and chemical characteristics, the following topics need to be focused on:

- Detection of **nanoparticles in biological matrices**. e.g. assess impact of nanotubes and buckyballs on cancer growth.
- Mode of entry/exit of nanoparticles into biological systems.
  Needed to determine worker exposure limits and biological decomposition.
- Methods to study nanoparticle **dissolution in biological fluids**.
- Development of improved *in vivo* methods to evaluate the data from *in vitro* experiments.



#### ••• • COMPUTATIONAL MATERIAL SCIENCE

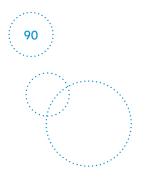
Computational material science tries to provide an understanding of materials' properties and to assist in the development of new functional materials. It does so by mapping the whole range of technologically relevant processes from chemical synthesis, through experimental characterisation of materials' properties, to industrial processing onto suitable models and by developing efficient algorithms for their simulation. This encompasses models capturing chemical detail on the scale of individual bonds (scale of about 1 Å) to the scale of the whole molecule, which, for macromolecules, can reach tens of nanometres. Structures in melts, blends and solutions can range from nanometre scales to microns, millimetres and larger. The corresponding time scales of the dynamic processes relevant for different materials properties span an even wider range, from femtoseconds through milliseconds to seconds or even to hours in glassy materials and large-scale ordering processes such as phase separation in blends. No single model or simulation algorithm can span this range of length and time scales.

#### Goals

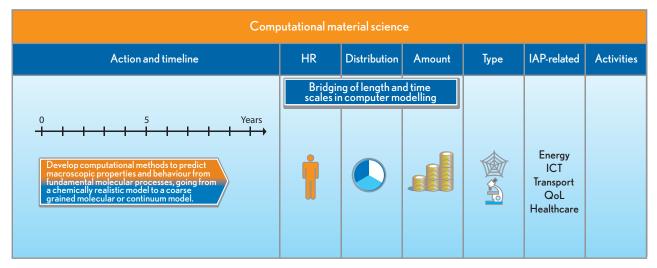
- Modelling of advanced materials and composites.
- Modelling of formulations to achieve controlled functional properties.
- Interfaces: design, characterisation and modelling.
- Surfaces: design, characterisation and modelling.
- Prediction of macroscopic properties.
- Understanding fundamental molecular processes.

This requires new and improved molecular models ranging from those for materials including quantum effects and electronic degrees of freedom, to chemically realistic, classical models, to coarse grained, particle-based 'mesoscale' models that retain only the most essential elements of the material to be simulated, to continuum models that describe the material in terms of, for example, density or composition variables.

- Bridging of length and time scales in computer modelling
- Development of applications software and user friendly interfaces for computational tools
- Specific interactions
- Analytical techniques for materials research via computer modelling



#### Bridging of length and time scales in computer modelling



The development of **computational methods** ranging from chemically realistic models to **coarse grained molecular** or **continuum models** is needed to predict **macroscopic properties** and **behaviour** from **fundamental** molecular processes.

Linking mesoscale molecular models and continuum descriptions is of paramount importance in the modelling of composite materials, the properties of which are determined by a hierarchy of structures on very different length/time scales. In addition to the mapping between models on different levels of chemical detail, parallel application of different modelling approaches will, of course, remain of great importance. A good example is in the area of organic electronics, where the relevant structural arrangement of the functional units has to be determined by force field based methods (chemically realistic or even on the mesoscale depending on their size) and the function, i.e. the response of the electronic degrees of freedom can only be described by quantum chemistry.



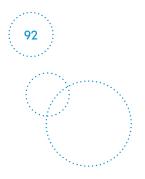
#### Computational material science HR IAP-related Activities Action and timeline Distribution Amount Туре Development of large-scale scientific applications software and new user friendly interfaces for computational tools Years $\rightarrow$ Energy Transport QoL Healthcare Energy Transport QoL Healthcare Energy ICT Transport QoL Healthcare

#### Development of applications software and user friendly interfaces for computational tools

The development of new approaches and **easy-to-use software** systems **for materials simulation**, both on **high performance computers** and on **personal computers** is needed:

- The development of hierarchical modelling approaches combining atomic-scale, molecular and mesoscopic modelling, as well as conventional engineering computing (finite element analysis, finite difference methods and boundary element methods).
- The application of simulation software to problems of technological relevance and the transfer of the acquired knowledge into industrial research.
- The workings of complex computer programmes should be as transparent as possible to help both user understanding and future development.
- A high level of 'user friendliness', including the presence of user friendly interfaces, educational modules, and intelligent tutoring systems is desirable.

- The interface must be easily customised, allowing for spreadsheet data input and mouse-based interaction with the model.
- Interfaces to other software tools like office and CAD products are necessary.
- The mathematical complexity of the solution needs to be masked by an interface applicable to both the power user and the average user.
- As these interfaces become more sophisticated, building and presenting models should become more intuitive.
- Output analysis tools for simulation need to include more guidance for users to prevent erroneous inferences. (The software needs to protect the non-expert user from making mistakes when interpreting the results. Additionally, the expert user needs better tools for constructing customised reports and capturing simulation information for later analysis).



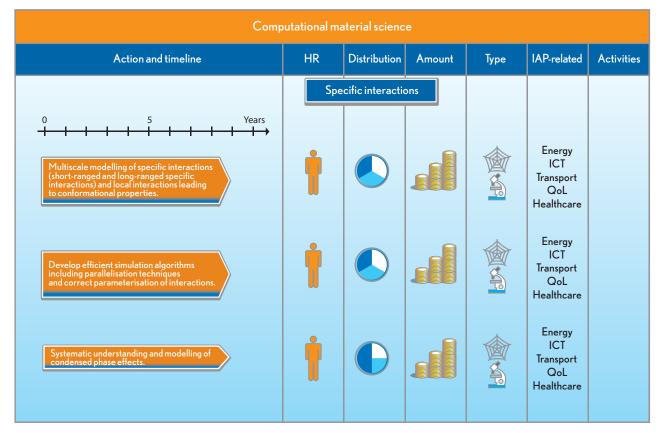
- Template models can help reduce the model development time and can provide valuable insight into the appropriate inputs to be considered when analysing a given process.
- The simulation environment for the interactive visualisation of 3D data, the visualisation of four-dimensional space time processes, and the design and implementation of parallel volume and surface oriented rendering in molecular and mesoscopic simulations have to be developed.
- The implementation of scientific multimedia functionalities and distributed virtual reality into materials simulation in parallel is of utmost importance for the development of high performance materials.

For **distributed computing** to be viable, software must be designed and implemented as components whose services can be accessed from any other component that needs it. Therefore adequate high speed network infrastructures have to be built and integrated.

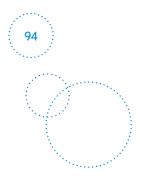
**Cooperation** with scientists and developers in the fields relevant to scientific visualisation will ensure proper leverage. This bilateral cooperation between groups from participating research institutes and industrial enterprises has to be supported through public funded projects providing the right framework conditions.



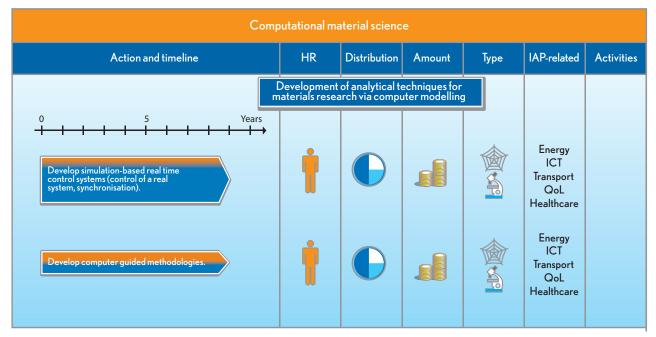
#### **Specific interactions**



A central and basic challenge which is becoming more and more urgent is the need for the quantitative prediction of the properties of matter (both "soft" and "hard"). The absence of that ability is increasingly a barrier to progress in modern industries ranging from molecular electronics to biotechnology. The primary fundamental challenge is to uncover the elusive connections in the hierarchy of time and length scales, and to unravel the complexity of interactions that govern the properties and performance of advanced materials. To overcome this barrier **multiscale modelling** of **specific interactions** (short-ranged and long-ranged interactions and local interactions leading to conformational properties) and the development of efficient simulation algorithms including parallelisation techniques and the correct parameterisation of interactions is needed. A systematic understanding and modelling of **condensed phase effects** like anisotropic interactions in liquid crystalline materials or long-range anisotropic strain fields is also needed.



#### Analytical techniques for materials research via computer modelling



Simulations of physical phenomena provide useful demonstrations that help to develop fundamental understanding and often reveal the essential nature of a process. The phenomena under investigation in modern physics and chemistry are usually too subtle, and the experiments too complicated to tackle with only analytical tools. Also, the experiments can be too difficult or expensive to perform or can raise environmental or safety issues. Simulations mimic the physical world down to the interactions of individual atoms and they are essential in the design of modern experiments. Analytical techniques such as high resolution transmission electron microscopy, scanning probe microscopy, X-ray and neutron diffraction, extended X-ray absorption fine structure (EXAFS), and various kinds of spectroscopy allow the examination of materials at the atomic level. These techniques like simulation-based real time control systems allowing the control of a real system including synchronisation need to be developed, improved, and extended further by integrating them with more powerful computers for rapid visualisation of data and comparison with computer models.

These techniques have a particular importance in the area of materials synthesis, where they can be used for manipulation and control of materials at the atomic and nano levels, as in atomic force microscopy. The modelling environment that links the simulation methods with advanced analytical techniques can supply a toolkit of common capabilities that permit, for example, the construction of new models, comparison of calculated and observed properties, and iterative adjustment to achieve maximise agreement. **Computer guided methodologies** are a centrepiece leading to the accurate understanding of physical/chemical processes and behaviour from the quantum level, to nanoscale, to mesoscale and beyond, so that phenomena captured in simulations can be applied to real complex systems without loss of intrinsic structural information.



#### Sustainable quality of life

The aim is to maintain and improve the quality of life of citizens through the application of SusChem technologies. A parallel aim is also to make citizens' life styles more sustainable and have lower environmental impact through the consumption of less energy, the use of fewer resources, and the reduction of emissions, either directly in citizens' own homes, or indirectly through the products which they buy.

#### Priorities in this section are:

- The home as self sufficient energy provider.
- The home as an eco-efficient environment.
- Waste treatment, soil and water remediation.

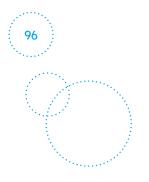
#### • THE HOME AS SELF SUFFICIENT ENERGY PROVIDER

While most houses still rely on traditional means for their energy requirements, technological advances and resource management techniques have made it possible to cut energy consumption by up to 90 % today. With the development of new technologies covering energy generation and energy consumption it will be possible for a home to generate enough energy to meet and even exceed its daily requirements.

#### Goals

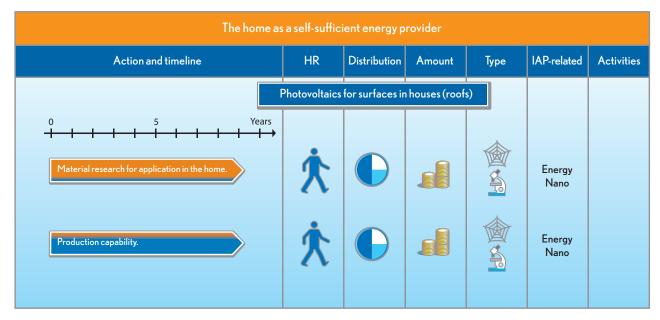
Create the core technologies and multidisciplinary capabilities to enable cost competitive and sustainable products and processes for energy generation and storage in the home environment. Attempts should be made to coordinate activities from the *Energy*, *ICT* and *Nanotechnology* sections to realise the Smart Energy Home visionary project.

- Photovoltaics for surfaces in houses
- Superior domestic batteries and alternative energy storage



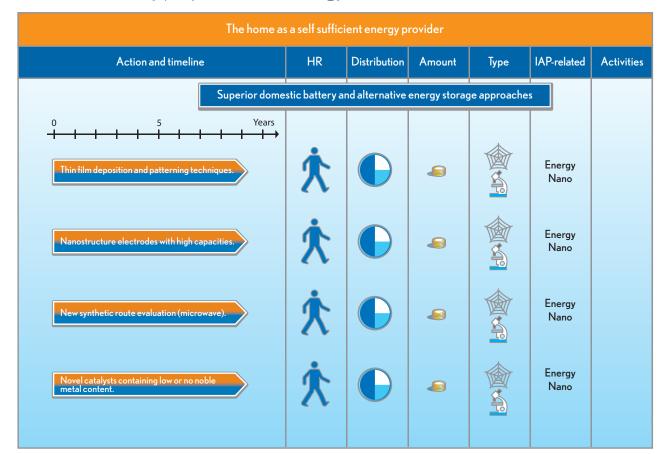
#### Photovoltaics for surfaces in houses

Element of visionary project: Smart Energy Home



Research needs to focus on superior **photovoltaics** (see also *Energy: Photovoltaics*) to maximise cost effective energy collection using silicon and conjugated polymer alternatives for the **home environment.** This needs to be combined with new solar panel **production approaches**, hybrid materials and new electrodes.

#### Superior domestic batteries and alternative energy storage Element of visionary project: Smart Energy Home



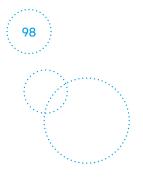
Priority activities in this area (see also *Energy: Fuel cells, Batteries & Supercapacitors*) are the development of:

- Lithium batteries for energy storage based on alternative electrodes/electrolytes and polymers, for example:
  - Nanostructured electrode materials of high specific capacity.
  - Mesoporous carbon electrodes and electronically conducting polymer electrodes.
  - Development of **new synthetic routes** for electrode materials, eventually assisted by **microwaves** (see also *Healthcare: Implantable biomedical devices*).

- Fuel cells:
  - PEM & DMFC.
  - Mesoporous carbon supported catalysts.
  - Electronically conducting polymer supported catalysts.

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- $\cdot$  Novel catalysts with low or no noble metal content.
- The development of thin film deposition and patterning techniques will lead to the production of smaller energy storage units, potentially leading to higher efficiencies and energy savings.
- Technology approaches such as supercapacitors and ionic liquids.
- Computer simulations.
- Ion-selective membranes which prevent deleterious ions via high flux permselectivity and demonstrate stability in harsh chemical environments.



#### **○** THE HOME AS ECO-EFFICIENT ENVIRONMENT

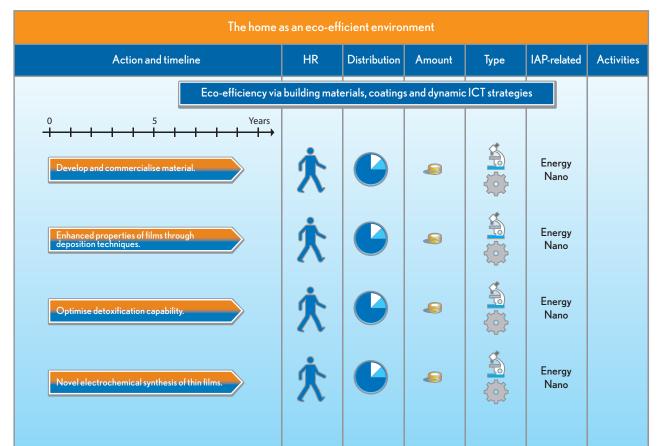
In addition to energy generation, most homes will require technology breakthroughs to reduce energy use and increase sustainability in a consumer friendly manner. Breakthroughs are required in areas such as building materials, decorations, home appliances, lighting and waste treatment.

#### Goals

The intention is the development of technologies, which enable the creation of highly eco-efficient products to assure energy conservation and improved convenience. This will lead to the "re-invention" of a wide range of products, including insulation materials, construction materials, kitchen appliances and domestic appliances and will create novel approaches such as self-cleaning surfaces.

- Eco-efficiency via building materials, coatings and dynamic ICT strategies
- Polymers from renewable materials for packaging, furniture, domestic water purification and recycling
- Household innovation





#### Eco-efficiency via building materials, coatings and dynamic ICT strategies Element of visionary project: Smart Energy Home

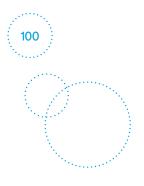
An important aspect of eco-efficiency that can be addressed through the application of smart materials is that of temperature (climate) control in the home and within appliances, using passive systems and appropriate control systems (**ICT strategies**). **Insulation** is the most important passive system. Materials which provide much improved insulation are available today, but new materials will significantly increase performance.

Priorities are therefore the development of:

- New high performance insulating materials (see also Energy: Insulation) including aerogel nanofoams potentially obtained by recycling waste and by-products.
- Photochromic coatings for glass.

Integrating these technologies with intelligent ICT components and sensors (requiring for example new conductive and non-conductive polymers and flat, lightweight, low-cost foldable and rollable displays) able to respond to parameter changes (such as temperature (interior/exterior), pressure or sunlight intensity) will lead to systems that efficiently monitor the home environment and react to changes thus allowing efficient home climate management and at the same time conserving energy. Active systems could be implemented through the use of mechanical or electrical devices that, for example, adjust the incandescent light or direct airflows through and within a building.

Indoor air quality has become an issue of increasing importance as many people spend most of their time inside buildings or vehicles. Processes or products that improve the



indoor environment can therefore bring about substantial health benefits. This can be accomplished by using devices that decompose any kind of pollutant (**detoxification**) or by producing **building materials** that are functionalised in order to passively perform the same function and thus create an improved environment. Low temperature nanoscale catalysts designed to decompose substances such as tobacco smoke, volatile organic compounds (VOCs) evolving from building materials, adhesives and cleaning products would significantly improve this capability. The increase in comfort and convenience brought about by new products for the home environment will also have significant impact on creating a "healthy home".

Photocatalytic films can also be used to improve the indoor air quality, but to make these very promising systems effective, affordable and reliable an improvement in the **deposition techniques**, an increase in the wavelength range of the utilisable radiation and a deeper knowledge of the processes taking place inside the photocatalytic materials are necessary. Also, new **thin film** coatings with inorganic, composite and conjugated polymer materials are needed.

Other developments of new materials to improve the ecoefficiency of the home include:

- Functional textiles with superior energy balance and flexible use for garments, home and construction, requiring lightweight and lower cost nanoporous systems, and self-healing and self-cleaning nanocoatings.
- Construction materials development of innovative (low temperature) cement compositions based on industrial scraps and recycled materials.

## 101

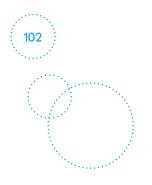
#### Polymers from renewable materials for packaging, furniture, domestic water purification and recycling

The home as an eco-efficient environment										
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities				
Polymers from renewable materials for packaging, furniture, domestic water purification and recycling										
0 5 Years										
Integrated research across disciplines.	X		-		Energy Nano					
Market-enabling approaches.	Ż				Energy Nano					

This area requires research in (see also *Bioeconomy*):

- Bio-based and self-assembly polymers.
- Nano and dielectric filtration techniques.
- Novel catalysts.
- Smart and dynamic packaging materials.
- Polymeric and dendrimeric materials bearing photoactive molecular switches in the side chains.
- Bacteriostatic-bactericidal properties of bioactive molecules.

If consumer products are to be developed from these diverse research activities, **market-enabling approaches** need to be investigated to achieve a quick time to market for the end products.



#### Household innovation

The home as an eco-efficient environment										
HR	Distribution	Amount	Туре	IAP-related	Activities					
Innovative and efficient household tasks: lighting, laundry, decoration, heating and waste treatment										
X				Energy Nano						
Ŕ				Energy Nano						
	HR	HR Distribution	HR Distribution Amount nold tasks: lighting, laundry, decoration, h	HR     Distribution     Amount     Type       nold tasks: lighting, laundry, decoration, heating and wa       Image: Constraint of the second sec	HR     Distribution     Amount     Type     IAP-related       sold tasks: lighting, laundry, decoration, heating and waste treatment       Image: solar stream of the strea					

In the home, many innovations are possible with the application of new materials and technologies ranging from an improvement in the efficiency of laundry processes by using new formulations or catalysts, to the implementation of (O)LED lighting and other low energy devices. Furthermore, activated surfaces incorporated in paints or wall decorations can combat odours created by cooking or household waste, and self-cleaning surfaces will reduce the amount of detergents and time spent on cleaning purposes. This broad area encompasses the following research:

- Light and energy management technologies.
- Appliances and consumer products with > 50 % reduced energy consumption and which are recyclable.
- The development of LEDs and OLEDs: LEDs based on conjugated polymers which will be crucial for the improvement of household eco-efficiency.

- Nanoscale controlled depositions (microcontact printing, nanotemplate patterning, etc.) on thin films and the integration into products like self-cleaning surfaces and functional materials (printed electronics etc.).
- Integrated appliance and chemistry design development.
- Innovative catalytic applications for tasks in the domestic environment such as:
  - Self-cleaning surfaces some applications have already been developed for building and painting materials but effort is needed to increase the range of applications.
  - Catalytic systems and **biosensors** coated on the internal surface of food packaging which are able to either decompose residual oxygen, thus prolonging storage lifetimes, or indicate by a change in colour whether the food is still safe for consumption or a combination of both.



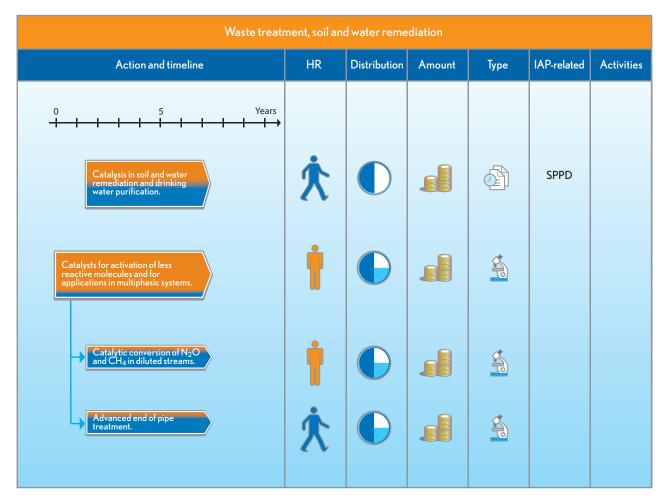
#### O► WASTE TREATMENT, SOIL AND WATER REMEDIATION

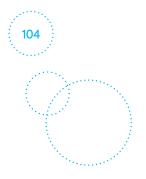
Catalysis provides innovative solutions to solve urgent environmental issues. In order to achieve and sustain a clean environment, technologies for water purification, soil and water remediation, waste treatment and the prevention of air pollution are required.

#### Goals

Develop a thorough understanding of the catalytic pathways involved in waste treatment/remediation processes. Use the knowledge gained for the identification of catalysts for waste treatment/remediation, using high-throughput methodologies.

- (Bio)catalytic solutions for **soil and water remediation** and **purification** of drinking water, targeting the conversion and removal of a wide variety of substances at low concentrations.
- Fundamental research targeting effective catalysts for the **activation of less reactive molecules** (e.g. CO<sub>2</sub>), and for applications in **multiphasic systems**.
- Catalysts for efficient conversion of greenhouse gases with high global warming potential, in particular N<sub>2</sub>O and CH<sub>4</sub>, in dilute process streams.
- Technologies for **end of pipe treatment** in process systems including separation methods, catalysis and utilising plasma surface etching, microwaves etc., thereby integrating efficient recycling and re-use strategies.





#### Sustainable product and process design

Aiming at more eco-efficient and environmentally benign processes and competitive production technologies in Europe, the following areas of research have been identified as highest priority:

- O Diversification of the feedstock base.
- Innovative eco-efficient processes and synthetic pathways.
- Knowledge-based manufacturing concepts for targeted and tailored products.
- Implementation and integration of intensified process technologies.

#### • DIVERSIFICATION OF THE FEEDSTOCK BASE

The main objective is to decrease the dependency of chemical production from oil by shifting the feedstock base towards alternative feedstocks. Biomass as a renewable resource is the preferred option, but efficient exploitation of gas and coal is also required, due to their more extensive reserves compared to oil.

For larger scale exploitation of biomass-derived feedstocks, whole value chains will have to be adapted and redesigned. Since the chemical industry is highly integrated this is a key challenge and a large scale analysis which goes far beyond a single transformation is necessary.

The introduction of new routes for natural gas conversion to chemicals and the efficient exploitation of coal as a feedstock requires the integration of knowledge of the selective activation of alkanes, development of new catalysts, new reactor engineering, and value chains in the chemical industry. This kind of expertise is currently only available in interdisciplinary teams.

#### Goals

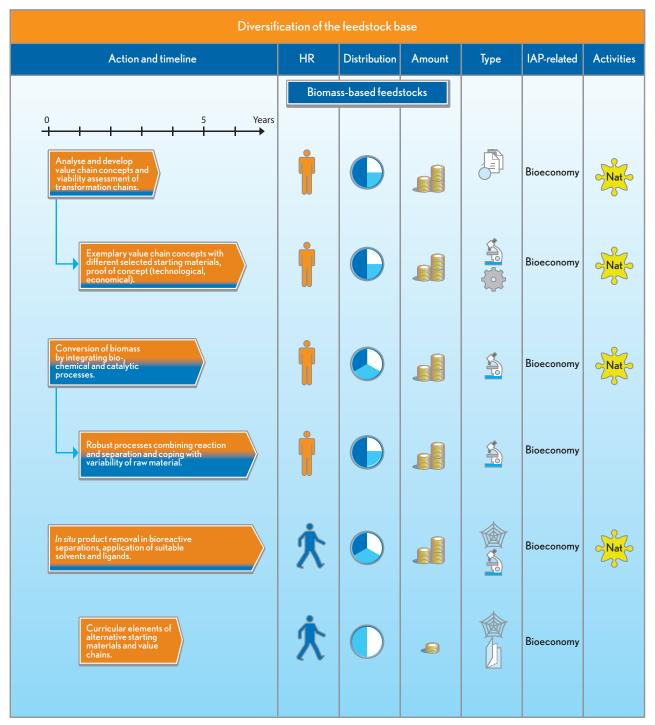
As a prerequisite for expanding the use of renewable, biomassderived feedstocks, a thorough analysis of value chains and development of alternative value chains starting from biomassderived feedstocks, including assessment of the economic viability of the transformation of the chains is required. This must be followed by the identification of easy entry points for the implementation of novel value chains. Technical key issues are the development of generic methods to cope with the variability of raw materials derived from biomass and their higher susceptibility to contamination by microorganisms, and of suitable catalysts for biorefineries.

Diversification of raw materials in petrochemical production by introducing new processes based on the direct use of natural gas as a raw material (e.g. acetic acid from ethane, acrylic acid from propane, methyl methacrylate from isobutene) will reduce the dependence of chemical production on oil and create competitiveness incentives. Conversion of natural gas produced in remote areas to liquids will allow the economic transport and enable its use as an alternative raw material, thus decreasing greenhouse gas emissions. New catalysts for the selective functionalisation of alkanes and gas to liquid conversion are required which should be integrated into smart and efficient reactor concepts, for example, for "at source processing" of natural gas.

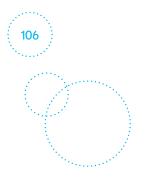
Short term targets are direct oxyfunctionalisation processes for ethane, propane and isobutene; longer term research should focus on using methane as a feedstock for chemical production which also requires development of new processes, avoiding the use of syngas as an intermediate, to convert it to liquid fuels.

- Biomass-based feedstocks
- Coal- and gas-based feedstocks

#### **Biomass-based feedstocks**



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A number of different actions seem to be suitable for the introduction of biomass based raw materials in the chemical industry:

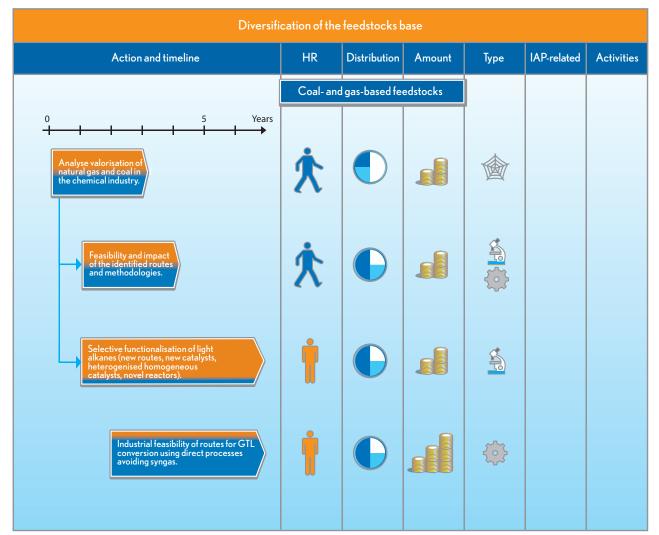
- The establishment of interdisciplinary study groups to conduct a survey analysing current value chains in the chemical industry and developing a concept for alternative value chains starting from biomass derived feedstocks, including lifecycle assessment of the economic viability of the transformation chains. Identification of easy and EU-based entry points for the implementation of novel value chains.
- The development and demonstration of **exemplary value chain concepts** requires a survey aiming at the conceptual development of an entry point value chain based on, for example, plant residues from biodiesel production (largely exceeding the requirement for feeding animals) and other starting materials such as lignocellulose, sugars, starches and seed oils. The use of these materials is in line with the proposed switch in farming from food production to providing raw materials for consumer chemicals. This switch would also have a beneficial impact on reducing subsidies in the Common Agricultural Policy and be a better use for land than set aside. The subsequent proof of concept for entry point value chains requires demonstration type projects.
- The development of novel synthetic routes for efficient conversion of biomass derived raw materials with high performance, stability and selectivity, by integrating bio-, chemical and catalytic processes. Synthetic pathways in which the complexity needed in a target molecule is already preformed in the biomolecule seem especially favourable.

- The development of **robust processes** based on new reactor engineering solutions to improve energy and process efficiency and economics, and which combine reaction and separation. Special attention needs to be paid to cope with the **natural variability** in the quality of raw materials.
- In situ product removal in bioreactive separations requires research and knowledge exchange in networks in respect of separation agents (i.e. adsorbents, "green" extractands), and fundamental research on transport processes through membranes and bioreaction mechanisms.
- The development and implementation of **curriculum materials** is essential to increase the awareness of chemistry students of alternative starting materials and conceptually different value chains.

#### **Existing activities**

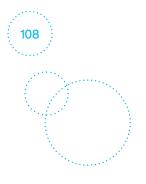
Some processes are traditionally based on biological feedstocks, such as in oleochemistry. In addition, the first projects to produce valuable chemicals from glycerol have been launched; also biopolymers and the conversion of wood are being explored. Novel activities could be based on the experience gained in these fields, but if novel value chains have to be developed, this experience is only of limited value. Problems, such as quality, variability and contamination with microorganisms, however, can probably also be solved in many cases on a generic level. Activities in FP6 focus on (conventional) processes rather than on innovative synthetic concepts and catalytic solutions.

#### Coal- and gas-based feedstocks



A number of different actions are essential for the introduction of natural gas and coal as a feedstock in the chemical industry:

- The establishment of interdisciplinary study groups to analyse possible routes for the valorisation of natural gas and coal in the chemical industry. Catalytic pathways coupled with new reactor engineering solutions, such as short contact time, catalytic membrane, electrocatalysis, seem especially promising.
- Research and demonstration type projects to assess and prove the technical feasibility, economics, sustainability and strategic impact of the routes identified and newly selected methodologies.
- The development of new innovative and clean methodologies for the selective functionalisation of light alkanes and reduction of the number of consecutive reactions: (i) coupling homo- and heterogeneous catalysts, (ii) use of new oxidants, (iii) supercritical operations in nanoreactors, (iv) new reactor options. Research should include the identification of methodologies which appear most promising in respect of the target products and alkane type.
- The demonstration of the **industrial feasibility** of routes to convert light alkanes to liquids using direct processes which **avoid using syngas** as an intermediate stage.



## SYNTHETIC PATHWAYS

The World Energy Outlook 2005 projects the world energy demand will increase by over 50 % between now and 2030 with corresponding energy-related CO<sub>2</sub> emissions 52 % higher than today. With strongly increased energy and resource prices, the increase in process efficiency in terms of energy consumption and resource use is more than ever a major goal for innovation in process technology from both an economic and an environmental perspective. Rather than incremental improvements of processes by stepwise re-engineering or adaptation of operational conditions, drastic performance enhancements are envisioned, which are eco-efficient and provide substantial competitive advantage. Exploring new reaction pathways and conditions, reducing the number of reaction steps, introducing intensified separation technologies and intensifying energy input are important steps in this context.

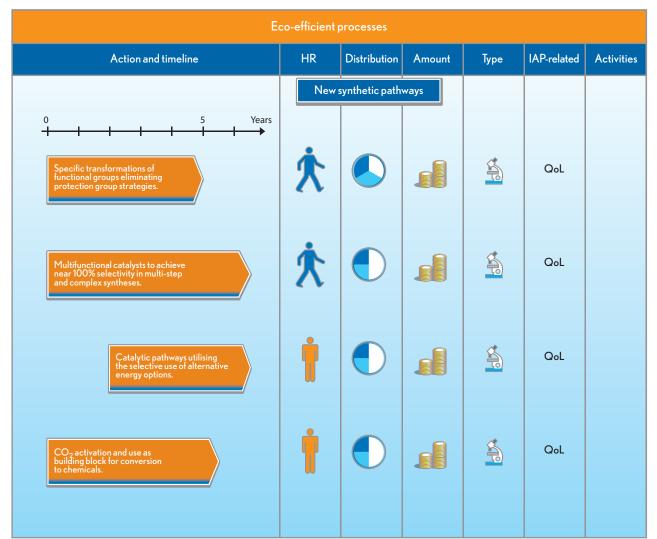
#### Goals

The following key activities aim at more eco-efficient chemical syntheses and corresponding processes with high resource efficiency and reduced amounts of waste. This includes the development and industrial implementation of more efficient chemical synthetic routes with a reduced number of reaction steps. Short term targets are the improvement of fine chemical synthetic routes, for instance by introducing catalytic steps instead of stoichiometric ones. On the longer time scale, large scale processes should also be reconsidered and possibly redesigned.

Complementary to synthesis strategies, the development of competitive and environmentally benign processes with reduced energy and resource requirements, replacement of conventional by alternative solvents, and greatly reduced waste formation are envisioned.

- New synthetic pathways
- Reduction of resources and waste

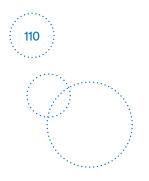
#### New synthetic pathways



- Research projects on more specific transformations of functional groups, circumventing the necessity to protect and deprotect which adds significantly to the number of steps necessary to reach a synthetic target.
- Catalyst engineering moving towards the design of the next generation of multifunctional catalysts by integrating knowledge on hetero-, homo-, single-site and biocatalysts, in order to achieve near 100 % selectivity in multi-step and complex syntheses. Fundamental research is required on the microkinetics of complex reactions on solid catalysts and the design of catalysts with organised sequences of active sites. The latter requires an understanding of the sequence

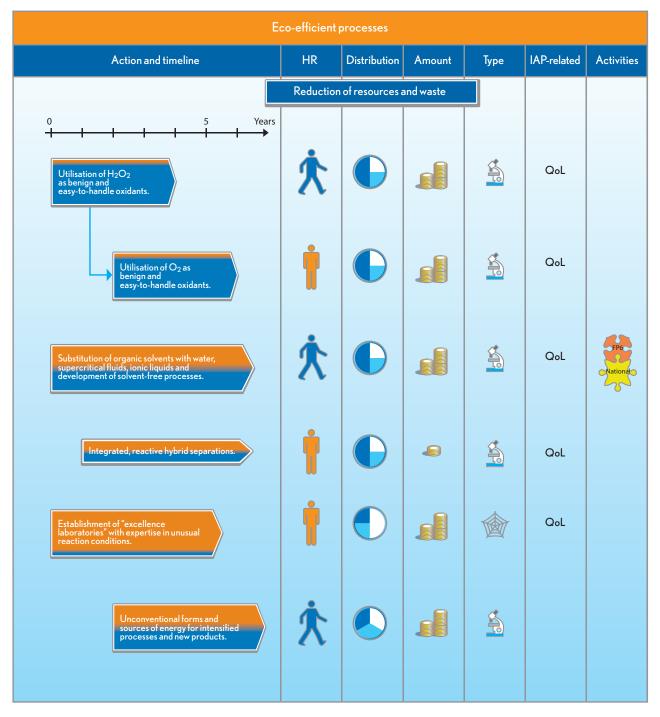
of steps necessary to make a complex catalytic transformation on the surface of a catalyst (not only in terms of active sites, but also in terms of the rates of the elementary steps) and of the possibility of assembling the active sites in the right sequence (also spatially), and with the appropriate reactivity. Furthermore the integration of homo-, bio- and heterogeneous catalysis in cascade reactions should be targeted.

 As a long term goal, catalytic pathways can be combined with the selective and local application of **alternative energy options** (e.g. photons, electrons, microwaves, ultrasound) to yield highest energy efficiency. This requires the collaboration of catalyst experts, engineers and engineering companies.



• CO<sub>2</sub> activation and subsequent use as a building block requires both fundamental research and the development of industrial applications in industry academia collaborative projects.

#### Reduction of resources and waste



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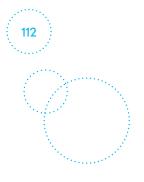
In order to reduce the use of resources and the production of waste the following actions are necessary:

- Increased use of benign and easy-to-handle oxidants with the short term focus on hydrogen peroxide. Part of the target must also be to reduce the production costs of hydrogen peroxide; this will stimulate the investigation of chemical routes using it. Applied research projects demonstrating the use of hydrogen peroxide and fundamental research of the catalytic requirements for its use are required.
- Exploiting the experiences with hydrogen peroxide as a basis, **molecular oxygen** seems to be the desirable and most cost-efficient and benign oxidant in the long run. Fundamental and applied research is required in order to identify new classes of highly specific catalytic systems, and to develop new preparation procedures for catalysts, which may optimise the cooperation of active sites.
- The substitution of harmful organic solvents by other systems, such as organic safer solvents, water, supercritical fluids – most notably carbon dioxide – and ionic liquids for reaction and separation/purification purposes, as well as solventless reactions in neat reagents. Required steps include surveys of prototypical examples analysing the costs and benefits associated with carrying out reactions or separations in a range of different solvents. Research projects are required with the aim of developing structure-performance relationships for ionic liquids to facilitate choice of specific ionic liquids. Further research projects have to be directed at the modification of catalysts and other compounds needed for specific transformations, for instance to increase their stability in aqueous environments, or their solubility in the respective solvent. An important aspect is also the appropriate selection of solvents for organic synthesis and purification/separation processes.

- Integrated reactive and hybrid separations are aimed at the total conversion of feed stocks and dramatically reduced energy consumption by combining (multi) reaction separation steps, or several separation processes, into one unit. Research in this area should be targeted at the design of integrated processes, adapted materials (i.e. membranes for hybrid separations), solvents (i.e. ionic liquids for extraction). Furthermore the development of suitable equipment is required.
- Development of clean, intensified processes using unconventional forms and sources of energy, such as microwaves, plasma, light or ultrasound, for manufacturing of functional products (including nanomaterials), and in particular products which are difficult to obtain using conventional processing methods. The targeted supply of innovative forms of energy will enable precise control of chemical transformations and reaction pathways, will allow novel reactions to yield new products with unique functionalities, and will boost the efficiency (rates, yields, selectivities) of existing processes carried out in a conventional way.
- **"Excellence laboratories"** having expertise in the handling of unusual reaction conditions, and working on example cases and best practise approaches, should be established and made accessible to interested users as a way of facilitating knowledge transfer.

#### **Existing activities**

Several national research projects and various groups in academia and industry have activities in alternative solvents, such as supercritical  $CO_2$  and ionic liquids. Novel activities could build upon these existing networks and nodes.



#### ••• • KNOWLEDGE-BASED MANUFACTURING CONCEPTS FOR TARGETED AND TAILORED PRODUCTS

Knowledge-based product engineering aims at the fast identification and development of the best process option for accurate targeting of product properties and fast and flexible manufacturing of tailored products. The ultimate goal is the mastery of product end-use properties through process design. Rather than addressing a single aspect or part of the process lifecycle an integration and intensification approach based on knowledge and understanding of the total process is required. Accordingly the entire process from discovery, through the development and pilot stages, to production and lifecycle management should be regarded and addressed in a complete way to achieve the overall goals of reducing the process time and focusing on the most competitive process options.

By targeting the total development chain of a process the final product is already considered in the early discovery stages. This requires highly interdisciplinary research and the highest level of integration and innovation.

#### Goals

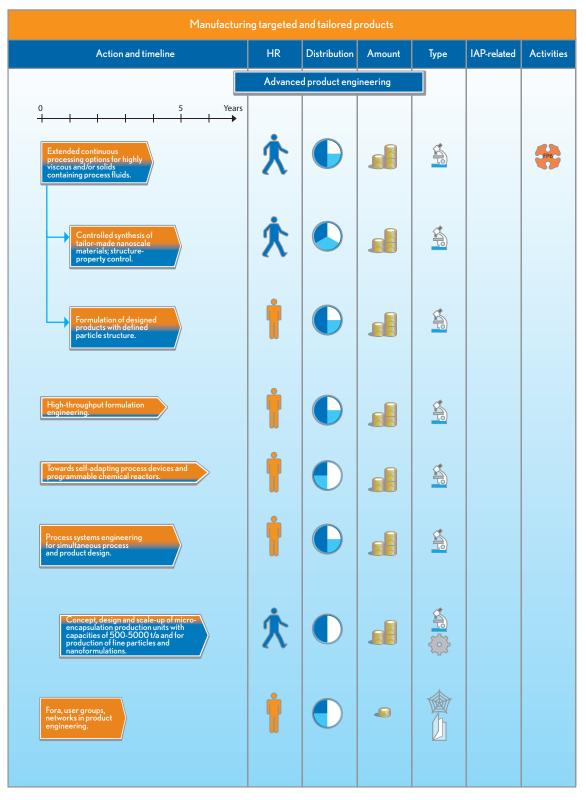
Within the next 10 years sustainable processes for targeted and tailored products - such as intelligent microencapsulated formulations with controlled release function - will be developed to meet the requirements for size, payload, chemical resistance, thermal stability, release control, physical strength, shelf life, taste masking and controlled (sustained, delayed or targeted) release rates.

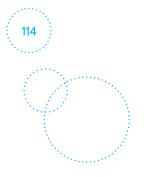
Some techniques (e.g. encapsulated pharmaceuticals and nutritional products with controlled release and herbicides with slow release) are already in commercial use. There is, however, a gap in respect of implementation in the broad field of technical products, which constitutes a large economic potential.

Strong academic industrial collaborative research is required on the intensification of processes for specifically targeted end-use properties, including research on accelerated scale-up methods from bench top to production scale. Particular emphasis should be placed on the interaction between chemistry and process design in the elaboration of supramolecular aggregates and structures. As the long term goal knowledge of structure property relationships should be developed as the basis to define the conditions necessary for precise, locally targeted process control in formulation engineering for rapid response to market and mass customisation.

### Key activities Advanced product engineering

#### Advanced product engineering





The following areas need to be developed to progres advanced product engineering:

- Methods for the continuous processing of highly viscous liquids and/or solids containing process fluids. In this context, particular attention must be paid to low cost intensified equipment for reduced capital expenditure on new plants and on retrofitting.
- New methods for the controlled synthesis of tailormade nanoscale materials and their assembly in 2D or 3D architectures. Focus should be on new preparation techniques to produce tailor-made nanoscale catalysts, with emphasis especially on producing organised thin films and hierarchically structured catalysts, and on studies of the nanostructure reactivity relationship.
- Formulation of designed products with defined particulate structure, size distribution, shape, morphology and surface. Target products are micro/nanostructured emulsions and dispersions with specific properties (e.g. dust free, hydrophilic/hydrophobic, controlled release, redispersability).
- High-throughput tools for formulation engineering are required for the rapid design, synthesis and testing of formulations, including computer aided multiscale modelbased techniques combined with experimental techniques to identify the optimal formulation (includes also aspects of manufacturing of the formulated product). The ongoing development and use of Dynamic Combinatorial Libraries for studies of receptors, catalysts, enzyme inhibitors and new materials, like multifunctional nanoparticles, will help to reach the goals identified. The results can also be used in related applications, like (gas-)sensors, biomarkers and receptive/ reacting materials (e.g. targeted drug delivery) – see also Nanotechnology.
- Pluridisciplinary projects (with engineers and material scientists) are needed aimed at self-adapting process devices comprising extremely flexible, high performance equipment developed through integration of self adapting materials (shape change alloys, piezoelectric components, etc.). The long term goal is the development of programmable chemical reactors whose local operating conditions adapt automatically to changes in feed composition, product specifications, etc. (for example the development of methods for design and validation of periodic operation of reaction separation systems).

- The development of **Process Systems Engineering** (PSE) techniques used for designing process and product together to ensure that products with the highest potential and the most appropriate processes are taken forward including rapid generation/screening of process product alternatives, systematic analysis and monitoring of product quality.
- A critical area for research is the **scale-up** from laboratory to pilot/demo plant scale especially for microencapsulation, and production of fine particles and nanoformulations; cost/risk sharing programmes are required to accelerate this essential step in developing new products; for microencapsulation, concepts, design methodologies and fast scale-up strategies are required. As a goal, pilot/demo scale production units with capacities of 500-5000 t/a are envisioned. The demand for tailored nanoparticles and multifunctional materials, like core shell particles, can only be satisfied by the development of new synthesis routes. Gas phase, wet chemical and critical phase production processes should also be a focus. Examples of research areas include studies on precipitation processes (e.g. miniemulsion, high gravity controlled precipitation, co- and jet-precipitation), sol-gel synthesis, hydrothermal methods, flame synthesis, plasma synthesis, hot wall reactors, desublimation and money intensive processes like rapid expansion of supercritical solutions (RESS), supercritical antisolvent precipitation (SAS), particle from gas saturated solutions (PGSS) and depressurisation of an expanded liquid organic solution (DELOS) - see also Nanotechnology.
- Fora, user groups and networks are required for communication, training and identifying common key opportunities for developments in product engineering, such as the design of experiments, multiscale modelling, product analytical techniques, etc. Chemical and pharmaceutical industries, engineering contractors, equipment manufacturers and academia should all participate.

#### **Existing activities**

A number of industrial applications already exist for microencapsulation, new release materials design and bioencapsulation; as does a network with several companies and engineering contactors involved in R&D.

Several national research projects and a number of groups in academia and industry have activities in this field.

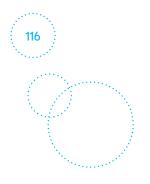
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#### • IMPLEMENTATION AND INTEGRATION OF INTENSIFIED PROCESS TECHNOLOGIES

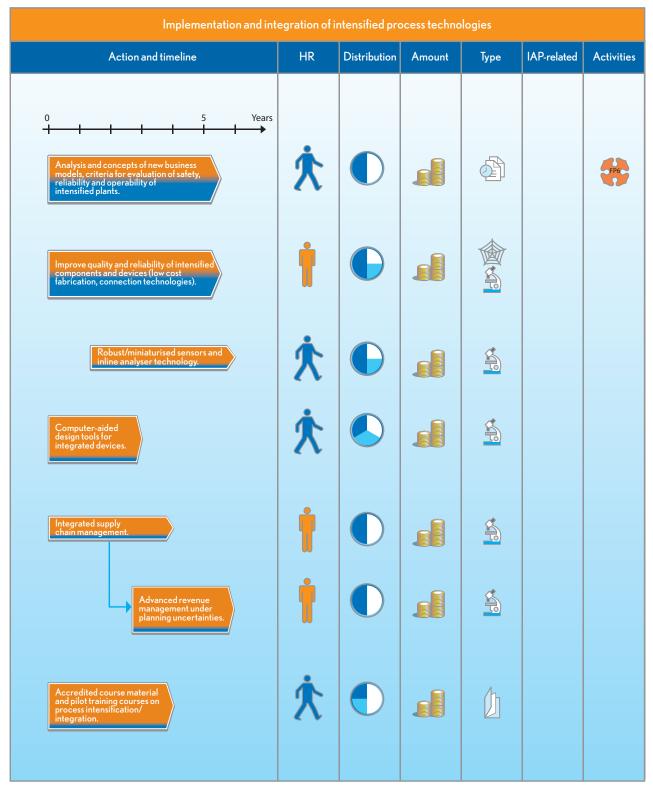
A competitive European chemical industry relies on innovative process equipment, with performance and control options which cannot currently be met, thus overcoming existing process limitations and enabling new manufacturing and processing methods. This requires widespread implementation of innovative equipment, advanced sensor and process analytical technology, and the introduction of sophisticated process design tools. Up to now the potential of intensified and integrated processes for manufacturing of tailored products has not been exploited. To allow for new business models based on, for example, distributed, on demand production or the integration of consecutive manufacturing steps, flexible supply chain management and planning tools are important.

#### Goals

The development and implementation of flexible intensified on site production plants situated in Europe, highly integrated in the value chains and employed on a routine basis for numerous chemical process applications over a wide range of production scales by 2025.



#### Key activities

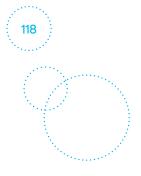


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Future leading European process technology is based on widespread implementation and use of intensified, high precision process equipment and devices together with a corresponding adaptation of plant management, supply chain organisation and business models. To achieve this the following areas need to be focused on:

- A thorough analysis and proof of concept of new business models and criteria for evaluation of the safety, reliability and operability of intensified plants are required through academic research projects, industrial collaborative research, user groups and networks.
- Improving the quality and reliability of intensified components and devices. Research should focus on low cost fabrication and connection technologies, robust materials, resistance to corrosion and clogging, and superior performance with respect to maintenance and reliability for applications under highly demanding conditions of temperature and pressure in aggressive and/or unusual media (supercritical fluids, ionic liquids, high temperatures, solvent-free reaction media, etc.). Networks (user groups/ fora) should define and discuss standards, fabrication and connection technologies.
- Collaborative research projects developing robust miniaturised sensors and inline analyser technology utilising advanced process analysers which meet the requirements of process analytical technology to enable local process control. On a global plant operation level, new monitoring tools for continuous assessment of plant component state and residual life time should be addressed. These developments are extremely important for the synthesis of tailored nanoparticles and materials (e.g. narrow particle size distribution, nanofoams).

- The development of **computer aided design methods and tools** for integrated multifunctional devices such as reactive and hybrid separation units, integrated reactor/ heat exchangers, integrated mass exchangers (solventbased separations), etc., to reduce waste and improve efficiency without compromising environmental impacts. In addition, the development of tools for the design or retrofit of sustainable chemical processes (including computer simulations, pinch analysis, mixed integer non-linear programming, multiple criteria optimisation, multiple criteria decision making, etc.) is required.
- As intensified and integrated processes lead to emerging new value and supply chains, advanced tools for integrated supply chain management are required. These include advanced network design for production and distribution systems requiring research in rapid model development for dynamic planning and scheduling and supply chain management models covering the entire product lifecycle. For validation of modelling strategies and tools, industrial case studies have to be investigated.
- As a further aspect of supply chain management advanced revenue management under planning uncertainties should be targeted. This research should include optimal safety stock planning with respect to demand forecast and service levels in order to reduce working capital. This requires fundamental research for multiobjective optimisation under uncertainties, adaptation and extension of combinatorial and stochastic programming methods to applications in supply chain optimisation and industrial case studies to prove research strategies.
- The dissemination of methods and techniques, and development of appropriate computer aided design tools; in particular, accredited course material and pilot training courses delivered through a dedicated network are required.



#### O LIFECYCLE ANALYSIS

Conventional lifecycle assessment (LCA) is a tool that can be used to assess the environmental impacts of a product, process or service from design to disposal i.e. across the subject's entire lifecycle. LCA is primarily intended for comparing the lifecycles of alternative processes and products designed to achieve similar objectives in order to discover which of them is the most environmentally sustainable. The reason for conducting LCA is to choose the options which have the lowest environmental impact and the highest benefit to society.

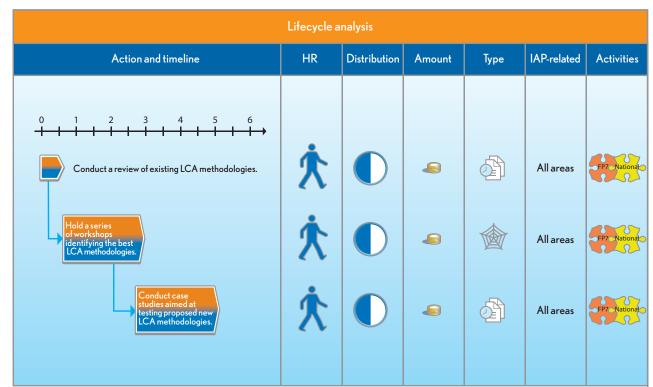
Sustainable Development seeks to deliver integrated solutions that optimise economic, ecological and societal goals. Whereas numerous instruments are used in practice for the ecological assessment of products and processes, a gap still has to be closed by developing social lifecycle assessment procedures to achieve an analysis of the entire sustainability potential. Recent initiatives have sought to develop further conventional LCA methodologies to include socio-economic aspects of sustainability (see for example "Assessment of the *Eco-toxicity Potential for Lifecycle Analysis, Eco-efficiency and SEEbalance*", P. Saling M. Silvani , *SETAC Europe*, 14<sup>th</sup> annual meeting, 22 April 2004).

Social lifecycle assessment procedures have been developed in order to improve the performance of a company's product portfolio and manufacturing processes.

#### Goals

A key priority for SusChem will be the further development of a harmonised European approach to lifecycle analysis methodologies aimed at achieving socio- and eco-efficient solutions. Based on existing industry/academia initiatives analysing product-related specifications of the environmental, economic and/or social sustainability dimension this harmonised methodology needs to be a comparative lifecycle assessment tool that seeks to integrate the examination of costs, environmental impact and social effects of different product or process alternatives in the search for socio-eco-efficient solutions.

#### Key activities



Work will build on the best practice development in the United Nations Environmental Programme (UNEP)/Society of Environmental Toxicology and Chemistry (SETAC) lifecycle initiative and the ongoing efforts at the JRC, Ispra, and industrial initiatives to create a European platform for quality assured data for LCA. Efforts will also be made to integrate learning from established practices such as the use of eco-profiles by the plastics industry and programmes sponsored at country level such as the PROSA project supported by the German Research Ministry (BMBF).

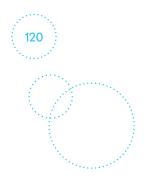
Activities will include:

- A review of existing LCA methodologies appropriate to SusChem.
- A series of **workshops identifying the best LCA methodologies** for achieving socio-eco-efficient solutions that will contribute to the development of a common European approach to LCA.
- Case studies aimed at testing proposed new LCA methodologies for achieving socio-eco-efficiency on selected SusChem technologies. These will include cost benefit analyses of the methodologies themselves.

The output will be a report (including the findings of the case studies) recommending ways to standardise LCA methodologies for sustainable chemistry (consistent with European LCA harmonisation initiatives).

The project will run for at least 5 years and will be led by an independent consultancy, with input from industry, academia, Member State governments and the EU Commission. Funding required is likely to be of the order of € 3 - 5 million and the fund will come from the European Commission and industry. An initial project with participation of a SusChem partner is already running under FP6 (CALCAS).

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#### Transport

Based on technological advances, the aim is to develop integrated, "greener", "smarter" and safer pan-European transport systems for the benefit of the citizen and society, whilst at the same time respecting the environment and natural resources; and securing and further developing the competitiveness and the leading role attained by European industries in the global market.

The following areas of research have been identified as those of highest priority:

- O Safety, information and mobility.
- O Eco-efficiency performances.
- Clean fuels and mobility.

#### **O** SAFETY, INFORMATION AND MOBILITY

To increase the transport efficiency, minimise costs, save time and reduce pollution, it is necessary to develop reliable systems and models to predict and to manage traffic flow through increasingly crowded infrastructures. Traffic monitoring is, therefore, a key element for the future both in terms of optimal management of existing traffic, and to future-proof development of new infrastructures and transportation modes for persons and goods.

#### Goals

The development of technologies and superior materials is necessary to achieve higher energy efficiencies, both in fuels and the economic viability of transport vehicles. In modern vehicles a reduction of 40 to 50 % of energy use should be possible through optimised energy management systems in combination with clean fuel systems. To face future challenges of urban traffic, the eco-efficient performance of future vehicles has to be combined with increased safety of all classes of vehicles within the transport sector.

#### Key activities

Adaptive human ergonomics



#### Adaptive human ergonomics

Safety, information and mobility							
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities	
	Adaptive	e human ergon	omics				
0 5 Years							
European Transportation Materials Development Centre.	X				Nano ICT QoL		
Functional materials & hybrids: synthesis of organic & inorganic hybrid composite materials.					Nano ICT QoL		

#### European Transportation Materials Development Centre

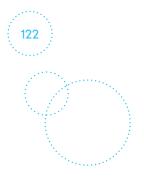
For increased safety in transport a holistic approach is necessary: this is called adaptive human ergonomics. This includes traffic management sensor systems (e.g. safety, collision avoidance and night vision), reliable on-board electronics in combination with self-repairing components, and instant diagnostics.

In order to develop the technologies required a **"European Transportation Materials Development Centre"** is proposed, whose sole purpose would be to investigate new **functional materials and hybrids** with enhanced properties (e.g. self-repairing coatings or bulk modifications), through modelling, synthesis and tribology, for the inclusion in technology devices (e.g. traffic management sensors, reliable on-board electronics and instant diagnostic systems). The purpose would also be to develop the production and testing of the novel materials and to determine norms and standards for the industry. For the automotive industry specifically, one focus will also be on the achievement of the "silent car and road" vision.

#### Functional materials and hybrids

For many years, everyday consumer and industrial parts and components have been coated using various techniques to enhance their properties. These are typically continuous thin film coatings that may be either organic or inorganic. Inorganic nanosized crystalline materials when embedded in such coatings offer tremendous opportunities in bringing the coating totally new functionalities. A thorough understanding of the physics of the fundamental properties of such nanoparticles, and how to modify those properties by varying the particles' size, morphology and chemistry (doping), will be required. Suitable support materials for the matrix will also need to be developed. Finally suitable high throughput deposition techniques for such hybrid nanocrystalline coatings will need to be developed:

- Since the field is very wide it would be too limiting at this stage to list specific functionalities. However the main series of deliverables would be in the form of having the right combination of nanocrystalline particles and support matrix that provides novel functionalities in high volume industrial and consumer goods (e.g. glazing, metal cladding for buildings, automotive etc.).
- The second deliverable would be to develop suitable industrially viable coating techniques.



#### **○** ECO-EFFICIENCY PERFORMANCES

Cars of the future require technological developments in terms of better safety, lower fuel consumption and lower environmental impact. Tyres are important parts of cars that, along with the other components, need to be improved to meet the high standards required in the future.

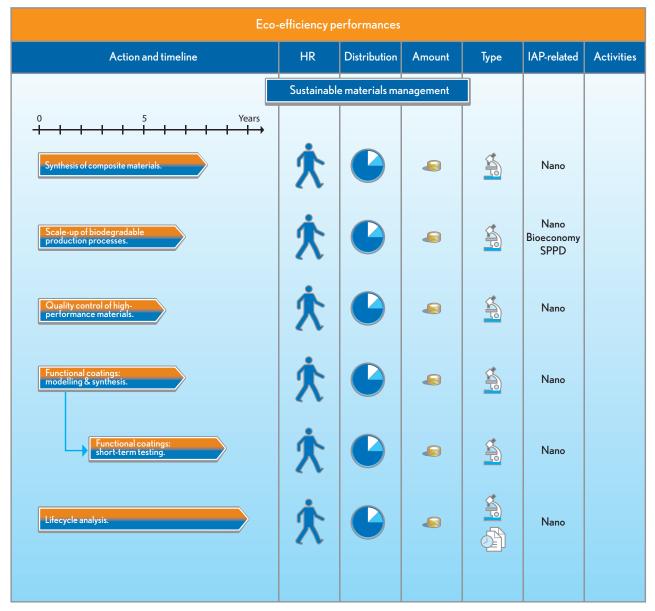
#### Goals

- Development of new materials for the lightweight construction of vehicles, including alternative assembly methodologies (e.g. the use of adhesives) and the replacement of heavy metal parts by conductive thermoplastics with enhanced mechanical properties.
- The further development of catalysts for the decomposition of green house gases.
- Development of eco-efficient vehicles composed of new materials with improved recyclability and with functional coatings to reduce biofouling of marine vessels.

#### Key activities

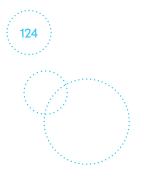
- Sustainable materials management
- Catalysts for COx, NOx, SOx decomposition
- Alternative body assembly technology
- Onboard H<sub>2</sub> production
- Elastomeric and thermoplastic products

#### Sustainable materials management



Lightweight, but strong, **(composite) materials** for diverse applications are increasingly required. **High performance materials** must conjugate with reduced environmental impact. In the transportation area, weight reduction leading to lower fuel consumption can be accomplished through the development of innovative elastomeric/thermoplastic products for structural parts such as:

- Tough thermoplastic foams.
- Organic fillers-based thermoplastic composites.
- Polymers with improved thermal resistance for further metal replacement (body panels).



In the area of safety equipment, more efficient airbag systems should be developed to bring the best degree of protection and a reduction in weight. A major environmental benefit in respect of a reduction in water pollution would also be obtained through the development of spun-dried flock and auto-activated flock for car interiors.

The availability of fibres offering a better cost/performance compromise would favour metal chord replacement in tyres giving a significant weight reduction and thus producing less rolling resistance and thereby reducing fuel consumption. Other important progress areas concern the fibre/elastomer adhesion system and the associated dipping operation where the need for a non-toxic dip is increasingly desirable.

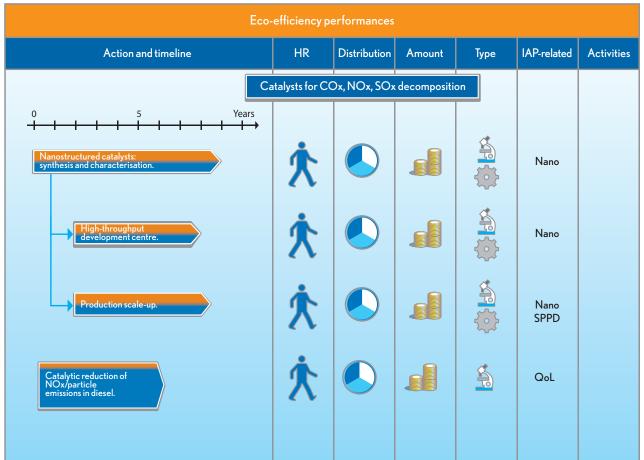
For eco-efficient hybrid vehicles new energy storage systems, like enhanced lithium batteries and supercapacitors, are needed to achieve the goal of a zero emission vehicle. To realise this vision, batteries and enhanced (PEM) fuel cells need to be coupled with supercapacitors which provide the required power peaks during acceleration and energy recovery during braking.

Next to fuel cell vehicles powered by stored hydrogen, systems with higher energy density and enhanced safety have to be developed. A possible fuel is methanol which could either be used directly in a DMFC (direct methanol fuel cell) or be reformed onboard to hydrogen to be used in a PEM fuel cell (*Japan Hydrogen and Fuel Cell Demonstration project (JHFC)*, http://www.jhfc.jp - G. A. Olah, A. Goeppert, G.K. Surya Prakash, *Beyond Oil and Gas: The Methanol Economy*, Wiley, Weinheim 2006) - also see further, *Onboard H*<sub>2</sub> *Generation*. The development of highly active catalysts with low or no noble metal content supported on mesoporous carriers will be crucial for onboard methanol fuel cell operation. Such catalysts will allow operation at low temperatures (< 250 °C).

Facilitated recycling operations to benefit the environment also need to be explored.

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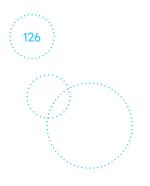
### Catalysts for COx, NOx, SOx decomposition



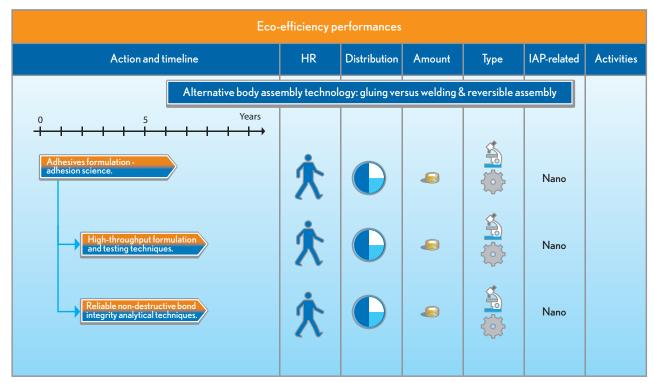
It has been proven that the decomposition of aromatic compounds and NOx from car emissions can be attained by the passive use of solar radiation acting on a photocatalytically active surface. So **photocatalysts** could be added to the pavement as a filler or as a film coating as a low cost method of achieving the decomposition of noxious compounds in car emissions. This is a very convenient way to instigate a distributed and *in situ* detoxification method, which has few drawbacks. However, research is required on some fundamental issues such as the development of more efficient catalysts and materials, sound and reliable methods to test the efficiency of materials, and **scale-up** from small scale operations to very large ones. Without this research, which can only be progressed through a multidisciplinary approach, this very promising method will not make any significant progress.

#### Catalytic reduction of NOx and particle emissions in diesel

Diesel engines have higher energy efficiencies (up to 30-35 %) than gasoline engines and they have undergone a significant technological evolution, in particular, with the development of the common rail system. Nevertheless diesel engines emit particulate matter and the presence of oxygen in the emissions does not allow the use of currently available catalytic devices available for NOx conversion. The development of catalysts able to convert the micro-pollutants present at a ppm level in complex mixtures, including with several other competing species and reactions, is required for effective control of the emissions. Significant research needs to be done on the preparation of **nanostructured catalysts** based on supported noble metals, for instance on NOx storage reduction catalysts, and on the interaction between NOx and particulates and on their conversion. Furthermore, the catalysts have to operate across a large range of temperatures, at very high space velocities and in presence of several deactivating elements.



#### Alternative body assembly technology: gluing versus welding and reversible assembly



To complement the move away from rigid assembly processes, in particular in the automotive industry, **adhesive/gluing technologies** need to be improved in order to replace welding as the standard assembly method. A bonus that results from using adhesives in the assembly process is the potential to reverse the process cheaply and efficiently by dissolving the glue away, particularly at the end of the lifecycle of the product. This will have enormous economic and environmental benefit. Research should focus on **high-throughput formulation** and testing techniques and the development of **non-destructive analytical tools**. Interaction with various manufacturing sectors will enable the rapid establishment of the technology.

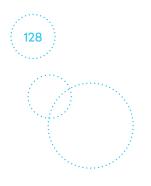


#### **Onboard H**<sub>2</sub> production

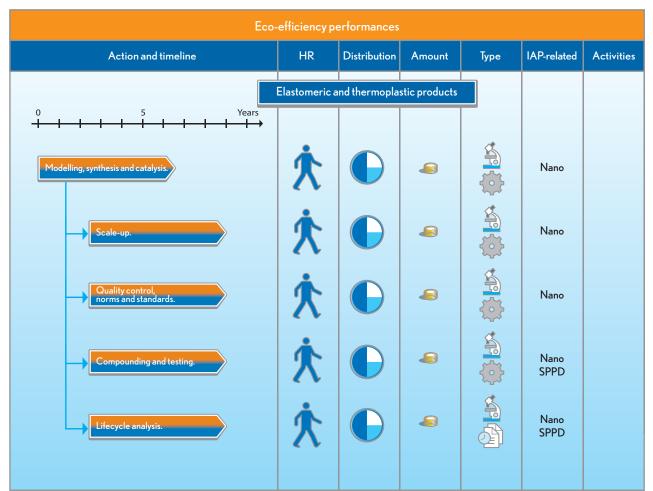
Eco-efficiency performances						
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities
	Onboard H <sub>2</sub> production					
$\begin{array}{c ccccc} 0 & 5 & Years \\ \hline + & + & + & + & + & + & + & + \\ \hline \end{array}$						
Catalysts and materials for microstructured reactors: synthesis and characterisation.	Ŕ				Nano	
Testing.	X				Nano	
Production scale-up.	Ŕ			<b>1</b>	Nano	

By definition H<sub>2</sub> is a clean fuel, but the development and application of a compact fuel reformer able to produce H<sub>2</sub> on board vehicles needs to be developed. This presents a substantial challenge: existing technologies are not able to satisfy the market needs in term of miniaturisation, efficiency, reliability, and durability. The fundamental step is the development of new, highly efficient and stable, nanostructured systems to be used as **catalysts** for **H**<sub>2</sub> **production** processes on small **scale**, such as reforming or catalytic partial oxidation. The preparation of nanostructures, with unusual metal/support interactions, represents the keystone in the development of advanced materials with the specific properties of high activity and stability. Nanostructured catalysts in which the interaction between metal and support is tailored are interesting because:

- Stabilised metal nanoparticles, in particular on oxides, display reactivities very different from those of particles with larger dimensions.
- Synergetic effects of promotion between the metal nanoparticles and the nanostructured support are present.



#### Elastomeric and thermoplastic products



New elastomeric and thermoplastic materials are required widely in transport applications, to improve durability, reduce fuel consumption and noise, and minimise environmental impact during the entire **lifecycle**. Copolymerisation, selective branching and chain terminations must be developed for better performance of these materials. The research focus should be directed towards better control of polymer chain architecture and polymer chain association in engineered plastics to achieve innovative supermolecular structures. Elastomeric and thermoplastic products have become a priority because of their large impact on sustainability, safety and eco-compatibility, and because of the potential for weight reduction across the entire transport industry.

The development of new fillers should also be investigated together with concomitant research on coupling agents for

an altogether better reinforcing system. Benefits would be longer lifecycle, enhanced safety and reduced weight. As a new family of materials, lightweight organic fillers need further promotion, and European cooperation is needed for adequate technical and financial effort and for an effective exploitation of the research results.

Development of new elastomers in order to facilitate their interaction with nanostructured fillers is needed. Co/terpolymerisation with different monomers, grafting reactions, selected chain terminations should be addressed. Chemicals for the vulcanisation process which give shorter vulcanisation times, better product performances and environmentally more friendly approaches (in particular which are sulfur free) are required. The use of aromatic oils and zinc free compounds in high performance compounds must become widespread.



#### O CLEAN FUELS AND MOBILITY

The development of efficient fuels, particularly in respect of their green house gas emissions, will lead to an improvement in the environment, while maintaining the mobility of citizens.

#### Goals

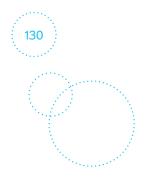
Development of fuels with low pollutant and reduced particulate matter emissions, while maintaining high fuel efficiency, in order to make their adoption by the European consumer feasible.

#### Key activities



Biofuels are likely to be selected for use as **fuels low in sulfur and aromatics**. Catalysts with specific properties need to be developed or improved for the different processes:

- The production of biodiesel requires the development of heterogeneous basic catalysts for transesterification with increased life time and tailored properties able to treat different streams (such as oils from plants, and waste oils from food preparation and cooking).
- The production of second generation fuels requires the development of catalysts with hydrotreating and de-oxygenation properties for the **production of low** oxygenated oils by catalytic pyrolysis.
- BTL (gas derived from biomass to liquid) processes require highly efficient and stable catalysts for syngas production based on high thermal conductive materials, which are resistant to deactivation by alkali metals and sulfur.



#### Resources – ways and means

#### **O** RESOURCE REQUIREMENTS

The SusChem SRA offers an unique opportunity to focus European spending in chemical R&D towards the most promising areas in respect of their impact on the overall goal of sustainability and achieving a high level of competitiveness. It is an ambitious plan that will require significant funding in order to be successfully implemented. Different funding sources including EU framework programmes, national and regional initiatives and private sector spending need to be accessed.

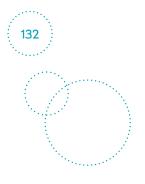


In the preceding chapters the resources needed to fulfil this Implementation Plan are given in detail. The amounts required, and the sources of funding in terms of private or public, European or national, have been estimated by the SusChem working groups for each of the activities pictured. The activities covered by this Implementation Plan - paving the way to achieving the SusChem vision - require funding in the order of € 9 billion for their completion. The table presents the distribution of funds - public (European Union, Member States funding agencies) and private (industry) sources - in total and their distribution among the different SusChem priority areas.

	Total project duration						
	European	national	private	total			
Bio-based economy	250	300	350	900			
Energy	600	600	1,000	2,200			
Health	150	150	200	500			
Information and communication technologies	350	350	900	1,600			
Nanotechnology	600	600	1,000	2,200			
Sustainable quality of life	50	50	150	250			
Sustainable product & process design	350	250	400	1,000			
Transport	100	100	150	350			
Overall	2,450	2,400	4,150	9,000			

On an annual basis, this roughly amounts to € 400 million each from European and national sources and € 700 million from private investment (based on an average activity duration of 6 years). This is less than that requested in the SRA since a further prioritisation has been applied in selecting topics for this Implementation Plan: the focus is on collaborative projects with a European component and only covers those projects which are most important to start within the next 2 to 3 years. The numbers in this table therefore represent the funding that needs to be committed within the next 2 to 3 years for the total duration of the projects. The estimated annual funding is thus valid for this initial period only. Afterwards the implementation plan will be revisited. Additional project proposals will come in thus increasing the required amount of annual funding in the coming years (with new projects starting and initial projects still running).

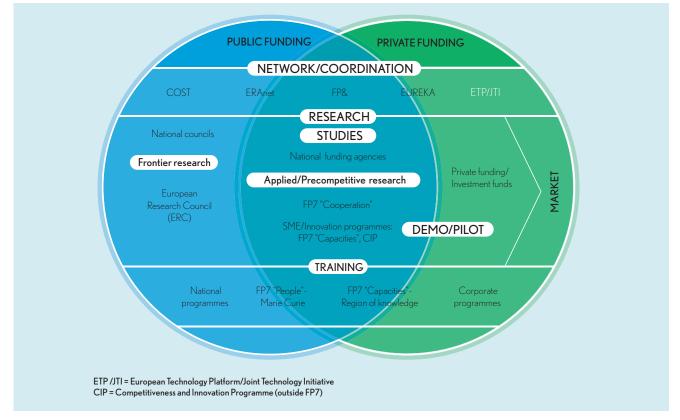
The figures show the expectations from SusChem stakeholders in terms of contributions especially from the European Framework Programme. They also give an estimate of the amounts the private sector should be willing to spend on SusChem R&D priorities provided that public co-financing is secured. Approximately 50 % of funding could come from industry which is an acceptable proportion for cooperative precompetitive research. However, industry funding of collaborative projects very much depends on the accessibility of public funds and how easy it is for private businesses to participate in funding programmes.



#### DETAILED DESCRIPTION OF POSSIBLE FUNDING SOURCES

The above is based on a relatively broad categorisation of funding sources. However, resources for SusChem activities will and need to come from a variety of programmes, agencies, entities, etc. that are all covered by these funding categories. The sources and possible connections to SusChem related work are described in more detail in the following. The diagram below shows an overview of available sources of funding for SusChem related research and innovation in Europe. The white boxes describe possible project types for activities as described in *Realising the SRA*.





The landscape for research funding in Europe is remarkably fragmented with a multitude of different pan-European, national, and regional players being involved. The European Union funding under the Research Framework Programmes accounts for only a small fraction of available funding.

For Europe to increase its competitiveness, and the value of its research funding, it is essential to coordinate available resources where this is feasible and meaningful. The SusChem Strategic Research Agenda, highlighting as it does the most promising research areas which have been agreed upon by industry, academia and other stakeholders in Europe, should be the key document when it comes to defining research programmes in chemistry, biotechnology and chemical engineering throughout Europe. While national and regional interests need to be taken into account in the respective funding programmes they should build on and complement the SusChem SRA.



ERAnets are a prime example of coordination of national research funding on the European level. Several ERAnets in SusChem related areas already exist:

- ACENET.
- ERA Chemistry.
- HyCo.
- Industrial Biotechnology.
- Matera.
- MNT.
- Photovoltaics.
- SUSPRISE.

SusChem will actively seek to continue its current collaborations with some of the ERAnets and establish coordination and alignment with others. Europe would gain significantly when projects which are financed through transnational calls in ERAnets, and which are at the same time relevant and related to topics in the SusChem SRA, are linked and aligned with the SusChem goals. SusChem will also disseminate information on related ERAnet calls through its stakeholder network to help to ensure that the best possible project ideas come forward and are selected.

The Member States Mirror group is another body that will help in aligning SusChem priorities and national research programmes with a view to achieving a more coherent European-wide research strategy and its future implementation. Thus, SusChem priority issues might be covered and (co-) funded by some national and regional programmes, where appropriate. The Member States Mirror Group carried out a survey of SusChem priorities to identify which of them are the most pressing in each Member State. With answers from 9 Member States the following 6 themes came up as the most important national priorities (in order of first appearance in this document). Consequently, these are most likely to be funded on national level as well.

- Improvement of biorefining technologies: the biorefinery concept (p. 25).
- Biomass and integrated biorefineries for energy generation (p. 29).
- Synthesis and processing of nanomaterials (p. 77).
- Nanostructured polymers, hybrid and mesoporous hybrid materials (p. 78).

- Innovative eco-efficient processes and synthetic pathways (p. 108).
- Implementation and integration of intensified process technologies (p. 115).

European Union Structural Funds allow the European Union to grant financial assistance to resolve structural economic and social problems. Resources are targeted at actions which help bridge the gaps between the more and the less developed regions. Four Structural Funds are currently available:

- The European Regional Development Funds (ERDF).
- The European Social Fund (ESF).
- The European Agricultural Guidance and Guarantee Fund (EAGGF).
- The Financial Instrument for Fisheries Guidance (FIFG).

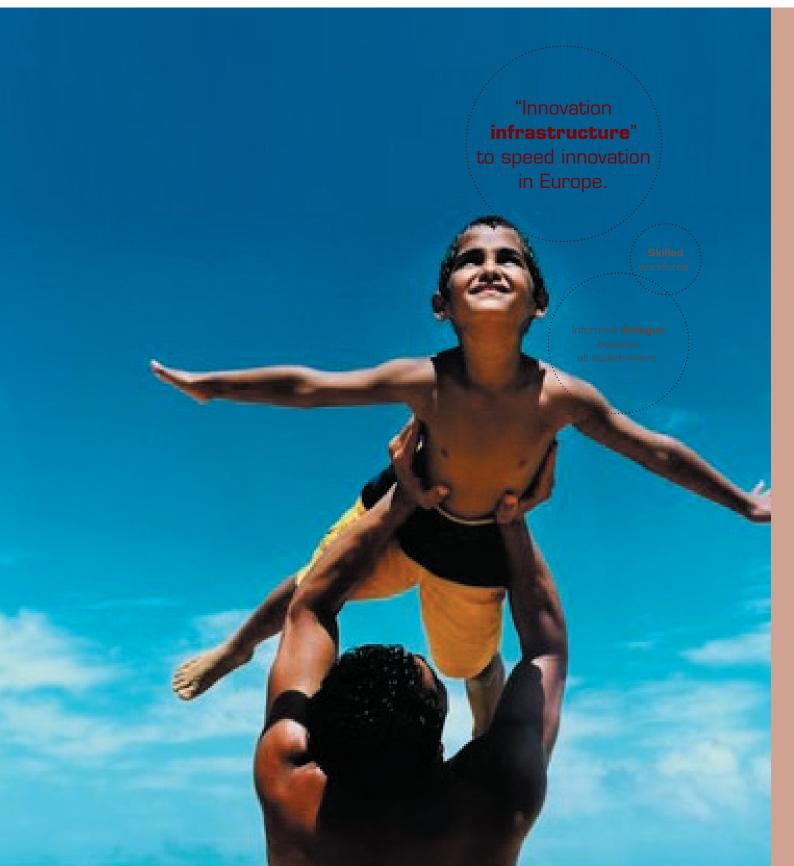
Of those, the ERDF could offer possibilities for project funding in SusChem related issues because it states that it will 'strengthen the research and development capacities of regions'. The regions referred to are categorised into Objective 1 (regions whose development is lagging behind) and Objective 2 (regions facing structural difficulties) regions.

Joint Technology Initiatives (JTIs), a new instrument in the 7th Framework Programme, are an opportunity for large scale and long term public-private partnerships in Europe. These initiatives, will mainly combine private sector investment and national and European public funding, including grant funding from the Research Framework Programme and Ioan finance from the European Investment Bank. Joint Technology Initiatives may be decided on the basis of Article 171 of the Treaty or on the basis of the Specific Programme Decisions in accordance with Article 166.

Although SusChem stated from the beginning that it cannot become a single JTI (due to the broad range of topics covered and the enabling character of chemistry in general) certain topics from the SusChem SRA might be best pursued if stakeholders join other JTIs, create smaller ones on specific topics, or generate similar structures (not necessarily under theumbrella of FP7).

A unanimous effort by European research funders, both public and private, to avoid duplication of research and to make the best use of the limited available resources will lead to a more efficient European Research Area. Innovation means turning new ideas into successful business. It needs excellent research and supportive framework conditions. Financial investment, commitment, public engagement, regulations, education, training and many other factors have a significant influence on industry's ability to innovate.

## Creating a supportive environment





#### Novel resources and business models

The business environment is increasingly governed by two factors - the increasing pace of technological development and the globalisation of the world economy. Customers, competitors, suppliers and collaborators may be located, quite literally, anywhere in the world. In consequence the requirement for companies to constantly strengthen their capabilities and find innovative ways to satisfy customer demands has never been greater. This is true for both Europe as a region and for the Member States: the Member States also need to find innovative ways to increase the capacity and attractiveness of their innovation and thus the competitiveness of 'their' businesses. The IAP refers to this need for a more supportive environment as the "Innovation Infrastructure" requirements. In this context SusChem considers innovation to be the entire process that takes new chemistry inspired knowledge and converts it into the products and services that will underpin future growth and jobs.

Although a variety of funding sources already exist in Europe, there is an urgent need for Europe to do more and better in terms of research and innovation support. In general, European innovation performance has been weak compared to competing regions in the world. This has been realised by the European Union and by different Member States. Consequently, several initiatives to promote research, and especially innovation, on a national level have recently been started or, in some cases, are already well established. These initiatives could serve as a role model for others (other Member States, the EU in general, or regions) to improve the overall (funding and support) situation for different players in the technology-based innovation arena. An effective innovation infrastructure requires appropriate resourcing and the examples presented in the following sections are illustrative of countries that are already developing better processes relevant to chemistry and biotechnology.

#### UK: TECHNOLOGY STRATEGY BOARD, KNOWLEDGE TRANSFER NETWORKS

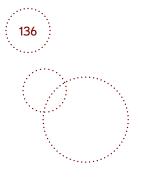
The UK government has acted to ensure that the promotion of technology innovation in business is led by business itself. The establishment of a business-led Technology Strategy Board in 2004 provided business the opportunity to directly influence government policies and to work together on common agendas. In taking forward the development of a national technology strategy, the Technology Strategy Board has focused on wealth creation and on driving forward business investment in R&D. The Board has adopted a twin pronged approach, namely the development of:

- Key emerging technologies which will underpin the high value-added areas of the UK economy and generate new streams of economic activity in their own right.
- 'Innovation platforms' where the integration of a range of technologies and the better coordination of policy and procurement instruments will result in a step change in UK performance.

In the innovation platforms government departments/agencies, research councils, regional organisations, business and the science base work together to identify and apply a diverse range of technologies (and other policy levers, e.g. standards and regulation) to deliver innovative new products and services for which there are significant customers in a potentially global market.

Over the period 2005-2008, £320 million is available to businesses in the form of grants to support research and development in the technology areas identified by the Technology Strategy Board. In spring and autumn each year, businesses will have the opportunity to compete for funding using the Collaborative Research and Development scheme whereby the UK government funds 50 % of the costs of approved projects which must involve at least one company and usually at least one academic partner.

In the spring of 2006 the UK launched a number of Knowledge Transfer Networks (KTNs) in selected technology areas. One of these is targeting chemistry innovation and two others focussed on different aspects of biosciences. The objective of a KTN is to improve innovation in UK businesses by increasing their ability to turn knowledge and expertise into new technology and products.



The Chemistry Innovation KTN and the Bioscience for Business KTN will make it easier for UK companies to seize opportunities and will bring together a number of organisations to facilitate innovation in the chemistry and biotechnology using industries, defined as those sectors that rely on chemistry and biotechnology to support their business.

#### THE NETHERLANDS: LEADING TECHNOLOGY INSTITUTES

The Dutch Leading Technology Institutes (LTIs) are partnerships for innovation between the business world, knowledge institutions and government. The LTIs are a unique and successful instrument that the government introduced in 1997 to boost the Netherlands' innovative capacity and competitive strength. Five of those leading institutes exist today:

- The Dutch Polymer Institute (DPI) focuses on research and development relevant to the polymer producing and processing industry.
- The Netherlands Institute for Metals Research (NIMR) enhances the competitiveness of the Dutch metal industry through strategic research into metal science, metal production and metal engineering.
- The Telematics Institute (TI) develops solutions for the innovative application of information and communication technology (ICT) in the business world and wider community.
- The Wageningen Centre for Food Sciences (WCFS) carries out strategic, fundamental research that boosts the competitiveness of the Dutch food industry.
- The Dutch Separation Technology Institute (DSTI) aims to improve the competitive position of the process industry by the development and application of breakthrough separation technologies.

Additionally, the Netherlands Institute for Industrial Biotechnology and LTIs around pharmaceuticals and plant genetics are currently being set up.

The LTIs are regarded as a best practice model of publicprivate cooperation for making the step from knowledge to innovation. They are playing an important role in Dutch innovation policy and are consistent with the increasing importance of networks, public-private cooperation, demand drive and programme funding. As an example in the SusChem arena, the Dutch Polymer Institute is a foundation, funded by industry, universities and government, set up to perform exploratory research in the area of polymer materials. The DPI operates at the interface of universities and industry, linking the scientific skills of university research groups to the industrial need for innovation. It performs pre-competitive research projects to add value to the scientific community through scientific publications and to the industrial community through the creation of intellectual property. The DPI integrates the scientific disciplines and know how of universities into the knowledge chain to optimise the conditions for making breakthrough inventions and triggering industrial innovation. It aims to combine scientific excellence with a real innovative impact in industry, thereby creating a new mindset in both industrial and academic research. Its mission is to establish a leading technology institute in Europe in the area of polymer science and engineering that is characterised by a strong, multidisciplinary, 'chain-of-knowledge' approach. The DPI is funded by industry (ca. 25 %), knowledge institutes/ universities (ca. 25 %) and the Dutch Ministry of Economic Affairs (max. 50 %).

Advanced Chemical Technologies for Sustainability (ACTS) is the key organisation for public private cooperation in sustainable chemistry in the Netherlands. ACTS focuses on catalysis, energy, chemical processes and biotechnology. ACTS has a LTI-like mode of operation, but is an independent entity within the Netherlands Organisation for Scientific Research supported by the Ministry of Economic Affairs.

#### THE NETHERLANDS: STRATEGIC TECHNOLOGY AREAS

In addition to the Leading Technology Institutes, the Netherlands decided to focus particularly on innovation activities and take advantage for opportunities for innovation by opting for 'Strategic Technology Areas', areas in which the Netherlands can excel now and in the future. Among the five themes chosen is 'chemistry'. The Dutch Ministry of Economic Affairs will support these areas through innovation programmes that involve collaboration of the business community, knowledge institutions and the government.

A business plan has been developed by VNCI (the Dutch chemical industry association) and the Netherlands



Organisation for Scientific Research. This business plan presents a coherent approach, starting with supporting fundamental research in the Netherlands up to entirely new initiatives concerning new company activities. The concept of 'Centres for Open Chemical Innovation' (COCIs) is being developed especially for new start-up companies. The COCIs should be located on existing R&D campuses typically belonging to major global operating companies. There is a particular focus on initiatives bridging the gap between (fundamental and applied) research and start-ups, i.e. public-private cooperation and innovation labs. The entire business plan requests investments (from all relevant parties) of approximately € 1 billion for the next 5 years.

#### O GERMANY: HIGH-TECH GRÜNDERFONDS

The successful transfer of results from R&D into marketable products is vital for the overall development and growth of an economy, since this stimulates innovation excellence and the structural changes brought about by the innovation. The complex interplay between R&D, economics, marketability and the technical and technological feasibility requires particular attention, since only successful implementation of R&D into innovation will lead to economic growth. From this interplay follows an intricate interaction between the various stakeholders (government, business, investors and scientists). In the early stages of technological developments, start-up companies can bridge these gaps. One of the problems they face is the lack of investment capital because investors feel uncomfortable with the perceived high technological and market risks.

In order to address this problem, the German model of a 'High-Tech Gründerfonds' (*High-Tech Gründerfonds* – *Chancen für Innovationen schaffen*, D. Jahn, 2005, Fraunhofer IRB Verlag, Stuttgart) could be expanded to European dimensions, a European High-Tech Fund (EHT), supported by the European Commission. In Germany, this model was established in 2005 and has been working successfully ever since. It was set up by the federal government, a banking consortium and several enterprises. The High-Tech Gründerfonds invest risk capital (around € 260 million for the next 5 years) in young promising technology enterprises that transfer research results into business. The enterprises will receive not only the badly needed seed capital but also coaching and support for their management. The proposed EHT fund concept consists of the formation of a fund into which business, European and governmental agencies place resources exclusively for the funding of high-tech start-up companies. As part of the funding agreement, start-up companies gain assistance from experienced coaches nominated by the EHT fund, who guide and support the burgeoning company through its early stages. Furthermore they benefit from the contact with the network of companies involved in the EHT fund, e.g. in order to gain market access. Through the careful selection of start-up companies, and the active assistance of coaches in the early stages, the chances of a successful product reaching the market is enhanced. This has the benefit for the EHT fund that the returns on investment and the original investments can be safeguarded to a certain extent, i.e. the risk is lowered.

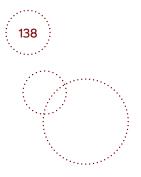
#### • FRANCE: PÔLES DE COMPÉTITIVITÉ

In response to the increasingly rapid changes in the global economy and their impact on the French economy, France recently launched a new wide-ranging industrial strategy focusing on the key factors of industrial competitiveness, particularly R&D-led innovation for manufacturers and service providers. This strategy offers a better balance between regional features, innovation and industry within the enlarged European environment and it outlines the context and issues of the competitiveness clusters (pôles de compétitivité) policy.

It was realised that industry is as important as the service sector:

- For France's competitiveness and attractiveness.
- Because of its spill-over effect on the rest of France's economy.
- For sales of related goods and services.
- For scientific and technical progress.

Innovation is obviously a key factor for industrial competitiveness. The effectiveness of R&D which is intangible and intelligence driven can be boosted by grouping players in clusters with global visibility. Pôles de compétitivité are designed to spark growth of industrial activities and jobs and to strengthen the regions. This tool is not just intended for emerging technologies (nanotechnologies, biotechnologies, micro-electronics, etc.) but also for more mature sectors.



Key issues for the competitiveness clusters policy are:

- Creating new wealth.
- Partnerships.
- R&D.

A call for these competitive clusters was launched in 2004 and ran until February 2005. Many pôles de compétitivité have been initiated and today, 66 clusters are operational. One is specifically dedicated to sustainable chemistry (Axelera based in the Rhône-Alpes Region), and one on the use of agroresources for industrial use (Industries and Agro-resources based in the Champagne Picardie regions). The Industries and Agro-resources pôle was created to respond to new industrial possibilities and emerging markets based on the conversion of biomass to new and innovative industrial products and to ensure new economical development of rural areas. Axelera has set up and shared with all its stakeholders a vision to switch from traditional chemical manufacturing to manufacturing techniques that seek to mitigate their impact and integrate environmental concerns from the start of design. Over the next ten years Axelera aims to move from being a curative chemical industry to a state-of-the-art industry integrating eco-design techniques, by completely rethinking its processes, products and reagents with a view to significantly improving environmental performance. Of its hundreds of stakeholders 50 % are SMEs.

#### SUSCHEM ACTIVITIES

Two specific project activities are envisaged to further develop the required "Innovation Infrastructure". Preliminary project scoping and evaluation work for these will be done using SusChem resources. However, assuming these projects can be shown to yield the expected benefits, more direct cooperation at country level will be required.

This could include working with individual country technology platforms, national associations, and Member States governments. The projects will also aim to work with and build on the various country innovation initiatives. The funding and resource needs of these projects will be defined during the scoping period. The first of these projects is a follow up study to update knowledge in terms of:

- The main funding and support models that currently exist at EU and country level.
- A first analysis of which of these are most relevant to SusChem, differentiating between those that directly fund public-private projects and those which fund public research organisations that should also be of value.
- A subsequent analysis of current best practices with an emphasis on the applicability to SMEs.
- Recommendations for concrete areas for improvement at all levels (EU, national, regional).

One outcome of the above project work will be to develop the information needed to initiate a SusChem Innovation Service to support SMEs. This is the second project and it would aim to develop a service that will speed up the adoption of "better practices" by smaller companies operating at the local level. Typical services would include:

- Awareness raising of support systems that already exist.
- An easy to access web database that would include some of the cost benefit data to support the next commercialisation steps (including potential funding).
- Networking seminars with a focus on how chemistry and biotechnology can enable downstream innovations.
- Outreach activities including communication/dissemination tools specifically designed to be used locally in the local language.

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### The innovation framework

#### • SUSCHEM CONTRIBUTIONS TO OVERCOME GENERAL INNOVATION CONSTRAINTS

There are extensive structural, social and political factors that significantly impact on the ability to innovate successfully as an industry. Several of these "innovation constraints" have already been referred to in previous SusChem documents and references. In this section the focus will be on clarifying aspects where SusChem can have a more meaningful impact on improving the "European framework for innovation".

Technology platforms are industry driven, so an ongoing challenge is to ensure an increased and longer term commitment to innovation by the leaders amongst the key companies. These leaders are ultimately responsible for generating the motivation and employee behaviour that cultivates an environment conducive to successful innovation. There are well documented challenges such as:

- Ensuring people in addition to those working in R&D are actively involved in the complete innovation process.
- Offering direct and visible support for new or different business models such as those that rely on open innovation and external collaboration.

In the above cases the role for SusChem will be to provide facts and figures that would validate such "new models" and help to quantify both the benefits and risks involved. This would be achieved as part of ongoing SusChem communications and workshop activities. It would also rely on networks remaining active so that success stories could be communicated directly to large company management teams as well as indirectly (For example, via national federations and technology platforms or using the channels available to the Member States Mirror Group) to smaller companies operating on a national level.

However there are other areas where sharing best practices will not be sufficient. An example of this relates to the fact that R&D is primarily considered as a cost rather than an investment. Thus as competitive intensity increases R&D costs will be further squeezed. This is aggravated by the cyclical nature of the industry which places additional pressure on longer term project spending during downturns. To develop an attitude within companies that would consider "Research & Innovation" as an investment will not be a simple task but further work in this area is needed to analyse potential positive stimuli such as fiscal incentives, increased reliance on external cooperative projects, and new risk sharing models with specialist financial institutions. An example of this latter point is the innovation initiative from the EIB (European Investment Bank) which is an area that SusChem has already started to develop.

#### Cooperative efforts to make partnering more productive

Framework conditions for FP7 have been finalised before publication of this document. However the need to continuously increase simplicity and relevance whilst reducing bureaucracy remains very critical to support a framework that is more conducive to innovation. SusChem will also be involved in other areas of public-private partnerships facing the familiar challenge of minimising resources committed to administration so as to maximise resources dedicated to the actual innovation process.

In this context the sharing of best practices where the SusChem network has direct experience would be a regular feature of the planned innovation workshops (see further). SusChem would also offer direct input to contribute to related governmental initiatives such as those aimed at improving the competitiveness of industry.

To act as project facilitator for individual technology projects would be beyond the resource capabilities of SusChem, however this would be more feasible for certain horizontal projects and for more generic advice for smaller companies or downstream customers. Information provision would include items such as:

- Identifying potential partners.
- Developing a semi generic process to help downstream users and SMEs to reduce bureaucracy with project submission.
- Ensuring effective links to the business development support that would need to follow a successful project.

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#### Speeding innovation in Europe

Societal challenges will require more innovative technologies whether seeking to address the future health needs of an aging population or the longer term energy needs as the availability of fossil fuels diminishes. These innovations will inherently carry different risks from today's current solutions. If too much time or resource is diverted in seeking to perfectly quantify these risks the critical (and typically more valuable) innovations will simply be driven outside the EU.

In the higher technology areas of innovation that SusChem is targeting, improving the trust of chemical and biotechnology industries will help towards the goal of achieving a better balance for risk-benefit sharing amongst SusChem stakeholders. This issue of building trust is also addressed in the wider stakeholder and social dialogue projects described in the next section. Industry's commitment for increased transparency will also help in this process. However this will need concrete, coherent and continued public support via key governmental institutions. In this context integrating feedback from risk management and stakeholder dialogue processes will be a crucial SusChem role, as facilitating such support and acceptance of new technologies will support the pace of market demand needed to make the new technology commercially viable.

#### Downstream linkages

Chemistry and biotechnology innovations primarily support progress at downstream customers. In general better cooperation up and down the supply chain should lead to increasing the probability of a successful innovation.

In this context a more structured interaction with relevant technology platforms provides a readily accessible means to create a better understanding of innovation priorities throughout the supply chains in which chemistry plays an important role. Workshops to stimulate this process would be the more visible contribution from SusChem, but the networking that ensues following such workshops provides the bigger boost to the innovation process. Ultimately this will require more effective use of the existing national, local and regional initiatives (including the national federations and technology platforms) as it is these existing associations that provide the most direct access to the SMEs and future downstream customers that SusChem is targeting. An initial objective would be to simply speed up the sharing of good practices but longer term a more strategic approach to such alliances might be envisaged.

#### Clarity of platform priorities

In today's highly competitive world industrial companies do not survive if they do not adequately respond to the needs of the market which in turn are driven by societal needs. These drivers form the basis for priorities within SusChem's research agenda. This should be equally applicable to the political priorities that also impact funding at both EU and Member State level. Thus ensuring a good match between these priorities and the work programmes within FP7, and the other key funding initiatives and organisations is essential. A good match will also increase the likelihood of the research work being further developed by industry and ultimately turning the generated knowledge into a commercially viable innovation.

A tracking system to ensure an adequate success rate for SusChem priorities within relevant EU and national R&D funding programmes would help in supporting this needed level of commercial viability. This process could also be applied to other areas of industry – governmental support programmes where SusChem interacts.

The two primary roles for SusChem would be to:

- Better define methodologies that can increase success rates and alignment between calls for projects and SusChem priorities for FP7 and related programmes. This would include ensuring the process remains as cost effective as possible.
- Maintain a systematic feedback process with appropriate experts such as the scientific officers that administer these programmes.



#### **Breakthrough innovations**

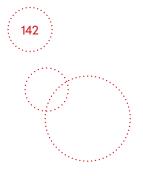
Today's society's relative affluence and stability creates a high aversion to risk and low tolerance for failure which contributes to a particular challenge for breakthrough innovations for companies operating in Europe.

SusChem's action plan to facilitate the implementation of innovative technologies in Europe is primarily reliant on the stakeholder dialogue in public engagement projects. These approaches help in building trust and demonstrating that industry cares about sustainability and social responsibility. It also helps strengthen the understanding of common core values and facilitates communicating on them with one clear voice. Finally, it also helps industry by proactively setting up processes to improve understanding and responding to societal concerns thus leading to more sustainable and successful product development. The results will be used to develop a societal approach for policy and strategy in the introduction of novel sustainable technologies, and will improve public trust in the sustainable chemistry sector and facilitate the uptake by society of these technologies.

#### Supporting innovative SMEs

Several of the preceding sections reinforce the fact that more effective interaction with smaller companies will be essential for improving innovation. This will be a continuing challenge where the SusChem network could be leveraged to propose specific services to SMEs.

To provide such services in an effective fashion would require ongoing financial support from the EU Commission for SusChem, for example to set up specific workshops, networking and communication support for SMEs. These workshops and their follow up would aim at increasing awareness of the most relevant SusChem opportunities, helping to navigate funding opportunities and directing access to companies which have related interests



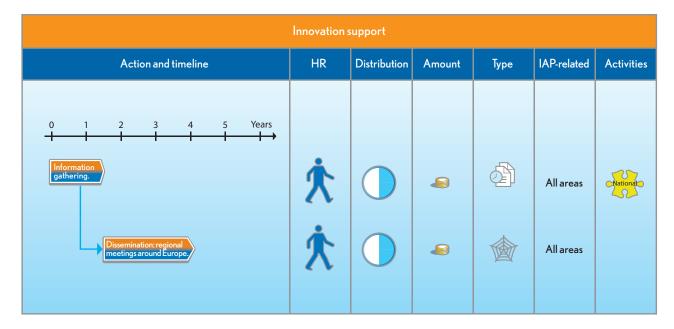
#### Innovation support project

Europe as a whole needs to significantly improve its innovation capabilities. Innovations in the SusChem arena also face the added challenges that extensive cooperation along the supply chain is normally needed and many of the stakeholders involved have a limited understanding of the role that chemistry needs to play in such innovations. As with many industries the main innovation opportunities are typically regional so activity to promote innovation has to take account of this factor.

#### Goals

With the above in mind a project will be developed to facilitate the exchange of best practice innovation know how at the regional level.

#### Key activities



The project envisages hiring an individual for a 3-4 year period to lead the initiative. The project would include the collection, dissemination and promotion of innovation know how. Collecting information would primarily focus on developing a portfolio of case histories and best practices. Dissemination would make use of all the modern methods but would crucially include extensive travel to the countries to ensure the required direct interaction with smaller companies will also be feasible. These regional meetings will also aim to get the managers of companies involved so that they gain a better understanding of innovation as an investment and the need to broaden the innovation process beyond the technology component. Effective cooperation with national federations, national technology platforms and any existing regional initiatives would be essential. Project costs are estimated at about €1 million. Funding sources would include both European programmes such as the CIP (Competitiveness & Innovation Programme) as well as the relevant country ministries (typically the Ministries of Industry or Economics).



#### O RISK ASSESSMENT AND MANAGEMENT STRATEGIES

The previous section described SusChem contributions to overcome some of the existing innovation constraints in Europe with a focus on chemical and biotech industries. In what follows some more detailed project ideas that have already been developed are presented. The focus will be on risk assessment and management strategies which have a significant impact on how innovative ideas can be pursued and transformed into market successes. The risk management portion of this activity would also need to quantify key financial aspects including an overall cost benefit analysis of the programme(s) as well as cost effectiveness assessments of the options proposed versus other alternative measures.

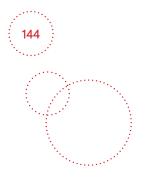
The introduction of emerging technologies requires reconsideration of the overall approach to risk assessment and management in the early stages of development. This is needed to ensure the objectives for growth and innovation, and the protection of health and environment, are not compromised. Especially in the light of long term investments into innovation, a reliable consistent risk-based framework is essential on the regulatory side and in the public debate.

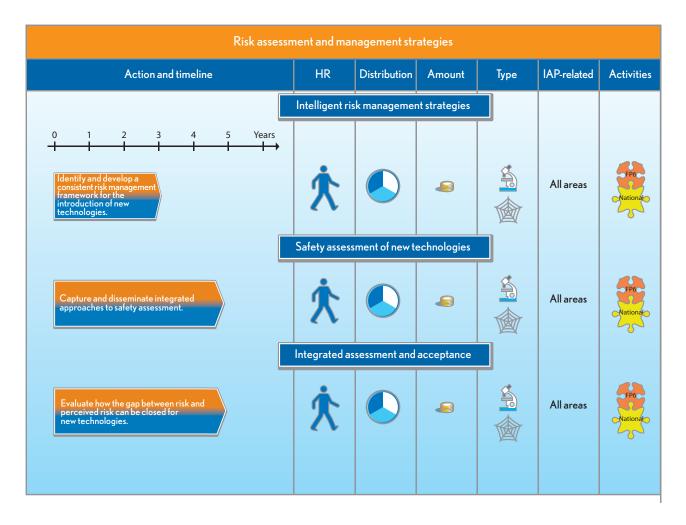
#### Goals

- The identification and development of a reliable consistent risk management framework for the introduction of emerging technologies – addressing the critical points throughout product use to allow for faster and more effective innovation.
- The capture and dissemination of integrated approaches to safety assessment within the context of regulatory decisions processes for emerging/breakthrough technologies.
- The evaluation of how the gap between risk and perceived risk can be closed for new technologies. The work should aim to define and characterise (i) risk, (ii) perceived risk, (iii) risk management options, and (iv) risk communication options to meet stakeholder concerns.

#### Key activities

- Intelligent risk management strategies
- Integrated assessment and acceptance
- Safety assessment of new technologies





#### Intelligent risk management strategies

The objective of this initiative is to identify and develop a reliable **consistent risk management framework** for the introduction of emerging technologies - addressing the critical points throughout product use to allow for faster and more effective innovation. Faster innovation implies carrying out multiple process steps in parallel. Accordingly these initiatives will be carried out where needed with the early involvement of bodies such as OECD, ISO and CEN. This will also help to speed up the harmonisation and information dissemination processes that are critical issues for emerging technologies.

The activity will involve:

- Compilation of retrospective and prospective case studies identifying risk points in product life cycle and/or supply chain and the impact of consistent vs. variable criteria regarding risk management. Additionally a cost benefit study be included as part of the process.
- Workshops on management/control strategies to identify optimum control options and to support confidence in the supply chain.

The main output of this activity will be guidance on risk management options and strategies for emerging SusChem related technologies that would inform evolving policy and permit regulatory and stakeholder acceptance.



The initial activities will run for approximately 3 years and will involve industry, competent authorities, the EU Commission, and academia.

Total required funding will be of the order of €3 - 5 million and potential sources of funds include pan-industry initiatives, the EU Commission and Member States. This work will also take note of and inform other risk management strategies of other technology platforms. Efforts will also be made to capture and incorporate the views of consumer groups, NGOs and international organisations such as the OECD and WTO. These groups would also provide input into the cost benefit studies.

#### Safety assessment of new technologies

The objective of this initiative would be to the **capture** and dissemination of integrated approaches to safety assessment within the context of regulatory decisions processes for emerging/breakthrough technologies.

Overall work will include the following activities:

- Regular periodic workshops on evolving safety assessment and other requirements for emerging technologies.
- A communication programme to provide information on research and regulatory needs to industry (including SMEs) and competent authorities.

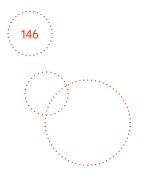
The main output will be guidance on best practice in safety assessment for emerging and breakthrough technologies. The initial work will run for a 3-5 year period and will include industry, competent authorities, the European Commission and academia. Total funding required is likely to be of the order of €5 million and potential sources of funds include pan-industry initiatives, the EU Commission and Member States. This work will also take note of, inform and contribute to the risk assessment activities of other technology platforms. A close collaboration is needed to avoid fragmented approaches.

#### Integrated assessment and acceptance

The objective of this activity is to evaluate how the **gap between risk and perceived risk** can be closed for new technologies. The work should aim to define and characterise (i) risk, (ii) perceived risk, (iii) risk management options, and (iv) risk communication options to meet stakeholder concerns. To make this work as tangible as possible a real case study is proposed (defined uses of nanomaterials) combining integrated risk assessment and societal dialogue.

The key deliverable would be structured guidance (including learning tools) on the steps necessary to close the gap between risk and perceived risk aimed at addressing stakeholder concerns and gaining stakeholder acceptance. These tools would ideally have generic application to other emerging technologies.

Work should run over 5 years with interim results after 2 or 3 years. Total funding required will likely be of the order of €5 million and potential sources of funds include pan-industry initiatives, the EU Commission and Member States. This work will also consider and learn from other activities. It will also form the basis for a comprehensive and constructive discussion with other technology platforms on their approaches.



## Building capacity and sharing knowledge

#### • COMMUNICATION, STAKEHOLDER DIALOGUE AND PUBLIC ENGAGEMENT

SusChem technologies involve a wide range of stakeholders with different views and interests, and have an important impact on society. However, public confidence in the chemical industry is generally low and some groups in society might perceive it as potentially high risk in terms of potential for negative impacts on health and the environment. Industry responses to such issues have been characterised as defensive, reactive and uncooperative. Many members of the general public are unaware of the sector's contribution to today's society and to sustainable development. Moreover there is often a gap between industry's vision of sustainability and how technology can contribute to it, and the vision of other stakeholders including the public. There is a need to understand what the underlying elements of these, often dissimilar, visions are, where the common grounds are and how consensus can be developed.

#### Goals

For the emerging SusChem technologies to be taken up by society and applied in a sustainable way, an informed dialogue between all stakeholders (industries, up stream and down stream sectors, academia, policy makers at EU and national level, consumer organisations, environmental groups, and other interest groups) is needed, as well as public upstream engagement, alongside innovative communication through media and targeted activities on the introduction of new products and technologies.

These approaches help building trust, demonstrating that "industry cares" about sustainability and social responsibility, strengthening common core values and communicating them with one voice, but also help the industry by proactively understanding and responding to societal concerns leading to truly sustainable and successful product development. SusChem can learn from existing examples such as:

 Responsible Care<sup>®</sup> (recognised as an integral part of sustainable development in the *Thematic Strategy on the Sustainable Use of Natural Resources*, COM(2003)572
 Final) activities already applied by many companies.  Downstream industries' voluntary approach towards informed dialogue to set up independent standardised crosscheck of products claims (e.g. industry self-commitment following existing norms and independent certification of biodegradable compostable polymer products (following the communication from the European Commission on environmental agreement at community level within the framework of the action plan on the simplification and improvement of the regulatory environment COM (2002)412 Final)).

The overall aim of this project is to develop an inclusive dialogue with all stakeholders to understand their concerns regarding the implementation of SusChem related technologies, and through the dialogue to build up an approach to address these concerns, including public engagement and communication activities.

#### Key activities

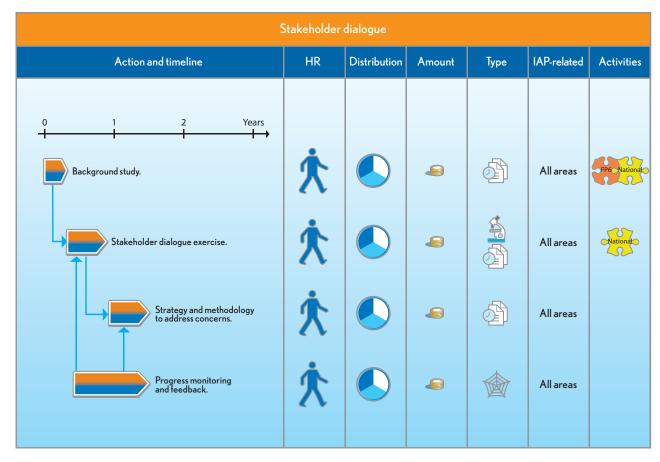
- Stakeholder dialogue
- Public 'upstream' engagement
- Communication plan

Three parallel activities are proposed on stakeholder dialogue, public upstream engagement and communication, which will set up the first steps towards a societal approach to the implementation of SusChem related technologies.

In order to initiate and operationalise these activities, a working group will be established, which will include representatives of industry and academia, social scientists and communication experts. Successful implementation of these activities is contingent upon commitment from SusChem stakeholders, including industry, regarding their active participation in this process, as well as taking on board the recommendations and best practices developed. Coordination with and leverage of ongoing activities will be ensured.



#### Stakeholder dialogue



The main objectives are:

- The identification of expert and stakeholder views regarding factors that can influence the implementation and commercialisation of novel chemical and biotech products and processes.
- The development of a dialogue process based on current and improved methodologies, together with a monitoring procedure, including impact assessment, to provide feedback and improve the process.
- The application of the dialogue process in SusChem context on all the identified influencing factors and concerns regarding emerging applications and products in sustainable chemistry, particularly perception, risk- and cost-benefit aspects.
- The formulation of qualitative and quantitative recommendations to the SusChem stakeholders on how to address the concerns, based on the dialogue results.

The process of stakeholder analysis and dialogue needs to be systematic. Various approaches to gain insight into consensus opinion regarding emerging risks and benefits associated with emerging technologies are reported in the literature and will be used in this study in order to refine methods.

The proposed project will facilitate an analysis of stakeholder views and improve public stakeholder dialogue. The results will be used to develop a societal approach for policy and strategy in the introduction of novel sustainable technologies, which in turn is likely to improve public trust in the sustainable chemistry sector and facilitate the taking up by society of these technologies.

#### Activities are:

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- To conduct a **background study**/survey on the existing stakeholder dialogue and communication activities; the issues already identified as creating concerns among the stakeholders and the public; and the new or future products perceived by the stakeholders and the public as new promising areas. It will be interesting to network with other technology platforms to learn from their experience (formal and informal) in stakeholder dialogue.
- To conduct a **stakeholder consultation exercise** to identify issues of concern specific to SusChem: The main objective is to identify and understand the views of stakeholders regarding innovative chemical and biotech products and processes.
- To develop a strategy and methodology to address the identified issues of concern in a transparent manner within the dialogue process.
- To monitor progress of the stakeholder dialogue both from a methodological and outcome perspective and to use this feedback for improving the dialogue process itself and the approach to address stakeholders' concerns.

Outputs of the entire work will include the following:

- A report summarising the findings of the survey on stakeholder views about SusChem technologies (concerns and potential success).
- Recommendations and guidelines regarding the development and maintenance of effective stakeholder dialogue on the implementation of innovative technologies.
- A raised level of awareness among stakeholders of the sustainability of SusChem technologies and the commitment of industries to sustainability.
- A well-defined consensus vision of what role sustainable chemistry could play in societal development along the three pillars of sustainability: people, planet, profit.
- Use and evaluation of innovative ways of communicating with stakeholders and the public.

The overall timeframe of the work will be 3 years and it will be steered by the SusChem working group on stakeholder dialogue, and carried out with the assistance of social and marketing researchers. Funding needs to come from the EU and from national research programmes, and may require industrial contribution. The budget for establishing the dialogue process will be of the order of €3 million and the continuation of dialogue activities will require further funding.

The proposed activities will serve to develop a network interlinking activities across other existing and emerging technology platforms, European and national activities for enhancing a societal approach to the introduction of emerging technologies.

#### Public 'upstream' engagement

The objectives of this activity are to set up a procedure for upstream public engagement on the introduction of the new technologies supported by SusChem and to increase the commitment of industry in terms of public engagement.

With the help of experts in public engagement procedures, the target groups for engagement as well as appropriate methodologies will be identified and defined.

A public consultation process to understand underlying concerns will be established starting, for instance, with identifying major concerns and issues to be addressed; results of this first exercise can be used as a basis for stakeholder dialogue. It is important that public engagement exercises are carried out as an integral part of the visionary projects of SusChem, e.g. how do people imagine their Smart Energy Home (see chapter *The SusChem visionary projects*). The activities and progress during this exercise will be monitored to provide recommendations for future public engagement activities.

This public engagement exercise will be carried out by independent experts with SusChem as an observer. The results will help SusChem to establish a work plan to involve industry proactively in stakeholder and public engagement activities. The issues and concerns emerging from the Public Upstream Engagement process will inform the activities in the Stakeholder Dialogue project.

Funding will be sought under FP7 and estimated budget as a first step for small scale study (e.g. focus groups) will be around €1 million. Further larger consultation and engagement projects will be based on the success of this first analysis and the recommendation of the stakeholder dialogue.



#### Communication plan

Some issues are already of concern to the public and decision makers and therefore need to be addressed rapidly in a coordinated way. The implementation of a communication strategy is a priority, although this will be continually refined according to new insights gained in other parts of the project. The following initial steps are required if an effective communication strategy is to be developed:

- Systematic analysis of existing communication activities regarding issues identified as relevant to SusChem, including how different approaches are focused on the needs of different target groups, and assessment of the impact of these communication activities.
- Prioritisation of the issues and target groups to be considered within the SusChem communication plan.
- Build-up of a network of science journalists, and development of information specifically designed for the press to increase their level of understanding of the SusChem technologies, and setting a reference point for press information.

Public communication activities developed on that basis could be initiated with a proactive emotion-entertainment-education based approach to raise public awareness and interest in the benefits of sustainable chemistry. The success of existing and novel communication activities needs to be evaluated and the key SusChem communicators need to be trained in public communication and media relations.

These activities go beyond SusChem actions; it is therefore crucial to identify groups efficiently setting up and carrying out communication plans and work with them on SusChem issues.

Taken together, the activities proposed within the *Communication and dialogue* section will facilitate the development of a consensus vision of what role sustainable chemistry could play in societal development along the three pillars of sustainability (people, planet, profit) which takes due account of the preferences and concerns of all stakeholders, end users, and members of society.

#### **O** EDUCATION, SKILLS AND CAPACITY BUILDING

In order to meet the SusChem goals it is important that there is an appropriately trained workforce in Europe.

#### Goals

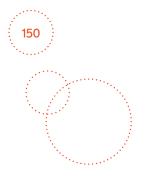
The priority for this area is to establish how best to build the skills and capacity, within academia and industry, required to realise the visions of the three SusChem technology pillars. In order to do this, an initial study is required to evaluate the adequacy of current European education and training programmes to meet the needs of sustainable chemistry.

There is also a need to identify effective curriculum materials and to disseminate these to pupils and teachers. Additionally networking opportunities are required and an e-learning portal should be established.

#### Key activities

Considering the first three actions (see roadmap on the following page), the work required includes:

- **Compiling information about best practice** for stimulating an interest in chemistry in school children and retaining the best students through to SusChem related university courses and producing a report outlining the best practice discovered.
- Conducting a **survey of industry** to establish the degree to which current education and training programmes will be able to provide appropriately skilled people to meet the demands of SusChem and preparing a report with recommendations based on an analysis of the data.
- Running a series of workshops with participants from higher education institutions, industry and other stakeholders aimed at disseminating the findings and stimulating the development of:
  - new education and training programmes and courses relevant to SusChem; and
  - programmes aimed at building-up an adequate supply of appropriately skilled people.



Education, skills and capacity building						
Action and timeline	HR	Distribution	Amount	Туре	IAP-related	Activities
0 1 2 3 4 5 Years	<b>i</b>			A	All areas	FP6 National
Compile information about best practice in education and training projects.	i İ				All areas	FP6 National
Run a series of workshops to communicate results.	t		<b>a</b>		All areas	FP6 National
Prepare inventory of curriculum materials.	ľ				All areas	FP6 National
Analyse gaps and develop new materials.	Ť			ð	All areas	FP6 National
Disseminate information.	ľ				All areas	FP6 National
Set up sustainable chemistry masters course network.	ľ				All areas	FP6 National
Investigate life long learning needs of industry, academia and teachers.	ľ		<b>.</b>	Ì	All areas	FP6 National
Develop e-learning portal.	Ť	$\bigcirc$	<b>.</b>		All areas	FP6 National
Summer schools.	Ť				All areas	FP6 National



The initial activities will run for over 5 years and will require input from:

- National and European chemical industry associations.
- Individual chemical companies.
- Academia.
- National and European chemical societies and academies.
- Government agencies (research councils etc.).
- Other European technology platforms (for benchmarking education practices).
- Networks and education initiatives, for example:
  - The European Chemical Employers Group (ECEG) and the European Mine, Chemical and Energy Workers Federation (EMCEF).
  - The European Association of Chemical and Molecular Science (EuCheMS).
  - The European Chemical Thematic Network.
  - ERAnets related to SusChem.
  - The AllChemE initiative.

The total funding for the above activities is estimated to be €500,000 for first 3 years for conducting two surveys and producing final reports. A further €200,000 will be required for workshops to disseminate the findings and to develop actions to be taken forward. Industry, the European Social Fund, and other sources will be approached for funding.

More generally actions are required to collect together and disseminate the best sustainable chemistry curriculum materials:

- Prepare **inventories of best curriculum materials**, both theoretical and practical, together with analyses of the effectiveness of those materials for teachers and lecturers at different educational levels including secondary school, undergraduate and masters.
- **Identify gaps** in curriculum materials and develop appropriate new materials.
- Disseminate information (through workshops, websites, etc.) about schools curriculum materials throughout Europe. The materials will have to be made available in a variety of languages.

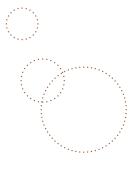
The workshops should aim to disseminate the information through demonstrating courses, and practical work which should be really viable. The courses should be directed at target groups of teachers who want to try out new things and learn. Other actions that need to be carried out are:

- Support for summer schools: either hands on techniques, or site visits, etc.
- Set up **network** to help with the development of **sustainable chemistry masters programmes**.
- Investigate the life long learning needs of industry, academia and teachers.
- Develop European sustainable chemistry e-learning portal.

In developing all the above activities the needs of industry from manufacturers through to end users, including the chemical using industries, should be borne in mind.

The overall budget for the education activities is likely to be of the order of €12 million.

Education plays a part in most other European technology platforms. There is a need to benchmark these other activities in the initial research phase of the study.



Sustainable chemistry has strong cross-sector importance and hence is particularly important for econmic growth in Europe. Showcasing its technological potential, networking and cooperation, monitoring and information sharing will further strengthen the foundations built by SusChem and its stakeholders.

# Strengthening the foundations





## The SusChem visionary projects

Results from the research proposed in the SusChem SRA will impact almost all areas of society, and thus promote sustainable development in Europe. Three visionary projects were described in the SRA that illustrate what will be possible in the future by applying the results of the research proposed.

Simply describing these project ideas is, however, not sufficient: SusChem intends to go a step further. In what follows, the steps necessary to realise some of these projects which demonstrate the full potential of the SusChem SRA are described.

Furthermore, an additional project with a special emphasis on reaction and process design has also been developed.

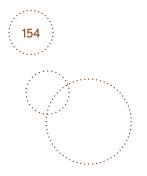
#### • THE SMART ENERGY HOME

Europe is already a world leader for new energy efficient construction materials, smart appliances, alternative energy systems in the home environment, insulation, sustainable consumer products, etc. Compared to other regions of the world, European homes are among the best in terms of energy efficiency. European companies have started to integrate new technologies into demonstration homes and developments. This strength and the available knowledge need to be fostered by speeding up the market uptake. Increased demand will also lead to more efficient mass production and thus reduced prices for such products.

The Smart Energy Home (SEH, formerly the energy generating house in the SRA) is a visionary project which will have a major impact on society in Europe and its energy consumption. Some of the technologies required to achieve the vision are already available but many others are yet to be developed. Energy conservation and home owner's comfort, health and convenience are integral parts of the concept of a Smart Energy Home. The realisation of this visionary project will require the involvement of many different stakeholders and the creation of new collaborations that can overcome technological and non-technological barriers that currently prevent innovation reaching the end user. In order to achieve the vision a drive needs to be provided and one such driver is to build the energy generating house as a vehicle for proving the feasibility of the employed technologies, and thereby showcasing the importance of chemistry and material development for a sustainable future in Europe.

In particular Europe will need to lead in the development of next generation high efficiency products that make extremely effective use of all raw material inputs from an overall lifecycle perspective. This also requires designing these products with the needs of the final consumer in mind, so that they develop into mass market opportunities rather than niche products.

"Living Innovation" will be an integral part of the Smart Energy Home. A wide range of materials, appliances, equipment and integrated technologies will be developed to create next generation efficiencies in areas such as energy use and consumer convenience. Such developments will create a portfolio of product innovations that can be scaled up for mass market sale (for example next generation appliances).



The Smart Energy Home concept: integrating energy efficiency, convenience, health and comfort



#### Energy/Resources

- Thermal insulation
- Fuel cells/Batteries
- Efficient domestic appliances
- Efficient lighting
- Phase changing materials
- Photovoltaics
- Water and waste management

#### Convenience

- Awareness enhancing technologies
- Domotics
- Smart materials
- Security
- Remote shopping

#### Health/Comfort

- Self-cleaning surfaces
- Remote diagnostics m
- Sound insulation
- Personalised nutrit
- Sustainable consumer product
- Air quality

In addition, the developments will create know how and design licensing opportunities in those cases where integration is a key feature of the development. Examples of this could include modular construction developments that could benefit from accelerated market development through public procurement programmes. Other examples include the technology needed to allow in house micro-cogeneration or mini-biogeneration of power with the required link-ups to enable alternative uses for that power such as sale to the grid or recharging fuel cells.

Finally the SEH will ensure all such developments are tested for consumer pull so as to avoid the trap of developing "greener" products that people do not buy.

#### The challenge

The challenge is clear and the message can be easily communicated to the public in terms of energy and household spending savings.

In western countries the energy used to heat buildings represents around 43 % of total energy consumption, generating the 2<sup>nd</sup> highest amount of greenhouse gases after transportation. A typical family with 2 children spends almost 70 % of its yearly energy consumption in the home. The vision is to put together a collection of technologies which will eliminate the use of this energy. This energy could be saved with the development and application of new products. A significant reduction of European energy consumption would be possible if such products were used in new and existing homes and in public buildings.

A future home that does not require an external energy source but is a self sufficient, or even a net positive, energy generator without  $CO_2$  emissions would address public concerns such as security of energy supply, climate change and independence of external energy sources - the energy efficiency in buildings is already mentioned in the Commission Communication on a broad-based innovation strategy for the EU (COM(2006)502 final). Addressing the current energy and climate change situation requires significantly increased energy efficiency in the short term - this was also expressed in the recent Action Plan for Energy Efficiency issued by the Commission (COM(2006)545 final).

The increased convenience and healthiness of the home would serve private needs of the individual consumer and thus lead to a natural uptake of such new products.



#### Innovation programme

This bold vision has major technical challenges with implementation horizons of more than 5 years. It requires a strong integration of policy, research, stakeholder input, and commercialisation routes. A single technology will not be sufficient. Compliance with current consumer habits and economical dynamics is critical for market penetration. Three specific areas need to be brought together.

The home as an energy generating source: Part of a family's energy requirement in the home could be provided by solar energy and also potentially through domestic versions of other alternative energies (wind, biomass, geothermal, etc.). Technology breakthroughs required include more flexible low cost photovoltaics based on hybrid silicon materials and conjugated polymers; one driver will be to move from solar panels to photovoltaic paints. In addition, superior battery technology with high flexibility and portability is required for domestic energy storage. To achieve this the technology breakthroughs required include superior electrolytes, nanostructured electrodes, ion selective membranes, modelling techniques and fuel cells (medium term).

The home as an eco-efficient environment: In addition to energy generation, most homes will require technology breakthroughs to reduce energy use and sustainability in a consumer friendly manner. The technology breakthroughs required for this include superior building materials for construction with nanoporous foams, and technology approaches such as nanocoatings for decorations, self-healing surfaces and photochromic coatings for glass. Appliances such as washing machines, heaters, lighting and waste treatment will need at least 50 % increased energy efficiency and ecoefficiency. Technologies such a nanofiltration, polymeric LEDs and multidisciplinary consumer product design are required. These developments need to be combined with renewable materials for packaging and efficient domestic water treatment.

The home as a sanctuary of health: To achieve rapid consumer and market acceptance citizens need to feel comfortable, safe and healthy in the home of tomorrow. This requires several e-health options for the diagnosis and sensing of body functions in the home environment. In addition, the home environment becomes the centre of healthcare, the basis for personalised nutrition and the use of sustainable consumer products. The creation of the relevant nutraceuticals, renewable materials and low cost diagnostics for consumers is required and the results need to be integrated in the home environment giving the consumer the choice with enhanced convenience. Furthermore these new technologies should, beyond providing medical assistance, play a role in providing a pleasant "atmosphere" in the home.

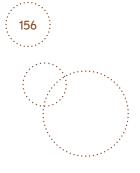
To build the Smart Energy Home a consortium with other technology platforms and industry needs to be established. Initial funding to build the consortium needs to be discussed with the EU Commission, industrial and academic partners. Initial work is required to gauge support for the project. Once sufficient support is forthcoming the consortium and management structures need to be put in place. The key task will be to raise the finances required to build the first house and coordinate the efforts of the various partners.

Once built, the house will act as a test bed for the technologies employed. Following a phase of technology optimisation, additional houses will need to be built in order to move towards commercialisation of the building techniques and technologies incorporated into the house.

In summary the Smart Energy Home will provide:

- A partner platform to facilitate testing and scaling up.
- A demonstration platform to showcase the importance of chemistry and material development for a sustainable future in Europe.
- Direct feedback from end users' 'Living Innovations'.
- A facility for implementing the results of leading FP projects in real life solutions for consumers.

With the right incentives considerable market uptake could be achieved within 3 to 5 years rather than 10 to 15 years.



#### O► THE INTEGRATED BIOREFINERY

Faced by global warming and limited fossil resources, and thanks to the development of new biological processes, the use of renewable raw materials derived from biomass becomes an attractive alternative as feedstock for producing fuels, innovative materials and chemicals, enhancing quality of life while reducing the industrial footprint on the environment. The integrated, zero-waste and diversified biorefinery is an integrated cluster of bioindustries, using a variety of different technologies to produce wide range of valuable commodities and end-products from biomass raw materials. This is a key concept in the realisation of the knowledge-based bioeconomy, and has the potential to revolutionise the way chemicals and energy are produced. Currently different technologies needed in a biorefinery from biomass pretreatment to improved bioprocesses and product development are being carried out in parallel. Sustainable use of resources and sustainable industrial development based on biomass will be maximised by making the best use of resources and strengthening cooperation between different industrial sectors along the value chain.

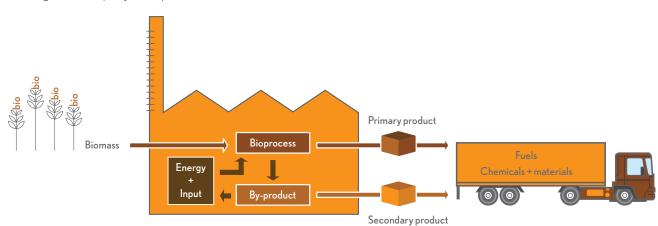
#### Motivation

In order to turn research into products, a crucial step is to establish proof of concept and carry out tests under industrial conditions. Because often full-scale manufacturing facilities or even pilot plants are not accessible to researchers, the concepts developed in R&D are not immediately applicable nor necessarily economically feasible on a larger scale. The focus therefore of the Integrated Biorefinery visionary project is on developing adequate industrial facilities to allow access to scale-up and pilot infrastructures during the research and development stage to develop and test industrial processes, thus reducing both lead time and investment. While pilot plants are not profitable ventures by themselves, they dramatically reduce the risk of introducing new technology on an industrial scale and therefore make a biorefinery venture much less risky for investors. Stimulating the construction of pilot plants is therefore one of the most important measures that can be taken in the development of the bioeconomy. Pilot plants enable the measurement of actual operating costs, and specific strengths and weaknesses of technological processes before costly, large-scale facilities are built.

#### Challenges

The integrated and diversified biorefinery will allow large-scale research, testing, and optimising of processes in the production of a wide range of products with the dual aim of using all fractions of biomass and exploiting their potential to produce the highest value possible in an eco-efficient way.

The initial construction of biorefinery pilot plants is a costly undertaking. Hence, specific scenarios for developing and funding flexible research oriented pilot scale activities need to be developed in Europe. Such projects will allow both feasibility and eco-efficiency studies and the demonstration of the benefits of the new technology in relation to the three pillars of sustainability: people, planet, and profit.



The Integrated Biorefinery concept



Through close cooperation in a research oriented pilot plant, such a project can facilitate the establishment of stronger academia and industry relations and understanding to support the translation of research into industrial innovation.

#### Innovation programme

Specific research and studies necessary to develop and optimise biorefineries are described in greater detail in *Bioeconomy*. Here are some of the key aspects on which biorefinery development needs to focus on:

- Biomass and pretreatment:
  - Selection of different biomass, including energy crops and dedicated non-food, based on eco-efficiency analyses including the production process.
  - Improvement of fractionation and pretreatment to develop more efficient but milder (in term of energy and input use) processes.
  - Use of the whole raw material for the best value and cost efficiency balance (energy use, inputs, waste retreatment, recycling or disposal).
- Processes:
  - Fermentation microorgansims that can withstand unpurified streams of feedstocks.
  - Integration of existing technologies and processing, both biological and chemical.
  - Valorisation of waste streams.
- Products:
  - Identification and process development of platform chemicals.
  - Development of biomaterials and products with new innovative properties.

Considering the current state of knowledge of biomass conversion, the technological approach will initially focus on improving and developing techniques for the processing of readily available and easily convertible standardised feedstocks such as starch, glucose, vegetable oils and proteins to produce intermediate and final products (ideally novel bioproducts). In a second stage, the biorefinery development will concentrate on adapting and optimising the well established conversion technologies to more diversified feedstocks such as raw biomass (non-separated).

#### The way forward

To develop this concept and the necessary industrial orpilot research oriented facilities, it is first important to ensure industry's commitment. A stakeholders' group including industrial actors (chemical, food and feed, polymers, biofuels industries, agricultural sector), academia, and other interested parties will be necessary to discuss issues requiring cooperation such as setting up a public private partnership, technology transfer, IPR management and sharing, and to develop best practices or guidelines for this novel framework. The stakeholders will have to define what research and testing will be conducted at such facilities, and establish an open scientific communication strategy to demonstrate the benefits of industrial biotechnology and its application in a biorefinery.

Funding possibilities have to be discussed with industrial and academic partners, the European Commission, Structural and Regional Funds, the European Investment Bank and the European Investment Fund. Decisions on types of biorefineries (raw materials, primary output and valorisation of bioproducts), and location(s) will be made after further research including the results from forthcoming FP7 projects to map existing biorefineries in Europe and develop models for their evolution.

As this project has a very broad scope and implications, it is important to develop it jointly with other European Technology Platforms such as Plants for the Future, Sustainable Forestry and Biofuels.

#### • THE F<sup>3</sup> FACTORY

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To meet the challenges laid down by the market and to combine product development with new manufacturing techniques, the implementation of an integrated technology initiative is needed, a technology and research spanning initiative for holistic product and process development: the F<sup>3</sup> Factory (fast, flexible, future).

#### Motivation

In recent years, product and process development in the European chemical and biochemical sectors has been characterised on the one hand by the development of new products and on the other by the optimisation of reaction conditions and the utilisation of economies of scale. One of the major drivers for the changes required in manufacturing businesses is competition from emerging countries where in the future large volume production will be cheaper and even sometimes more flexible. Additionally customer needs will change in all European business areas driven by market reaction time. A higher product diversification and more fast and flexible future (F<sup>3</sup>) production strategies will result from these customer demands.

In the long run upcoming competitive business models will be based on new manufacturing technologies and a holistic approach to process development. The synthetic processes of the traditional chemical industry will be strongly affected by biotechnology and by process intensification, for example, microreaction technology. The flexible integration of inherently safe process technologies with small hold-up volumes will be a key to the success of future products. Future sustainable chemicals production must combine a much broader range of production scales with interlinking technologies and logistics. Issues both in scale-down for 'ultra' small-scale production of extremely high value-added products early on in the development stages, and scale-up for 'precision engineering' of product properties for high-tonnage sectors need to be addressed.

#### Challenges

Future products will have to be developed whilst keeping in mind the need to:

- Increase product diversification.
- Shorten the time to market.
- Develop production capacity in accordance with product and market developments.

An important strategy to meet these challenges is "process intensification" in chemicals production. Process intensification is a strategic and interdisciplinary approach employing different tools (e.g. microreaction technology, modularisation) in order to improve processes holistically. Process intensification strategies vary depending on how demanding the goals set are: if, for example, safety aspects or the optimised control of reaction conditions of highly exothermic or endothermic reactions are a key factor, then a microreactor may be the answer. Moreover, as the approach is business driven, the strategy must address the total process or situation including raw materials, energy flows, staffing requirements and logistics issues.

The F<sup>3</sup> Factory aims to push radically new and upcoming technologies allowing product development and manufacturing with higher added value compared to current technologies. The realisation of this project will be a crucial step and a prerequisite for the development of successful and competitive future processes in Europe.



#### Innovation programme

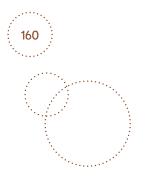
This technology initiative is aimed at the development of new process and plant concepts for speeding up the development of new products and for improving the product lifecycle. A major objective will be to achieve a substantial drop in capital expenditure for new plant and/or for retrofit of high performance intensified devices into existing infrastructure.

An important task of the technology initiative is to analyse the whole value added chain of production processes and to:

- Enable new products using new processing technologies and production concepts.
- Encompass the full lifecycle to optimise the whole value added chain.
- Minimise the use of resources and improve the eco-efficiency.
- Deliver demonstration plants and a technology platform for future processes.

The general aim of the project is to build up flexible demonstration plants on which existing scientific concepts will be bundled and implemented. Integrated process units and combined unit operations will be linked with process modelling tools, inline monitoring, model-based process management and advanced process control to form a centre for fast process development. This highly integrated technology platform will generate new opportunities and will lead to future factory concepts. These production assets will come together in F<sup>3</sup> Factories made in Europe. The technology initiative will address four different areas of product development. Each product category exhibits productspecific needs, but a strong interlinking of market size (with respect to volume) and product and process development can also be found. Focus areas of product development are:

- Value chemicals, intermediates and active ingredients: flexible and safe production on demand, process intensification, model-based process management.
- Specialised customised polymers by modular plants: small footprint, simple, modular, flexible, inherently safe, modelbased process management.
- New functional (nano and microstructured) materials by multipurpose plants: flexible, inline monitoring, on demand.
- Life science products by new production technologies: modular, multifunctional, highly integrated, safe, small footprint.



The developments within these fields can be divided into product and process developments and plant design and logistics.

#### a) Product and process development

- Development and application of microtechnology.
- Process intensified production technologies, as new catalyst technologies, for example, through heterogenisation of catalysts in micromodular devices.
- Reduction of process steps through the integration of unit operations in a single device.
- New multifunctional reaction units such as disposable reactors and fermenters.
- Eco-efficient products with small footprints.

#### b) Plant design and logistics

- The development of new concepts for the supply chain of multi purpose continuous plants and dedicated modules.
- Flexibilisation of production through modular plant design and process equipment.
- New concepts to analyse quality relevant parameters (online process monitoring).
- Improved process control.
- Adaptation of production capacity to lifecycle in high value applications.
- Scale production on demand: tailoring to needed volume (easy numbering up).
- Local logistics collaborative supply chains when using capacities at different sites (close to the customer).

The F<sup>3</sup> Factory: Different elements for the new production paradigm





#### Detailed project scope

The picture on the previous page illustrates how the different elements of a complete "supply chain" for the new production paradigm of the  $F^3$  Factory can be put together. All elements will then be combined to result in a structure that answers the need for a more flexible, modular production.

The elements are as follows:

- A focus on renewable resources for the new production paradigm.
- Research into novel synthesis pathways directly adapted to process intensification should be utilised. Nanotechnology for catalysis will play an important role (e.g. catalytic nanofactory). Dedicated product design based on the advantages of the F<sup>3</sup> Factory can be conceptually developed.
- Specialised hardware must be designed, developed and tested. In particular this will cover microreaction technology.
- Concepts for how to devise production facilities must be developed and implemented.
- Computer models supporting process management and optimisation will be developed taking into account the overall control through model based concepts.
- Supply chain design and implementation will be conducted for the new production world. The fact that a completely integrated approach - called "Collaborative Supply Chain Optimisation" - will be implemented will allow future chemical production to be closer to the customer in many respects.

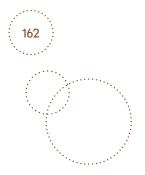
#### Implementation

The F<sup>3</sup> Factory visionary project will be both a coordinated cluster of projects and a demonstration facility. Industry commitment and academic support must be clearly visible with industry leading the project. The project is planned to be conducted in the following steps:

- Identification of a small number of partners from Europe; each covering one of the aspects delineated in the detailed project scope. Each of partners should identify a group of additional subproject partners for cooperation to run one of the subprojects that together form the cluster of projects (early 2007).
- Feasibility study to establish a more detailed project plan and a framework for partner commitment (1<sup>st</sup> half of 2007).
- Based on the findings of the feasibility study the project plan will be finalised and concrete preparatory work will be conducted (2<sup>nd</sup> half of 2007).
- Execution of the final project plan: the project cluster should consist of 6 projects including a demonstration facility. The latter does not necessarily have to be in one location but could be a virtual facility at multiple sites (2008-2010).

#### O DIALOGUE AND ENGAGEMENT

Since all visionary projects will have a high societal impact and will be showcasing SusChem's technology potential, it is important that all projects include stakeholder dialogue and public engagement as an integral part of the development and realisation of these projects.



### Integration, cooperation and networking

Sustainable chemistry has strong cross-sector importance beyond the chemical industry. It will be a key contributor to the competitiveness of many of Europe's industries and hence is particularly important for economic growth in Europe. Accordingly, a strong relationship between SusChem and other sectors' activities exists.

The first deliverable of all technology platforms is the creation of a multi-stakeholder forum with representation of a broad stakeholder base. This is a very important step in terms of integration and networking of activities. SusChem has been successful in this respect and will continue to welcome other stakeholders who are interested in actively participating in the platform. The different SusChem groups (Board, technology working groups, Horizontal Issues Group, Member States Mirror Group) all contribute to the improvement of European integration, cooperation and networking in the field of sustainable chemistry research. This cooperation needs to be further developed for SusChem to achieve its vision. Only a truly multi-stakeholder platform embracing the different voices of various players will allow SusChem to successfully define widely supported European priorities.

The SusChem Board is responsible for setting the SusChem strategy and direction. The Board composition ensures broad high level support from all important stakeholder groups. The technology groups align priorities of a multitude of research groups both in industry and academia on a technical level. Thus, they are most important for the networking of researchers across Europe and across the boundary between public and private research. The Member States Mirror Group allows for alignment and networking between the SusChem stakeholders and national research funders thus bridging the gap between overall European and specific national goals.

The implementation of the SRA as described in this document will only be possible with a coherent European-wide approach. Only coordinated approaches and networking among different actors will ensure that the required high quality research will be performed in the quickest, most effective, and most economic way with the highest possibility of success. Linkages will also be established with other players who are not currently directly involved in SusChem activities.

#### • INTERACTION WITH OTHER EUROPEAN TECHNOLOGY PLATFORMS

On a European level, close interaction between SusChem and other technology platforms is of utmost importance, as chemistry and biotechnology are enabling technologies, delivering solutions and materials for a wide range of other areas like the consumer care, information technology or transport industries. SusChem aims to exchange ideas with other platforms on the possibilities and value of cooperation and common activities at organisational as well as at expert level.

Meetings between researchers from academia and industry in chemistry and biotechnology with experts from downstream industries are a key to success of future SusChem activities. Such meetings are needed to identify overlaps, to agree on cooperation models and to find solutions for common problems.

SusChem has identified several technology platforms which either promise significant synergies with SusChem activities and/or cover important technologies for chemistry and biotechnology along the value chain. Bi- and multilateral consultations with these platforms will be continued or organised in the future.

The technology platforms which are essential for SusChem are:

- Biofuels.
- Construction.
- EuMaT.
- Forestry.
- Hydrogen and Fuel Cells.
- Manufuture.
- Nanomedicine.
- Photonics 21.
- Photovoltaics.
- Plants for the Future.
- Textile.
- Water Supply and Sanitation
- Zero Emission Fossil Fuel Power Plants.



The following table describes relevance and contributions of the SusChem IAP to other technology platforms (and their respective sectors) in more detail.

					н	ligh	Medium	Low	Visonary project
Technology Platform	Bioeconomy	Energy	Health	ICT	Nano	SQ₀L	SPPD	Transport	Visionary projects
Advanced Engineering Materials and Technologies (EuMaT)		Extreme materials	Extreme materials: ceramics	Extreme materials	Extreme materials		Extreme materials: production	Extreme materials: steel/alloys	
Advisory Council for Aeronautics Research Europe (ACARE)					Materials			Materials for transport applications	
Biofuels	Biorefinery	Biofuels					Bioprocesses	Biofuels	Biorefinery
Embedded Computing Systems (ARTEMIS)				Materials	Nanoapplications		Materials		
European Construction Technology Platform (ECTP)		Energy efficient building			Nanoapplications in energy efficient building	Energy efficient building			SEH
European Nanoelectronics Initiative Advisory Council (ENIAC)				Materials	Nanoapplications				
European Rail Research Advisory Council (ERRAC)		Materials						Materials for transport applications	
European Road Transport Research Advisory Council (ERTRAC)		Biofuels			Nanoapplications			Materials for transport applications	
European Space Technology Platform (ESTP)		Photovoltaics		Materials	Nanoapplications				SEH
European Steel Technology Platform (ESTEP)		Materials			Nanoapplications		Production	Production	
Food for Life	Biomass/-fuels; use of organic wastes as feedstock				Production		Food processing, packaging and distribution		
Forest-based sector Technology Platform (Forestry)	Lignocellulose- based biorefinery	Biomass/biofuels			Nanoapplications				Biorefinery; SEH
Future Manufacturing Technologies (MANUFUTURE)		Production			Nanoapplications	Production	Production/ manufacturing technologies	Production	F <sup>3</sup>
Future Textiles and Clothing (FTC)	Enzymatic processes		Materials		Materials & processes			Materials	
Global Animal Health (GAH)									
Hydrogen and Fuel Cell Platform (HFP)		Materials for fuel cells; bio-based hydrogen sources	Application of fuel cells in medical devicecs		Nanoapplications in fuel cells	Implementation of fuel cell technology in the home	Process technologies	Application of fuel cells in the transport sector	SEH
Industrial Safety (ETPIS)					Nanoapplications		Risk management inherently safer processes	·	
Innovative Medicines for Europe (IME)			Materials for targeted and smart drugs		Nanoapplications				
Mobile and Wireless Communications (eMobility)				Materials for ICT devices					
Nanotechnologies for Medical Applications			Materials; enzymatic functionalisation of drug delivery		Nanoapplications	Implementation o materials for medica applications in	f <sup>al</sup> Application		
(NanoMedicine) Photonics21			material	Photonic material	Nanoapplications	the home			
Photovoltaics		Photovoltaic materials		development	Nanoapplications in photovoltaics	Photovoltaic materials in the home	Production of photovoltaic materials	Applications of photovoltaic materials in the transport sector	SEH
Plants for the Future	Biomass optimisation and crops for industrial use	Biomass optimisation for biofuels and energy						Biomass optimisation for biofuels	Biorefinery
Robotics (EUROP)				Materials	Nanoapplications				
Water Supply and Sanitation Technology Platform (WSSTP)	Clean enzymatic processes				Materials & processes	Water and soil remediation			SEH
Advanced Engineering Materials and Technologies (EuMaT)					Materials			Materials	
Zero Emission Fossil Fuel Power Plants (ZEP)		CO <sub>2</sub> reduction			Materials			Catalytic CO <sub>2</sub> /NO <sub>x</sub> /SO <sub>x</sub> conversion	

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#### **O** ERANETS

ERAnets represent a very promising approach to start aligning national with European programs without losing the national perspective. ERAnets like ERA Chemistry and ACENET play an important role in the planning of future integration of national and European funding activities in chemistry, chemical engineering, biotechnology, and related areas. SusChem will actively cooperate with the ERAnets by discussing the SusChem Strategic Research Agenda and the Implementation Action Plan with the ERAnet members.

Such activities will help create strong interactions and exchanges between funding and networking activities on the national and European level envisaged by SusChem. As described in *Resources - ways and means*, SusChem will attempt to moderate and facilitate the process of further alignment of national and European funding programs in areas related to its priorities. The SusChem Member States Mirror Group will also play an important part in this process.

#### **O** NATIONAL TECHNOLOGY PLATFORMS

SusChem is a European wide initiative. National technology platforms for sustainable chemistry or similarly named initiatives have been created in several countries throughout Europe. They serve as a means to bundle national input into SusChem, to focus the SusChem messages to the individual country's interests, and to increase the participation especially of small and medium enterprises. SMEs are often discouraged by the idea of European wide organisations, but are more likely to join initiatives on a national level.

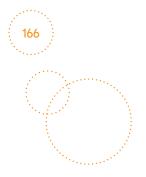
These national initiatives thus present a unique chance to foster chemistry, chemical engineering and biotechnology research on a national and European level and to create a European understanding in these disciplines. SusChem will further support the creation and continuation of such national platforms and initiatives. SusChem is especially willing to support the establishment of national nodes in the eastern European countries and is ready to discuss and exchange ideas for common European and national activities.



#### O NETWORKING ON A EUROPEAN LEVEL

National chemical and biotechnology business associations are important SusChem partners to increase visibility and participation on a national level, especially with respect to SMEs. Most of these associations carry out additional research and innovation activities that need to be leveraged as much as possible. To give just one example, in Italy, the Italian Federation of the Chemical Industry (Federchimica) has developed specific framework cooperation agreements with Italian research bodies designed to enhance technology transfer and to allow companies, particularly SMEs, to make better use of those institutions.

The chemical and biotechnological societies in the Member States have a special role in the networking process as they can act as conduits for integrating dialogue on the SusChem ideas via many additional stakeholders and other interested parties. Networking, distribution of documents and ideas and feeding back national opinions and perspectives into the SusChem process can easily be facilitated by these organisations. In addition to the cooperation with the national technology platforms, SusChem will continue its successful cooperation with societies like RSC, GDCh and DECHEMA. On a European level, industry federations (Cefic and EuropaBio) and research societies such as ESAB (European Federation of Biotechnology Section on Applied Biocatalysis) are already involved as SusChem partners. Others such as EuCheMS (European Association for Chemical and Molecular Sciences) or EFCE (European Federation of Chemical Engineering) are currently represented through some of their member societies (RSC, GDCh, DECHEMA). Some of them are also involved in AllChemE, the Alliance for Chemical Sciences and Technologies in Europe. Greater cooperation between SusChem and all the AllChemE partners (Cefic, EuCheMS, EFCE, COST Chemistry and Molecular Sciences and Technologies, CERC3 - Chairmen of European Research Councils Chemistry Committees, and ECTN - European Chemistry Thematic Network) will be sought to further enhance networking and cooperation on a European level.



# Role of the SusChem Technology Platform

After developing and publishing the Strategic Research Agenda and the Implementation Action Plan SusChem will continue its work during the implementation phase. Fostering chemistry and biotechnology research and innovation in Europe will remain the key goal. SusChem's role in the future is thus a logical continuation of its recent and current work. Its aim will remain that of achieving the conditions necessary in Europe for innovation in chemistry, industrial biotechnology and chemical engineering by monitoring the implementation of the SRA, by actively engaging in the political debate in Europe, and by providing support to researchers and innovators.

In addition to promoting its vision, reviewing progress and updating a rolling programme of research, it is essential for SusChem to meet and satisfy the needs of its stakeholders and to continue to be a forum to turn dialogue into actionable outcomes. Therefore, SusChem will take on a role as an information platform facilitating networking and exchanges between researchers and manufacturers, funders, governmental bodies, academic institutions and NGOs. SusChem intends to provide a service that clearly differentiates it from other networks in the minds of existing and potential members so that it is seen as the preferred point of entry into all SusChem-related technologies.

#### **O** IMPLEMENTATION MONITORING

The Implementation Action Plan sets out the activities necessary to follow through with the SusChem SRA. Monitoring this implementation is essential to ensure a smooth process and continuous alignment of activities and requirements. The IAP will need adjusting based on the results of current and future projects, and on developments in Europe, and in other parts of the world.

Accessing and activating necessary resources (both finances and people) and successfully registering necessary modifications requires a monitoring system. SusChem will thus:

- Establish an implementation monitoring system encompassing both European and national programmes.
- Prepare a yearly assessment of achievements based on the monitoring.
- Promote yet unmet SRA and IAP priorities with policy makers, funding bodies and other SusChem stakeholders. This will include the organisation of review meetings between the SusChem Board and European Commission and Member States' representatives to agree on improvements and priorities for the future.
- Update its Strategic Research Agenda and Implementation Action Plan when appropriate. The current expectation is that the SRA will be updated every 5 years, and the IAP every 2 years.

SusChem also expects to take a more active role in respect of horizontal issues. Whilst the technical issues are likely to be taken up and driven by industry, the framework programmes and national programmes, the same may not be the case for cross-cutting issues. SusChem will therefore closely monitor the development of the Horizontal Issue projects. The Horizontal Issues Group will, if necessary, commission small pieces of work to initiate actions in particular areas. The funds for these actions will be provided by the SusChem partners and, where appropriate industry, the European Commission and national bodies will be approached for support.



With the above in mind it will be essential to keep the horizontal network active. Ongoing sharing of best practices amongst interested parties will be one means of doing this as will maintaining interactions between prospective partners for the proposed projects. This will be done both via the existing Horizontal Issues Group as well as via targeted representatives of organisations that can reach stakeholders where SusChem does not have effective working relationships.

Practical examples of the expected deliverables from maintaining such networks are essentially already provided by the activities outlined in the previous chapter. In addition to facilitating and monitoring progress here SusChem would also plan to initiate cost-benefit assessments of its work in this field. More sustainable chemistry solutions will enable more sustainable innovations downstream. Thus through interactions with potential downstream users (via for example knowledge transfer activities) the industry should be able to better understand their future markets. At the same time stakeholder dialogue work will help SusChem to react better to likely societal concerns. By integrating the combination of this market pull and critical consumer concerns into the technology push industry should be able to substantially improve innovation progress. The generation of at least semi-quantitative measures of the costs and benefits of this approach will be needed to both justify future resourcing of this area and to improve the effectiveness of these approaches.

#### **O** PROMOTING THE SUSCHEM VISION

Promoting sustainable chemistry in Europe and fostering research and innovation in this area will require continuing dialogue with a wide variety of stakeholders such as policy makers, authorities, consumers and the public at large. Due to its multi-stakeholder nature, SusChem holds an important and ideal position in the debate on these issues. Activities which are necessary include:

- Continued advocacy for chemistry and biotechnology research and innovation at a European level.
- Activities, such as public engagement and innovative communication, aimed at increasing public awareness and perception of sustainable chemistry.
- Follow up work on visionary projects.

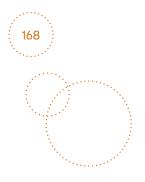
#### Link to national SusChem platforms and funding programmes

With the majority of public European research funding originating from national and regional sources, the implementation of the SusChem SRA will have to rely on these sources for funding in addition to funding from FP7 and private sources. Close collaboration and coordination with national initiatives is therefore of utmost importance (see under *Implementation Monitoring*).

National SusChem platforms have already served as important champions of the SusChem cause in their respective countries and will continue to serve in this role in the future. They have also brought, and will continue to bring, specific national interests into the European platform. The SusChem Member States Mirror Group also acts as an intermediate between SusChem and national funding agencies.

During the implementation phase SusChem will therefore engage in:

- Keeping a direct contact to national SusChem platforms and ERAnets as well as supporting the establishment of national platforms where they do not already exist.
- Remaining an important communication link between EC Directorates and national funding organisations (e.g. via the MSMG).
- Working towards alignment between FP7 and national programmes.



#### **O** SUSCHEM SUPPORT

SusChem aims to support research activities relevant to its SRA at European, Member State and regional level. This requires involvement in different activities related to research projects.

#### SusChem will:

- Engage in activities to provide a communication link between EC Directorates, national funding agencies, and SusChem stakeholders.
- Act as a dissemination platform for SusChem related information on calls for proposals, projects, etc. via:
  - The SusChem website.
  - Regular newsletters and electronic mailings.
  - Press releases.
  - Meetings including stakeholders, user group members and project representatives.
  - Presentations at relevant fairs.
- Support activities to facilitate partner searching for those working in SusChem areas. Possibilities currently under consideration are for example the publication of stakeholder interests on the SusChem website or the organisation of partnering activities in specific cases.
- Work to establish and organise dedicated user groups and fora for widespread implementation of concepts and results from SusChem related projects.

#### **O** SUSCHEM DYNAMICS

Further SusChem activities might be considered and included in the future as a response to the needs of its stakeholders. The SusChem Board and partners invite all stakeholders to remain actively involved in all SusChem activities to continue its success story. As an open stakeholder forum, it is the SusChem stakeholders themselves and their ideas and actions that will drive SusChem now and in the future.

# Glossary

ACENET	ERAnet for Applied Catalysis	I ICT	Information and Communication Technologies
ACTS	Advanced Chemical Technologies for Sustainability,	ILD	Inter-level Dielectric
	The Netherlands	IPR	Intellectual Property Rights
ALD	Atomic Layer Deposition	ISO	International Organisation for Standardisation
AllChemE	Alliance for Chemical Sciences and Technologies	ITO	Indium Tin Oxide
	in Europe	JRC	Joint Research Centre, European Commission
ATP	Adenosine 5'-Triphosphate	JTI	Joint Technology Initiative
BMBF	Ministry for Education and Research, Germany	KTN	Knowledge Transfer Network
BTL	Biomass to Liquid	LCA	Lifecycle Analysis, Lifecycle assessment
CAD	Computer-aided Design	LED	Light Emitting Diode
Cefic	European Chemical Industry Council	LPG	Liquefied Petroleum Gas
CEN	European Committee for Standardisation	Matera	ERAnet Materials
CERC3	Chairmen of European Research Councils'	MCM	Mobil Composition of Matter - Type of
	Chemistry Committees		Mesoporous Material
CMOS	Complementary Metal Oxide Semiconductor	MNT	ERAnet Micro- and Nanotechnology
COCI	Centre for Open Chemical Innovation	MOF	Metal Organic Framework
C₀E	Centre of Excellence	MSMG	Member States Mirror Group
COST	European Cooperation in the Field of Scientific and	MTBE	Methyl Tert Butyl Ether
	Technical Research	NGO	Non-governmental Organisation
DECHEMA	Gesellschaft für Chemische Technologie und	Ni-MH	Nickel Metal Hydride
	Biotechnologie, Germany	NMR	Nuclear Magnetic Resonance
DELOS	Depressurisation of an Expanded Liquid Organic Solution	NOx	Nitrous Oxides
DMFC	Direct Methanol Fuel Cell	OECD	Organisation for Economic Co-operation
DNA	Deoxyribonucleic Acid		and Development
EBN	European Biocatalysis Network	OLED	Organic Light Emitting Diode
EC	European Commission	OTFT	Organic Thin Film Transistor
ECTN	European Chemistry Thematic Network	PDMS	Polydimethylsiloxane
EFCE	European Federation of Chemical Engineering	PEM	Proton Exchange Membrane
EH&S	Environment, Health and Safety	PEO	Poly Ethylene Oxide
EHT	European High-tech Fund	PGSS	Particle from Gas Saturated Solutions
ERA	European Research Area	PPO	Polypropylene Oxide
ERDF	European Regional Development Fund	PSE	Process Systems Engineering
ESAB	European Federation of Biotechnology Section on	PV	Photovoltaic
	Applied Biocatalysis	QoL	Quality of Life
ETBE	Ethyl Tert Butyl Ether	RESS	Rapid Expansion of Supercritical Fluids
ETP	European Technology Platform	RSC	Royal Society of Chemistry
EU	European Union	SAM	Self-assembly
EuCheMS	European Association for Chemical and	SAS	Supercritical Antisolvent Precipitation
F D:	Molecular Sciences	SBA	Santa Barbara Types of Mesoporous Materials
EuropaBio	European Association for Bioindustries	SEH	Smart Energy Home
EXAFS	Extended X-ray Absorption Fine Structure	SETAC	Society of Environmental Toxicology and Chemistry
FP	European Framework Programme for	SME	Small and Medium-sized Enterprise
FTID	Research and Development	SOx	Sulfur Oxides
FTIR	Fourier Tranform Infrared	SPPD	Sustainable Product and Process Design
GDCh GPCR	Gesellschaft Deutscher Chemiker	SRA SUSPRISE	Strategic Research Agenda
	G Protein-coupled Receptor		ERAnet Sustainable Enterprise
GTL H-PDLC	Gas to Liquid Hala angelia Palance Diagona d Liquid Canatal	UNEP UV	United Nations Environment Programme
	Holographic Polymer Dispersed Liquid Crystal	VOC	Ultraviolet Veletile Oceanie Commenced
HyCo	ERAnet Hydrogen and Fuel Cell Implementation Action Plan	WTO	Volatile Organic Compound World Trade Organisation
IAP			

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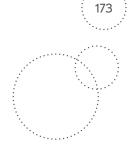
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