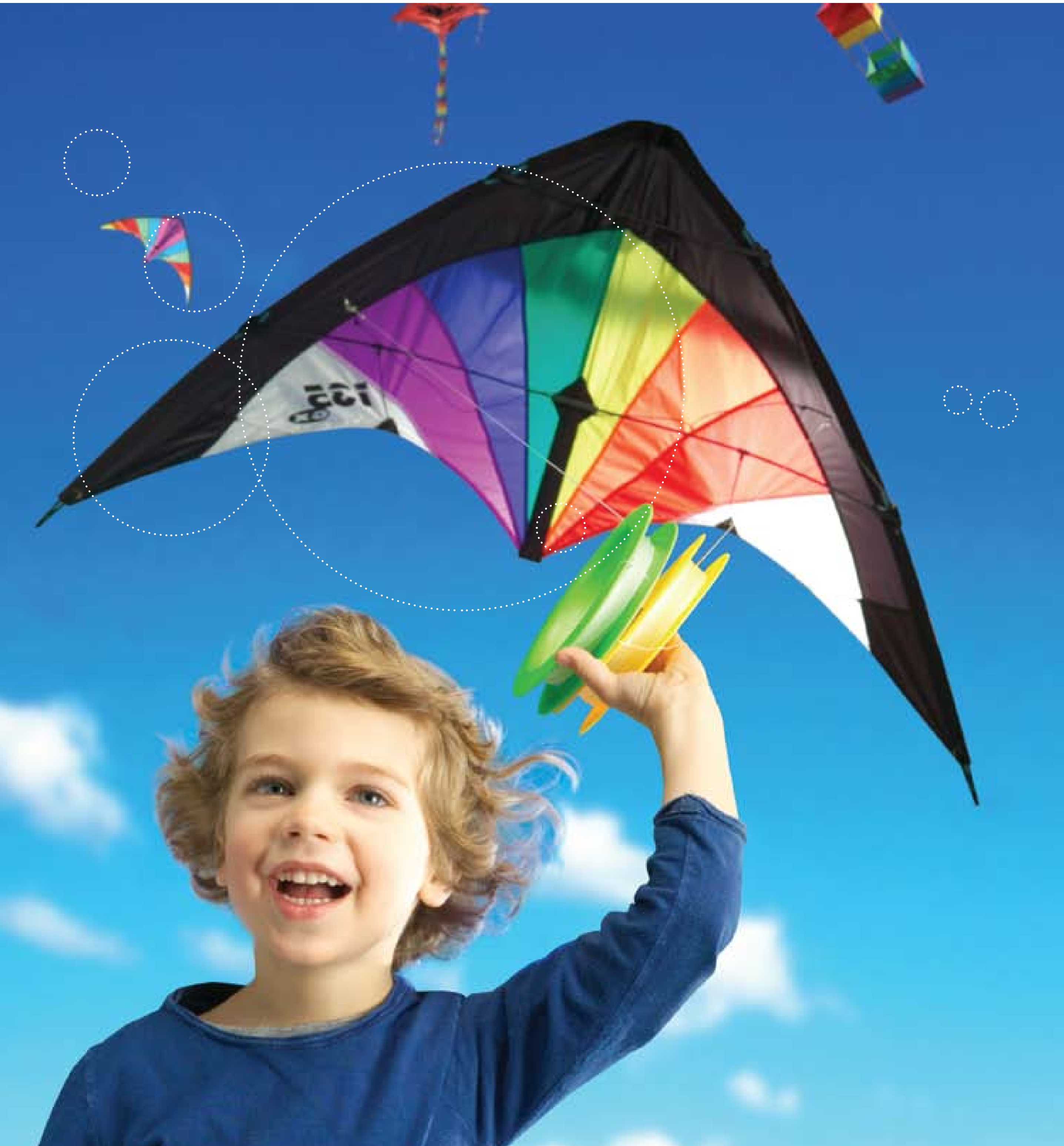
SusChem
European Technology Platform For
SUSTAINABLE CHEMISTRY

SusChem IAP Update 2009

Materials Technology



1. Materials Technology IAP Update

1.1 Introduction

The SusChem Materials Technology Group, chaired by Prof. Rüdiger Iden of BASF, Germany, consists of European experts in topics related to the design, preparation, analysis and application of new materials and nanomaterials in functional systems or devices. The group has been responsible for the Materials content of the SusChem Strategic Research Agenda (SRA) and the respective contribution to the Implementation Action Plan (IAP). In the latter document, Materials Technology topics are in particular represented in the chapter "Sustainable Nanomaterials and Materials design".

Following the finalisation of the SRA and IAP documents, the group has been reviewing and assessing the take-up of Materials Technology topics in the FP7 work programmes. Based on this analysis, the group has continued to recommend strategic goals as well as specific topics for future calls.

The group acknowledged that Materials topics have been well represented in the FP7 calls in 2007 and 2008, in particular in the NMP work programme, but also in the KBBE, Health, Energy, Environment and ICT programmes. In particular, calls in the field of nanotechnology had an impressive overlap with one or several topics of the SusChem IAP. The uptake of IAP proposals was generally satisfying for funded projects in the NMP and ICT theme, as far as data were available. The group recommends to carefully assess the subscription rates and quality of proposals in areas, where research fields have been combined and, based on this, to consider following, more focussed future calls in these areas.

In review some fields of strategic importance were identified that did not receive sufficient funding. These include energy management topics such as wind power, efficient lighting, batteries, and supercapacitors. The work group members evaluated more than 60 new research topics that were received from stakeholders. Topics that were proposed by several stakeholders were given priority and grouped in four clusters that emerged naturally from the analysis:

- **Energy managing nanomaterials and electronics**
  - Battery materials, nanoscale contacts at low dimensions, charge transport at interfaces, printable electronics, efficient lighting, transparent conductive electrodes
- **Lightweight and functional materials**
  - Nanoporous hybrids, functional nanocomposites, construction materials, in-line analyzers, optical applications
- **Design and safeguarding of bio-nano-interactions**
  - Environmental, Health and Safety (EHS) aspects of nanocomposite material, nanomembranes to separate/recover nanomaterials from liquids, controlled biokinetics and drug delivery
- **Corrosion**
  - Novel tools to predict and analyse corrosion cracking, corrosion of polymers, corrosion in very demanding conditions such as fluorine or chlorine, ionic liquids, high temperatures

Following on from this a number of topics with high urgency and low levels of recent funding were selected and elaborated into specific research proposals. These proposals are described in the subsequent pages of this document.

As a general theme, life-cycle-analyses as well EHS aspects should be included proactively into all projects concerning nanomaterials. This will help to generate data and facts needed to ensure early awareness and identification of problematic areas in nanotechnology. It will also allow the development of nanotechnology in a sustainable way and communication of this to the general public.

Batteries have been a long-standing priority topic of SusChem and have finally received recognition in the Recovery Plan of the EU in the sector Green Cars. Specific proposals for further research in this area are found on the following pages.

One of SusChem's visionary projects (the **Smart Energy Home**) found its mirror in the sector Energy-efficient Buildings of the Recovery Plan. Construction is a traditional, highly cost oriented sector which makes adoption of new materials and techniques difficult. Industry members of SusChem have taken action through the Smart Energy Home initiative to speed up the uptake of available technologies (nano and non-nano) which can reduce the CO_2 emission of new or existing residential buildings. The Smart Energy Home is executing a specific set of action lines that together complement the range of initiatives already being taken by governments including subsidies, regulations and guidelines. The construction industry will greatly benefit from nanomaterials with new functionalities and enhanced performances. Directly and indirectly the construction industry is one of the biggest consumers of energy resources and accordingly, one of the biggest emitters of greenhouse gases. Also here, new materials can help the sector to reduce its carbon footprint.

1.2 Recommendations for IAP update and future FP7 calls

1.2.1
Theme: Energy managing nanomaterials & electronics
Topic: Battery materials – Anodes and cathodes for high power applications researched by high throughput methods

Battery materials for high power applications are essential prerequisites for the electric vehicles for future sustainable surface transport. Current state-of-the-art materials for high power Li-Ion battery electrodes provide insufficient energy storage densities of about 150 Wh/kg (450 Wh/l) leading to a short operational range for electric vehicles.

It is already foreseeable that the materials currently under optimisation even after further development steps can only achieve at maximum a vehicle operational range of 100 to 150 km with an acceptable battery mass of 200 kg in the future. Additional issues are safety problems and high costs related to current materials technologies. Therefore a new approach starting from basic materials development is necessary.

1.2.1.1 Relation to SusChem IAP

This topic is an extension of key activity "Batteries - Develop nano structured electrode materials of high speed specific capacity for lithium batteries" in IAP chapter "Energy - Batteries - Develop high capacity electrodes and safe electrolytes".

1.2.1.2 FP7 Uptake of this topic

Development of novel battery materials was already addressed in call **NMP-2007-2.2-3 Advanced Materials architectures for energy conversion.** There are still major technical hurdles to be overcome and so this topic has not been sufficiently covered by this call. An approach based on more basic materials research is necessary to achieve the long-term goals of the Green Cars initiative.

1.2.1.3 Gaps

- High throughput methods (complete work flows including meaningful testing) to identify new compositions for anode and cathode materials for high power batteries
- Battery materials with an energy storage density of 250 Wh/kg and 600 Wh/l

1.2.1.4 R&D objectives

- Development of methodologies for **high throughput screening of battery materials** and materials combinations (complete work flows from synthesis to assembly of test batteries and testing)
- Identification of new **alternative materials** combinations for **safe, low cost, high power batteries** of the future with an energy storage density of 200-250 Wh/kg and 600 Wh/l for improved Li-Ion batteries and of 300-350 Wh/kg for batteries based on alternative materials

1.2.1.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects or for large projects oriented to basic materials research including application-oriented testing addressing the challenges of the topic.

1.2.2
Theme: Energy managing nanomaterials & electronics
Topic: Charge transport at interfaces; nanoscale metal contacts in low dimensions

Manipulation, assembling and integration of low dimensional nanostructures (LDNs) in high performance devices are primary goals of nanotechnology, where it is expected that LDNs will maintain their unique properties when they are assembled and integrated within these devices. These materials show properties and performances in applications that are different from their traditional bulk counterpart. A deep understanding of the electronic structure of LDNs and control of their integration would allow design of tailored functional systems. However, despite the current need, the processes of assembling and integrating individual LDNs and the question of how their unique properties evolve are still far from being fully developed and understood. The key step of integration of LDNs into functional devices is the engineering of the electrical contact. To achieve low-resistance ohmic contacts with LDNs, e.g. carbon nanotubes (CNT), and thus further advance their integration in new nano-devices, investigation of the metal-CNT interaction focused on detailed understanding of the physics and chemistry of this interface, is essential.

1.2.2.1 Relation to SusChem IAP

This topic is an extension of the key activities defined in the "Information and Communication Technologies", and "Nanotechnology" IAP chapters. Key relevant activities are "Interface Engineering", "Development of analytical techniques" and "Computational material science".

1.2.2.2 FP7 Uptake of this topic

So far, the SusChem Focus Area Development of analytical techniques for materials research via computer modelling has not been sufficiently taken up by FP7 calls.

1.2.2.3 Gaps

A lack of knowledge of detailed understanding and control of the interface physics and chemistry of LDNs, enabling their effective integration into larger scale devices and manufacturing flows including:

- Lack of appropriate characterisation tools at this scale
- Limitations in both computing power and theoretical methods mean that calculations are now commonly performed on less realistic small test systems containing at most only a few hundred atoms (Quantum chemical calculations are typically order N^3, i.e. doubling the number of atoms in simulation increases the computing requirements by a factor of eight. This places a severe limit on the size of calculations possible).

1.2.2.4 R&D objectives

- Develop new **theoretical and experimental tools** capable of detailed analysis of LDNs' interface formation and characteristics
- Develop suitable experimental and theoretical test case LDNs in order to explore specific aspects of such interface behaviour e.g. **carbon nanotube metallic contacting**
- Transfer this new knowledge to development for **pilot production** and eventually industrial high volume manufacture

1.2.2.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects with an emphasis on satisfying the key R&D objectives listed above.

1.2.3
Theme: Energy managing nanomaterials & electronics
Topic: Charge transport at interfaces and interface engineering

To improve the performances of organic-based photonic devices (such as OLEDs and organic photovoltaic cells) the charge transport between organic (photoactive material) and inorganic (electrode) layers must be well understood and optimised. In this view, interface engineering (via self-assembled monolayers, specific surface physical treatments, and molecular design aimed to energy level tuning, etc) will deliver decisive know-how for the appropriate tailoring of organic-inorganic interfaces, with the organic material being carbon nanotubes (CNTs) or any other organic semiconductor/conductor (as for example conjugated polymers or molecules). One of the main points that still needs full elucidation is the rationale for the relations between the functionalisation type (particularly in the case of utilisation of SAMs (self-assembled monolayers), or wall-linked molecules for CNTs), assembly topology (i.e. standing vs. tilted, uniform vs. island-covered, etc.), and the effects of these treatments on the charge transport at energetic levels of the interface. The same investigation must be applied to the organic functionalisation of new emerging nanostructures based on semiconducting III-V, II-VI materials. These materials are still poorly characterised but have demonstrated great potential in organic optoelectronics.

1.2.3.1 Relation to SusChem IAP

This topic is an extension of the key activities defined in the "Information and Communication Technologies", and "Nanotechnology" IAP chapters. Key relevant activities are "Interface Engineering", "Development of analytical techniques" and "Computational material science".

1.2.3.2 FP7 Uptake of this topic

So far, the SusChem Focus Area Development of analytical techniques for materials research via computer modelling was not taken up sufficiently by FP7 calls.

1.2.3.3 Gaps

A lack of knowledge for detailed understanding and control of charge transfer at interfaces, enabling effective integration into larger scale devices and manufacturing flows:

- Lack of appropriate characterisation tools at this scale able to probe the single device (e.g. nanosensors) at working conditions. Gas induced mass transport of the ad-layers are for instance important phenomena that can change completely the properties of the interface. It is therefore important to develop spatially resolved (at the nanoscale), chemically and surface sensitive tools for characterisation.

1.2.3.4 R&D objectives

- Develop state-of-the-art tools **integrating spatial resolution** and **chemical sensitivity** to overcome material and working condition gaps
- Application to development of **organic/inorganic interface systems** with improved **charge transfer** properties

1.2.3.5 Recommendation

Address this topic with several research oriented calls for small/medium scale projects with an emphasis on satisfying the key R&D objectives listed above.

1.2.4
Theme: Lightweight and functional materials
Topic: High-performance light-weight composites

Over the near future, the European aircraft industry demands a weight reduction in airplane structure of 30% and cost savings in the manufacturing process of 40%. These goals can only be reached by the development of novel high-performance composites, manufactured by liquid composite moulding (LCM) techniques (such as RTM, DP-RTM, SLI) instead of the presently used pre-preg technique. The application of these resin injection techniques for advanced composite manufacturing is particularly appropriate for complex structures and such structures are not limited to modern airplane production and use. However, the application of LCM techniques to carbon fibre-reinforced polymer (CFRP) frames is presently obstructed by the following drawbacks which have to be overcome:

- Matrix shrinkage, which deteriorates the dimensional stability of frames ("spring-in effect")
- A lack of electrical conductivity (no lightning protection)

It is anticipated that the doping of the neat resin with suitable nanostructured particles can be used for effective shrinkage reduction. In addition, a combination of such matrix doping and a tailored fibre coating should be developed in order to achieve an improved electrical conductivity and antistatic properties. Lastly, the combination of classical fibre-reinforced composites with nanostructured materials is expected to result in a generally enhanced material performance level, especially with regard to safety-critical properties such as crack resistance, impact behaviour and damping properties.

1.2.4.1 Relation to SusChem IAP

This topic is an extension of the key activity "Transport – Sustainable materials management". The original key activity and its extension comprise key technology developments for sustainable chemical manufacturing.

1.2.4.2 FP7 Uptake of this topic

Novel light-weight high-performance composites were addressed in the call for Large-scale Integrating Collaborative Projects NMP-2009-2.5-1 "Light high-performance composites". While this call addressed radical advances in composite materials, it is necessary to overcome the technological hurdles described above which were not sufficiently covered in this call.

1.2.4.3 Gaps

Although promising initial data regarding the use of nanostructured particles in composites are provided in the scientific literature, significant efforts to extend the scientific knowledge addressing the effect of nanotechnology in the field of composites should be realised. Functional relationships between the particle parameters such as size, functionalisation or volume fraction and relevant composite properties, including shrinkage, mechanics or conductivity, must be developed prior to their adoption in safety-critical applications. In addition, process simulation should be enhanced with respect to reaction kinetics and curing behaviour in order to enhance the applicability of such materials for modern processing techniques. Last, but not least, multi-scale modelling of the cured materials is as yet a missing factor.

1.2.4.4 R&D objectives

In detail, the following objectives should be addressed:

- **Development of novel tailored nanoparticles by highly-efficient design and manufacturing** in order to substantially enhance - **at low content levels (≤ 5%) - the mechanical performance of the matrix (reduced resin shrinkage; improved impact resistance)** in comparison to state-of-the-art resins
- **Generation of new light-weight fibre-reinforced nanocomposites** to be used with different resin injection techniques characterised by a higher mechanical performance in comparison to state of the art CFRP from LCM techniques **(matrix shrinkage: minus 50%; impact resistance: CAI (compression after impact) plus 20%)**
- **Improved dimensional stability of complex shaped structures** from composite moulding processes
- Establishment of an **evaluation standard for the spring-in effect**
- **Significant reduction of structure weight** by enhanced material usage, reduced safety factors and/or a lower matrix density in comparison to conventional, equivalent CFRP components
- **Enhancement of electrical conductivity up to 10^5 S/m** (from 10^4 S/m) for carbon fibre-reinforced composite structures
- **Establishment of design rules for fibre-reinforced nanocomposites** considering the particle surface functionality, particle volume fraction, and targeted composite shrinkage and electrical conductivity
- **Development of standard methods** for characterisation of the material's performance, particularly with respect to composition/make-up and its effects
- **Multiscale understanding** of the materials performance and its application to process design
- **Development of new/customised equipment types**

1.2.4.5 Recommendation

Address this topic with a research-oriented call for small/medium scale projects or a large call including demonstration activities for intensified product engineering addressing the challenges of the topic.

1.2.5.
Theme: Lightweight and functional materials
Topic: Nanoporous hybrid materials

Nanoporous materials are of interest with respect to catalysis, separation and purification, as well as chemical and biological sensing and optical communications. They are usually made by hydrothermal methods, which are not well understood yet. The understanding of the synthesis mechanism is essential for controlling pore architecture at the nanometre scale. The new type of nanoporous hybrid materials, covering organic-inorganic frameworks like MOFs, COFs or ZIFs, have led to a number of conceptual developments with respect to tailoring these materials as efficient catalysts and sorbents for the production of chemicals and fuels as well as components for electronics and photonics, through application of environmentally friendly and energy saving procedures.

1.2.5.1 Relation to SusChem IAP

This topic is part of the activity "Materials: Nanostructured polymers, hybrid and mesoporous hybrid materials" in the IAP chapter "Nanotechnology".

1.2.5.2 FP7 Uptake of this topic

"Organic-inorganic hybrids for electronics and photonics" is addressed in the "Cooperation Work Program 2010 – NMP" with the call identifier NMP-FP7-2010-2.2-1. Inorganic-Organic Hybrid Materials for sorption and catalysis were subject of the call NMP-2008-2.4-1.

1.2.5.3 Gaps

- Current technologies for the preparation of catalysts and adsorbents are mainly based on single-step conversions, however, the real needs are targeted in the direction of multi-step conversions and region-selective processes.
- Understanding of the synthesis mechanism of nanoporous hybrid materials
- Intelligent use of the tremendous number of available functionalised organic linkers

1.2.5.4 R&D objectives

- Development of innovative promising **organic-inorganic hybrid** materials with advanced properties for use as components for **electronics and photonics**
- Development of **synthesis mechanisms** for the hierarchically-structured organic-inorganic hybrid materials
- Development of **process technologies** for low-cost syntheses
- Investigate the functionality of **nano-engineered structures** of organic-inorganic hybrid materials

1.2.5.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects.

1.2.6
Theme: Design and safeguarding of bio-nano-interactions
Topic: Triggered drug delivery

The interaction of nanomaterials with biological matter is a Janus-headed topic: one research community seeks to exploit the designed properties of engineered nanomaterials for diagnostic and therapeutic purposes, while on the other side we have to quantify the hazard potential of unintentional interactions by nanomaterials in human contact or released into the environment. Both aspects synergistically share the need to understand bio-to-nano-interactions on a molecular level.

The controlled biokinetics of nanocontainers involves uptake and accumulation in the human body, and enables enhanced medical imaging and smart sensors and, in a further step, drug delivery by triggered release of actives behind compartmental barriers that are impenetrable to the active substance without the particulate carrier (container).

Traditional drug screening tests have been developed for molecularly dissolved drugs, and need to be modernised for formulated and/or encapsulated systems.

1.2.6.1 Relation to SusChem IAP

This topic extends the key activity "Materials development for drug delivery" in IAP chapter "Health". Today, the aspect of triggered release is perceived as essential, and the impact on pharmaceutical formulations is broad due to the proposed platform concept.

1.2.6.2 FP7 Uptake of this topic

Research outcomes and concepts can be used, but must be combined and refined from projects that answered the earlier calls HEALTH-2007-1.2-3, HEALTH-2007-1.2.4-1 and NMP-2007-4.0-4.

1.2.6.3 Gaps

- Assays and test methods for bioavailability from nanostructured formulations are not available.
- Release due to a specific trigger (other than pH and T, and pro-drug conjugates) is in general not available, but some examples such as insulin release due to local glucose concentration have been demonstrated.

1.2.6.4 R&D objectives

- Develop a **nanocontainer concept**, which can serve as a platform for drug formulation (encapsulation) and/or multiple surface coatings to be exposed successively in different biological environments in order to combine **multiple functionalities**: cross compartmental barriers, localise in specific body compartments, **triggered release** of actives; demonstrate an enhanced response per dose after barrier passage, reduce side effects.
- Develop **abiotic test methods for bioavailability** that are adequate for container systems.
- Develop **high-throughput cell-based screening assays** for bioavailability that are adequate for container systems.

1.2.6.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects.

1.2.7
Theme: Design and safeguarding of bio-nano-interactions
Topic: Nanostructured membranes: materials, processes and upscaling

Nanostructured membrane materials have a great potential to separate nanomaterials both from wastewater and from other liquids containing nanomaterials. Other possible applications are separation of noble metals from highly diluted streams, isolation of (bio)nanomaterials in production processes, and purification of liquid streams from (bio)nanomaterials like bacteria or viruses. Further research is needed to fully understand the parameters for controlling the performance of porous materials at the nanoscale. New organic as well as inorganic materials are necessary that reach high fluxes and high selectivity combined with long term durability. Robust and powerful characterisation methods are required to test the performance 'post mortem' as well as under real process conditions. The tailor-made design of new (co)polymer materials, as well as inorganic materials, will help to adjust the porosity and other relevant properties. This field is fast developing and has recently shown promising results. However further efforts and new concepts are necessary to enhance performance in order to make the materials applicable for industrial environments.

While small amounts of tailored materials with appropriate nanoporosity are already available it is essential for the technology of nanostructured membranes that i) robust processes based on nanostructured membranes are developed and ii) processing and scaling up of the nanoporous materials themselves is addressed. Further research is needed to transfer laboratory results on promising new materials to processes.

1.2.7.1 Relation to SusChem IAP

This topic is an extension of the key activity "Nanotechnology – Materials and Novel production technologies" and also "Sustainable product and process design". The original key activity and its extension comprise key materials and technology developments for sustainable chemical manufacturing.

1.2.7.2 FP7 Uptake of this topic

Nanostructured membranes were addressed by the calls "NMP-2008-2.1.1 Nanostructured membrane materials" and "NMP-2008-2.1.2 Processing and Upscaling of nanostructured materials". In the first call radical new approaches were addressed while in the second call the processes were the focus. A holistic approach should overcome the gap between fundamental research and industrial applications.

1.2.7.3 Gaps

There is still a lack of high flux and high selectivity materials in both organophilic as well as aqueous nanofiltration applications. Even worse the processes suffer from stability and long term durability issues which are serious hurdles for their exploitation. Further research is required to design high performance nanoporous materials with respect to the specific requirements.

1.2.7.4 R&D objectives

In detail, the following objectives should be addressed:

- **Development of novel tailored nanostructured membrane materials** with high fluxes and high selectivity and enhanced stability, of both organic and inorganic nature
- **New stable nanostructured membrane materials for aqueous and organophilic nanofiltration**
- **Development of enhanced polymers with intrinsic microporosity (PIM)** with long term durability for organic solvent nanofiltration (OSN) on the most suitable supports
- **Development of processes for processing and upscaling** of nanostructured membrane materials
- **Demonstration of membrane modules** with new and enhanced materials in relevant industrial processes

1.2.7.4 Recommendation

Address this topic with a research-oriented call for small/medium scale projects including demonstration activities for process engineering addressing the challenges of the topic.

1.2.8
Theme: Design and safeguarding of bio-nano interactions
Topic: EHS aspects of nanocomposite materials

Products that contain nanostructured materials continue to penetrate consumer markets. Those nanostructured materials that come into consumer contact are to a great extent nano-composites with internal nanostructures. Such internal structures are generated a) by the compounding of nano-objects (particles, platelets, fibres) in continuous matrix materials, e.g. in coatings and light-weight materials, or b) spontaneously due to the synthesis process, e.g. in concrete or phase-separating plastics. Previous research on nano-objects (especially particles) has established that a general nano-hazard does not exist, although some materials do show a higher toxic potential when dispersed on the nano-scale, especially when dust atmospheres of nano-objects become inhaled. Nano-objects tend to be much more relevant to production worker safety than for product safety.

1.2.8.1 Relation to SusChem IAP

SusChem has always advocated that the development of novel materials must be accompanied by an appropriate risk assessment (IAP topics p. 87-88; SRA horizontal issues p. 97-98).

1.2.8.2 FP7 Uptake of this topic

There has been a yearly 'open window' on safety aspects of nanomaterials in FP7 with calls in NMP, KBBE, ENV and HEALTH.[1] Strong priority has been given to studies on nano-objects (engineered nano-particles, not nanocomposites) and to hazard studies (not to exposure, except aerosol measurement techniques). Following the call NMP-2008-1.3-1 no project was successfully commissioned. The OECD's Working Party on Manufactured Nanomaterials (WPMN) includes nanocomposites in its work on Exposure Assessment and Mitigation.

1.2.8.3 Gaps

- Release and Exposure: little is known about the degradation mechanisms and potential degradation products from nanocomposite materials due to weathering, recycling (shredder), combustion and landfill disposal. Anecdotal evidence exists on abrasion on a limited range of materials.
- Hazard: Validated methods to quantify hazard are not complete. In-vitro methods do not yet converge with in-vivo methods. A generally accepted testing strategy may be developed from OECD guidelines.

1.2.8.4 R&D objectives

- Release and Exposure: **quantify released substances** from different classes of nanocomposites by **different degradation mechanisms**
- Exposure: **life-cycle analysis** of different classes of nanocomposites, including possible **bioaccumulation**
- Hazard: **compare physiological effects** of degradation products with the effects of the materials before compounding
- Hazard: develop a **testing strategy that is compatible with REACH**, including nanocomposite materials (change of hazard potential by formulation and compounding)

1.2.8.5 Recommendation

Address the hazard aspect of ecotoxicology and human toxicology separately in research-oriented large scale projects in order to include a broad methodical portfolio; collaborate on the testing strategy with regulatory bodies on the European or national level. Address the exposure aspect with small scale projects (with industrial leadership) that focus on nanocomposites and their life cycle, but ensure methodical comparability.

[1] Relevant are NMP-2008-1.3-1 and -2; NMP-2007-1.1-1; NMP-2007-1.2-2; NMP-2007-1.3-1; KBBE-2007-2-5-03; KBBE-2007-2-4-02; ENV.2007.3.3.1.1; HEALTH-2007-1.3-3.

1.2.9

Theme: Corrosion

Topic: Low cost production of complex corrosion resistant coatings in ionic liquids for high temperature applications

Significant progress has been achieved in developing chemical processes based on the use of ionic liquids (such as filtration, extraction etc.). For several industrial applications at high temperatures, e.g. energy conversion, increases in overall performance can only be achieved by increasing the in-service temperature, but at the same time coatings are needed to protect the materials at these elevated temperatures. The production of complex coatings with specific properties at lower temperatures, i.e. in ionic liquids, is considered to be a major breakthrough as the substrate material properties are maintained while at the same time offering a wide range of metal combinations, and finally the production costs may be considerably decreased. This proposal aims at broadening the use of ionic liquids in the field of high temperature corrosion protection. Production of complex coatings including reactive elements at low temperatures represents a challenge and a significant step forward for the surface modifications of materials in harsh environments.

The use of ionic liquids, which exhibit a low vapour pressure, would reduce the common hazard and exposure issues encountered with classical volatile solvents. This represents some significant advantages for the engineering costs of a global process.

In addition, technological developments obtained in the course of this proposal will be beneficial for other applications using electrodeposition techniques, i.e. thermoelectric materials, photovoltaics etc.

1.2.9.1 Relation to SusChem IAP

The subject "Coatings" is covered in various chapters of the IAP such as "The home as an eco-efficient environment".

1.2.9.2 FP7 Uptake of this subject

This topic was marginally addressed in call NMP-2007-2.1-2.

1.2.9.3 Gaps

Considering the electrodeposition of classical metals (Al, Cr) together with reactive metals (Y, Hf) for the production of corrosion resistant coatings, there is a considerable lack of knowledge in optimising the electrolysis process. This is especially true for co-deposition processes or the electrodeposition of complex coatings with gradient-type properties or with well defined microstructures to enhance selected surface or catalytic properties.

In addition, most of the processes currently developed must be conducted under inert atmospheres because of either the sensitivity of the ionic liquid to moisture or the use of metal chlorides as the metal source. A considerable step forward would be achieved with the development of an open electrolysis process insensitive to environmental conditions.

1.2.9.4 R&D objectives

- The research will remarkably strengthen the **dual approach of modelling and experimentation** to gain valuable data on the physico-chemical properties of ionic liquids to produce the required complex coatings.
- The selection of the ionic liquids for use should consider the following points i) **environmental** (minimisation of organic solvents to produce the ionic liquids) ii) **economic** (evaluation of the process costs) and iii) **scientific and technical** (hydrophobic, viscosity, melting point).
- The second key point deals with the electrolysis process itself. The work will be focussed on the design of cells to produce **adherent and protective coatings on complex geometries** (e.g. turbines blades).
- One of the key issues to overcome is the development of a **continuous process for the metal supply** (soluble anode, metal dissolution).
- The investigations will provide new complex coatings with specific properties which will be tested under **oxidising or aggressive environments** simulating **industrial** processes.
- Finally, special attention will be paid to the **reprocessing** of the electrolysis melt and the safety issues (hazard and exposure) linked to the use of ionic liquids. This approach will lead to a **prototype** process at a significant industrial scale.

1.2.9.5 Recommendation

This subject should be addressed by a research oriented call for small/medium scale projects. This will improve the technology transfer from universities and research centres to industry, active participation by industrial partners will reflect the relevance and impact of the research effort. The participation of ionic liquids producers, manufacturers and end-users in plants represents an added value for the proposed activities.

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