SusChem

European Technology Platform For SUSTAINABLE CHEMISTRY

SusChem IAP Update 2010

Materials Technology

Foreword

The first SusChem Implementation Action Plan was published in 2006 with the purpose of describing how the research priorities identified by SusChem in its Strategic Research agenda (SRA) could be implemented in trans-national and other research programmes across Europe.

Many of the project topics described in the 2006 IAP were subsequently incorporated, in part or as a whole, in one or more of the calls in the European Commission's Seventh Framework Programme for Research and Development (FP7) or in other trans-national and national research programmes.

However, research and technology do not stand still and in a highly competitive world it is important that economically and socially significant gaps in current research are swiftly identified and responded to.

This 2010 IAP Update is the result of discussion and debate within the three SusChem Technology Working Groups: Industrial Biotechnology; Material Technology; and Reaction & Process Design. The topics selected in this document will feed into and enrich relevant research and innovation programme formulation discussions across Europe including future FP7 calls.

SusChem has now introduced an annual process for updating the IAP to ensure the relevance and timeliness of European sustainable chemistry stakeholders' input to the formulation of future European research programmes.

To achieve a sustainable future requires sustainable technologies that are welcomed by society. SusChem invites contributions from all interested parties and is open to engagement with all sections of civil society to help build a truly sustainable future for all.

To learn more about SusChem activities contact us at suschem@suschem.org

www.suschem.org

Materials Technology IAP Update

Introduction

This SusChem Materials Technology Implementation Action Plan (IAP) update 2010 has been written from scratch, proposes novel topics, and implements the original vision and strategy of SusChem in today's world.

The SusChem Materials Technology Group, chaired by Prof. Rüdiger Iden of BASF consists of European experts in topics related to the design, preparation, analysis, and application of new materials and nanomaterials in functional systems or devices. Since 2009 new members of the group have broadened the foundations of the group in the chemical sector, and have taken responsibility for specific end-user sectors.

Following the finalization of the SusChem Strategic Research Agenda (SRA) in 2005 and the IAP in 2006, the group has been reviewing and assessing the take-up of Materials Technology topics in FP7 work programmes. Based on this analysis, the group has continued to recommend strategic goals as well as specific topics for future calls. Starting with the IAP update of 2009 a continuous process of yearly updates has been initiated which allows current societal, scientific and economical challenges to be taken into account.

The Materials Technology Group has gathered proposals from its academic and industrial partners followed by extended discussions to prioritize and select topics for this current update. Compared to the 2009 update, the selected topics in the 2010 update follow a more specific approach. To coincide better with the timing of the drafting process of the FP7 work programmes, an earlier publication date for the update has been decided. Being finalized by end of January 2010 allows both the IAP updates of 2009 and 2010 to be considered in the drafting process of the FP7 Work Program for 2011.

As with the 2009 IAP update, topics in this update have been grouped in four clusters to directly address some global societal challenges. This cluster approach will be continued over future years to organize specific topics. The scope of the clusters will be refined to match changing global societal challenges. Currently the four clusters are:

Energy managing nanomaterial and electronics

- ➔ Organic photovoltaic modules;
- ➔ Efficient lighting: New materials with improved properties for OLED lighting;
- ➔ Energy storage: Li-Ion batteries with improved safety and performance.

Energy efficiency

- ➔ Lightweight thermoplastic composites for easy assembling of structural elements;
- ➔ Heavy duty tires for better fuel efficiency.

Environment, health, and bionano

- ➔ Materials-based sustainable life-cycle of drugs;
- ➔ Catalysts for clean air – designed materials for NOx-reduction.

Smart and resistant materials

- ➔ Smart coatings for robust building exterior.

In line with the above process, the scope of the fourth cluster has been extended from the original theme “Corrosion“. This allows for a more general approach to materials with improved properties that are useful to society. Some of the proposed topics are very tough scientific challenges and will require extensive cooperation between the most experienced academic and industrial labs, including specialized research infrastructure for nanoscale characterization.

In addition, several topics have been proposed and selected for the current update in the context of the new Public Private Partnerships “Green Cars“ and “Energy Efficient Buildings“. The latter is especially welcomed as a natural extension of SusChem’s visionary project The Smart Energy Home (SEH).

The proposals elaborated in this IAP update 2010 concentrate on topics with high urgency and a low level of current funding. In order to keep the document focused, some promising themes that merit funding have been omitted. Examples are thermoelectric materials in the field of energy management and super capacitors as a mean for high volume, short-term storage and release of electric energy. These and other topics will be looked at in future updates.

As proposed earlier, life-cycle analyses as well as environment, health and safety (EHS) aspects should be continued to be included proactively in nanomaterial research. This will help to generate the knowledge and data needed to ensure early awareness and identification of problematic areas in nanotechnology. This will also allow the development of nanotechnology in a sustainable way and enable effective communication on this topic with the general public. There can be little doubt that general acceptance by the public will be decisive for the further success and commercial implementation of nanotechnology.

Recommendations for IAP update and future FP7 calls

1 Theme: Energy managing nanomaterials and electronics

Topic: Organic Photovoltaic Modules

Organic solar cells (also known as bulk heterojunction or 3rd generation) offer the potential to lower the cost of photovoltaic (PV) cells through raw material and process economies. However their structures are radically different from the planar solar cells in production today. A bulk-distributed interface is needed for to achieve adequate efficiency. Both organic-inorganic hybrid structures, such as dye-sensitized solar cells (DSSC), and 'pure-play-organic' (OPV) approaches need an increase of efficiency and of stability, and the development of an appropriate manufacturing technology.

The efficiency of this technology must be raised to 10% at industrial scale production by 2015, if they are to realize their long term potential. The increase in the performance of organic solar cells requires improved basic understanding of the device physics, the synthesis of novel materials and the development of advanced cell concepts (multi-junction or special interfacial morphology).

Breakthroughs are needed in improvement of stability, in particular the intrinsic stability of the organic materials used in the active layer, the cells' nanomorphology and the contact between metal conductors and organic semiconductors.

Work in these three areas and progress in the field of low-cost encapsulation techniques (also needed for organic LEDs and organic electronic circuits) should result in modules with a stability of at least 15 years.

1.1 Relation to SusChem IAP

This topic is an extension of the key activities defined in the "Nanotechnology" IAP chapters. Key relevant activities are "Interface Engineering" and "Development of analytical techniques". Europe is well placed to remain at the cutting edge of R&D and production of organic solar cells because of its strong position in the related field of organic electronics and manufacturing machinery.

1.2 FP7 Uptake of this topic

Development of organic PV materials was already addressed in call ICT-2009-3.3 *"Flexible, organic, large area electronics"*. ENERGY-2007-2.1 contained a specific call for DSSC resulting in the project *"ROBUSTDSC"*. No large projects are running in the field of pure OPV. Some projects of broader scope may address indirectly the needs of organic PV.

1.3 Gaps

The following gaps were identified:

- Understanding of the degradation mechanisms;
- Transparent flexible ultrabarriers to oxygen and moisture;
- Transparent flexible conductive electrodes;
- OPV efficiencies are still insufficient for commercial exploitation;
- Large area high speed deposition processes.

1.4 R&D objectives

- Printing technology for contacting and current-generating layers and the electronic circuitry for an integrated printing process;
- Materials and process for flexible transparent ultrabarrier to oxygen and water at large scale;
- More transparent, less resistive, more cost effective, large scale electrode layers;
- Understanding of degradation mechanisms;
- Organic-inorganic (metal) and organic (donor)-organic (acceptor) interface characterization, from the electronic point of view; more effective charge transfer across border layers;
- Materials and processes for controllable and more stable nanostructure;
- Process for homogeneous fast large area deposition.

1.5 Recommendation

Small or medium-scale focused research projects focusing on some of the above R&D objectives.

2 Theme: Energy managing nanomaterials and electronics

Topic: Efficient lighting: New Materials with improved properties for OLED-Lighting

Solid-state light (SSL) sources, like organic light-emitting diodes (OLEDs), may in the future outperform almost all other light sources in terms of efficiency and thus provide a saving potential of about 50% in terms of electrical energy[1]. Therefore efficient lighting is one of the quickest ways to energy and CO_2 reduction, and also represents huge cost savings.

The lighting market today demands higher energy efficiency and longer lifetime. SSL is a perfect answer to these requirements, since it offers the potential for the highest efficiency light source in the future.

OLEDs for lighting consist of a multilayered stack of different organic and inorganic materials. Improved materials with tailored electronic, optical and chemical properties are the key success factor for efficiency and increased lifetime of an OLED-device. For a breakthrough in OLED lighting, massive investments in research and development are required.

In addition, OLEDs have strong synergetic effects with many other organic electronic domains with several technologies based on similar materials and processes. OLED lighting materials and encapsulation solutions can be shared with technologies such as the display screens and OPV. Even if the materials itself may not be able to be shared, development results can definitely provide benefits. In particular, OLEDs and OPV have very similar requirements concerning their fundamental technology. For instance, the methods and processes of R2R (roll-to-roll) processing for OLED and OPV by printing show substantial overlap. The development of materials for R2R processing will help to speed up development overall.

2.1 Relation to SusChem IAP

This topic is an extension of the key activity “efficient lighting” in the IAP chapter “energy conversion / efficient lighting” – identification of suitable materials and composites with increased lifetime and efficiency. Furthermore the topic has a strong relation to the SRA of the new OLAE-stakeholder platform (Organic and Large Area Electronics), recently proposed to the European Commission.

2.2 FP7 Uptake of this topic

This topic was addressed in a call NMP-2007-2.2-1: *“Organic materials for electronics and photonics”*, but the call offered a relatively broad spectrum to all major application areas of organic electronics. Approximately, already 46 M€ have been devoted on research on OLEDs for lighting. Due to the high impact of OLED lighting on innovation, for example the expected quick wins for energy efficiency, a new call should be focus on improved materials for OLED-lighting.

---

[1] Ad Hoc Advisory Group ICT for Energy, Consultation Group lighting & Photonics Technologies (2008)

2.3 Gaps

Despite of the progress achieved in several EU-projects (FP6 and FP7, ICT programme), a lot of challenges in material research remain to be solved. Attention should be given to:

- Maximize the external quantum efficiency, reliability and lifetime of OLEDs at higher brightness levels;
- Cost-effective and reliable encapsulation enabling longer shelf life should be developed;
- The development of flexible, conformable, large area devices, including suitable breakthrough materials such as highly efficient (blue) emitter, charge transport, injection materials, substrates, barrier layers, electrode materials are needed;
- Materials special suited for high speed solution processing, or materials optimized for high temperature vapour phase deposition, with the reasoning of shortening throughput times are required;
- Attention should also be given to cost effective alternatives for (printable) Indium Tin Oxide (ITO) and other transparent electrode materials.

2.4 R&D objectives

- Projects should cover an integral and holistic research / development plan because of the different material properties and limitations. Therefore projects should consider in an adjusted approach a set of different materials rather than an isolated strategy;
- What is needed: Highly efficient emitter materials and materials for charge transport, injection and barrier layers. Understanding of the charge transfer mechanisms at the interfaces by advanced nanoscale characterization. Alternatives for (printable) ITO and transparent electrode materials. Encapsulation materials enabling high shelf-life;
- Critical performance indicators of the materials for OLEDs: Efficiency >100 lm/W, brightness levels >5000 cd/m^2, lifetime / shelf life >10years, high quality white >90 CRI, flexible. Compatibility with low cost and high throughput production processes such as printing, lamination, vacuum deposition or combinations thereof.

2.5 Recommendation

Address this topic with a research / development oriented call for small / medium or large cooperative projects, covering the above mentioned R&D objectives including application oriented aspects. The challenge of this topic needs an appropriate participation from industry.

3 Theme: Energy managing nanomaterials and electronics

Topic: Energy storage: Li-Ion batteries

Due to their superior performance with respect to energy density and cycle life compared to other battery systems, Li-Ion batteries have received great attention over the past decades. However, the present electrochemical systems are insufficient with respect to performance and costs for supporting the most important new market sector: electromobility (e.g. battery electric vehicles or hybrid electrical vehicles). Still higher performance and increased safety at lower costs are required together with more environmentally acceptable materials.

These limitations can be overcome only by major advances in new materials that have to be available in large quantities at low costs. Nanotechnology appears to have a key role to play in this context. New nanostructured materials, combined manufacturing approaches, and the development of new (or revisited) electrochemical systems are the main sources for breakthroughs in this field.

3.1 Relation to SusChem IAP

This proposal is an extension of the original IAP topic on energy storage (pg. 41-42) and complements the IAP update 2009, chapter 3.2.2.

3.2 FP7 Uptake of this topic

This topic is crucial for the sustainable development of transport, through applications in electric vehicles. Despite of this, the number of granted projects related to battery developments is low.

3.3 Gaps

The following gaps have been identified:

- ➔ There is still a strong need for high performing electrode materials with high energy density, high cycle life, high calendar life, tolerance to low and high temperatures that consist of easily available and low cost, environmentally benign raw materials, which are easy to process, and which can be recycled;
- ➔ Low cost materials (e.g. based on Mn for cathodes) do not yet provide the required performance for energy density, cycle life and longevity to be useful for electromobility applications;
- ➔ High performing anode materials which are not based on Graphite (e.g. Si) have not progressed from laboratory trial status yet;
- ➔ Green production: Alternatives to Co, Ni based cathodes and further enhanced separators. Solvent-free electrode manufacturing and adequate recycling processes;
- ➔ Cathode materials based on Fe do not provide the required energy density and are difficult to process resulting in production costs that are not competitive;
- ➔ The potentially highest performing battery systems will be based on metal/oxygen chemistry (e.g. Li/ air) but these promising systems are still in an early stage regarding stability and safety.

3.4 R&D objectives

- Improve performance of existing chemical systems especially of low costs materials (e.g. by using nano-scale materials). Increase energy/power density and stability e.g. by new nanocomposite active materials and new electrolytes. Understand structural and electronic behaviour of nanocomposites under actual working conditions;
- Reduce production and processing costs for active battery materials, replace rare and costly elements;
- Green production with active materials based on water-soluble binders, new separators. Concepts for recycling processes;
- Improve temperature tolerance of cells (performance at low and high temperatures);
- Develop high-voltage systems to increase energy density. This would also need high-voltage tolerant electrolyte systems;
- Long-term: Develop stable and safe metal/oxygen systems.

3.5 Recommendation

Small and large projects are appropriate for these topics; joint call NMP / Transport in close collaboration with the Green Cars PPP initiative.

4 Theme: Energy efficiency

Topic: Lightweight thermoplastic composites for easy assembling of structural elements

The replacement of structural metallic elements with lightweight composite materials is an important potential driver to generate consistent weight reduction when applied to road vehicles and aircraft. As a consequence, significant advantages in fuel consumption and compliance to future requirements on air emissions are possible.

The use of fibre reinforced, semi-crystalline thermoplastic structural composites shows clear potential advantages versus thermosets. These include high mechanical strength, absence of monomers and solvents, ease of processing, life cycle assessment and recyclability at end of life.

To meet targets, specific knowledge has to be developed concerning:

a) The design of materials and parts to reach relevant targets and safety requirements as replacements for metals;
b) The development of predictive modelling tools to simulate and optimize the resistance of parts in conditions of stress (crash, fatigue, temperature endurance etc.);
c) The development of innovative, industrially scalable techniques to directly join and assemble multimaterials, such as polymer composites with themselves and with metals. This includes surface activation treatments and interface compatibilization.

4.1 Relation to SusChem IAP

This topic modernizes and specifies in more detail the theme of the original IAP 2006 "*Alternative body assembly technology: gluing versus welding & reversible assembly*". In the IAP update of 2009, topic 1.2.4 "*High-performance light-weight composites*" was specific to nanofilled thermoset composites and addressed clearly distinct market requirements for aircraft applications.

4.2 FP7 Uptake of this topic

The proposals from the original IAP 2006 received no significant funding in FP7. Calls that are related to the present topic include ENERGY.2007.2.3.1 "*Development of components and systems for turbines and wind farms*" and NMP-2008-2.5-1 "*Functionally graded materials*". The present proposal will benefit from methods developed in projects funded by NMP-2007-2.5-2 "*Modelling of microstructural evolution under work conditions and in material processing*". However, none of the earlier calls addresses the specific needs of the present topic.

4.3 Gaps

The following gaps have been identified:

- Simulation of mechanical behaviour of thermoplastic composites: significant progress is required in the development of reliable models and simulation tools to predict the behaviour of composites based on semi-crystalline thermoplastic polymers at the micromechanics level. This is particularly urgent for models for both endurance (fatigue, creep, temperature) and crash behaviour;
- Joining technologies: present technologies are not sufficient to guarantee long term adhesion on hybrid materials (thermoplastic polymers / polymer reinforcements / metals) and for compliance with mechanical requirements of structural parts. In addition, the management of interfaces (including polymers / reinforcing agents) is not sufficiently mastered or modelled.

4.4 R&D objectives

- Develop new technologies suitable for the production and transformation of thermoplastic, semi-crystalline structural composites to replace metals in structural and safety parts of vehicles (e.g. shock absorbing chassis elements, seat frames). Provide solutions with the required advantages for the car industry regarding weight reduction and full compliance with functional and safety requirements of the parts;
- Develop new solutions for the assembly of such structural elements, through the use of joining and soldering technologies and surface activation, in order to assure maximum interfacial adhesion, time endurance and mechanical resistance to structural elements. To characterize and understand the behaviour of metal-polymer interfaces;
- Develop micromechanics simulation tools and models to predict the mechanical behaviour of structural parts on the basis of the material geometry and structure; acquire competencies to simulate both invasive test conditions (crash) and long term endurance behaviour (fatigue, creep);
- Provide sustainable solutions regarding life cycle assessment versus traditional technologies, particularly concerning eco-compatibility, recyclability at end of life, CO_2 balance, etc.;
- Weight reduction target would be 10 to 15% on a medium sized car. As a reference, 10% weight reduction would imply around 5% saving of fossil fuel, or an increase of 60 to 80 km in the range of an electric car.

4.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects or a call for large projects oriented to basic materials research including application-oriented testing addressing the challenges of the topic. A “large” projects call would offer the chance to establish a ‘European Task-force for Innovative Lightweight Vehicles’ with wide-scale cooperation involving the most experienced academic and industrial labs.

5 Theme: Energy efficiency

Topic: Heavy duty tyres for fuel efficiency

The Tyre Industry has to meet the growing demands of the transport sector in terms of energy efficiency and CO_2 emissions reduction. The EC Regulation No. 661/2009 which was signed on 13/07/2009 by Parliament and the European Council defines for all tyres the requirements in terms of maximum levels for rolling resistance and other key parameters (such as wet adhesion or noise). For truck tyres, this standard is scheduled from 2016 with a more restrictive threshold in 2020.

The use of highly dispersible silicas as reinforcing fillers of tyre treads is already an industrial solution in the market for Light Vehicle tyres: more than 50% of the tyres sold in Europe are "Green Tyres". The challenge is to transpose this silica-technology to the heavier weight transportation where natural rubber is the usual elastomer material.

5.1 Relation to SusChem IAP

This topic is an extension of the theme *"Ecoefficiency in transport"* of the original IAP from 2006.

5.2 FP7 Uptake of this topic

FP7 has not yet opened calls regarding green tyres, particularly for heavy duty vehicles. The proposal provides a concrete research objective coherent with the NMP work programme 2010, theme 4, in particular in *chapter II.5.3. "European Green Car",* which includes, as a major pillar, *"research for heavy duty vehicles",* including improvements in special tyres with low rolling resistance.

5.3 Gaps

The following gaps have been identified:

- ➔ In the state of the art, the tyre tread of the heavy weight transportation is constituted from carbon black filled natural rubber to avoid excessive heat build-up and to be resistant to frequent use. The classical highly dispersible silica / polysulfide silane combination, developed for light vehicles is not directly transposable to such elastomeric compositions, containing natural rubber;
- ➔ The main challenge to introducing silica is to fine-tune the interface between the silica and the natural rubber using new interfacial agents (specific silanes for instance) to improve the trade-off between reinforcement (wear resistance and long-term durability) and reduced energy dissipation (rolling resistance);
- ➔ An additional gap is to implement predictive modelling methodologies, allowing correlations between the microstructure (tyre composition and morphology) and tyre behaviour (e.g. rolling resistance).

5.4 R&D objectives

- Development of innovative silica-rubber materials with advanced properties for use as tyre tread components for the truck and other heavy weight transportation vehicles;
- Development of state-of-the-art micromechanics simulation tools to understand the relationship between the structure of these silica-rubber materials and their reinforcement and energy dissipative reduction properties;
- Quantification of the gap in truck tyre performance, focused on the reduction of rolling resistance with a challenging target of more than 15 % (which translates to a 5% reduction in fuel consumption) related to the market standard, keeping the same level of wear resistance and long-term durability;
- Use predictive simulation tools to correlate morphology, interface and mechanical behaviour of tyres through micromechanics computer modelling.

5.5 Recommendation

Address this topic with several research oriented calls for small/medium scale projects focused on the four R&D objectives, including cooperation with non-EU countries.

6 Theme: Environment, health, bio-nano

Topic: Materials-based sustainable life-cycle of drugs

The availability of innovative biotherapeutics at costs bearable by public healthcare systems constitutes a major societal need. Recovery of innovative high potency drugs from the synthesis process as well as the targeted delivery of the drug substance to the patient depend on the proper development and choice of suitable materials, which are typically nanostructured.

Integrated and intensified processes including optimized downstream processing and efficient delivery to patients, as well as effective wastewater management and regeneration will be key in reducing the downstream processing costs of new biotherapeutics. These are currently perceived as major cost drivers.

High potency drugs act in minute amounts and require special precautions in the research lab. Therefore, specifically tuned processing concepts including formulation and delivery steps are necessary. Equally important is the consideration of the "post-therapeutic" process, considering the physiological release of any non metabolized drug, and especially the disposal of unused therapeutics by patients or in hospitals into the wastewater system. Therefore, a direct link to the goals and concepts discussed in the WSSTP (Water Supply and Sanitation Technology Platform) is also required.

6.1 Relation to SusChem IAP

This is, in part, an extension of earlier segmented proposals, involving the combination of "materials" aspects with aspects of "reaction & process design", and tied to issues raised in the WSSTP 2011 IAP Update.

6.2 FP7 Uptake of this topic

This integrated approach towards biotherapeutic materials along their diagnostic and therapeutic R&D and life cycle has not been previously addressed in FP7 calls.

6.3 Gaps

An integrated consideration of materials aspects across the whole life cycle of novel biotherapeutics is required with regard to:

- ➔ New concepts driven by health care economic constraints;
- ➔ Stratified medicine approaches;
- ➔ High potency drugs;
- ➔ Access to and responsible use of the required water (in terms of both quantity and quality).

6.4 R&D objectives

- Design and manufacture of nanostructured materials and membranes with much higher selectivity than available today for efficient capture/retention of therapeutics from synthesis and removal of residual products from waste streams, tuned to the production processes and cleaning process technologies in which they will be employed;
- Development of suitable sensors to detect biotherapeutic materials in the sub-microgram region for drug delivery and/or water purification/decontamination systems. In case of porous materials, to address stability, tuneable metrics, organic and inorganic functionality with permanent and dynamic porosities regarding uptake and release of the compounds under investigation;
- Exploration of the interface of biological function with nanomaterials and establishment of structure-size-property relationships relevant for assessment of the therapeutic efficacy and the environmental control of such materials by, for example,.X-ray transmission spectromicroscopy or alternative appropriate techniques for the nano-bio-interactions;
- Develop model-based approaches to describe, optimize, and finally predict materials impact on therapeutic efficacy and the ecological impact.

6.5 Recommendation

The scope and relevance of this topic require large cooperative projects and a joint call between NMP and Environment is suggested. Links to the JTI-IMI should be set up.

7 **Theme: Environment, health, bio-nano**

Topic: Catalysts for clean air - Designed materials for NOx-reduction

The classical inductive, empirical process of catalyst discovery and optimization is costly and time consuming and typically involves many iterations of formulation design, optimization and testing. In contrast, the reduction of emissions from internal combustion engines follows very stringent rules in terms of legislation, costs and timeline to market. Moreover, due to the variety and complexity of these systems there is a need to investigate new approaches for the identification and validation of material sets for future catalyst technologies employed in emission control systems for mobile sources.

For this a fundamental catalyst development effort is required based on a combination of structure versus function relationship investigations together with *ab-initio* materials modelling. This approach includes modification of the nanostructure of the active catalyst, as well as the optimization of the support and of the catalytically active components. In order to validate the expected benefits, catalyst systems for the fuel lean conversion of Nitrogen Oxides (NO_x) should be investigated, as the reduction of NO_x is one of the most challenging aspects of emission control for modern fuel efficient, lean burn engines, in particular diesel engines.

Catalysts are key materials for many sustainable technologies enabling much higher energy efficiency and clean-up of exhaust emissions. The topic of catalysts for clean air will maintain a high impact/ profile in Europe and with European car manufacturers and the automotive supply industry in future as it will take several decades before a larger percentage of vehicles are fully electrically powered.

7.1 Relation to SusChem IAP

This topic is an extension of the IAP chapter transport, eco-efficiency performances, catalysts for CO_x, NO_x, SO_x decomposition.

7.2 FP7 Uptake of this topic

This topic has not been covered in prior FP7 calls. The calls *NMP-2007-2.4-2 “Nanostructured catalysts with tailor-made functional surfaces”* and *NMP-2010.2.4-1 “New materials and or membranes for catalytic reactors”* were focussed on chemical production processes and the call
SST.2008.1.1.1 “Clean and efficient power trains” were focussed on engineering aspects of power trains and exhaust cleaning systems and not on breakthrough improvements for catalysts for NO_x decomposition.

7.3 Gaps

The following gaps have been identified:

- Material science has, in the last ten years, started to provide the basis for the use of ab-initio calculations for material development. In recent years this method has increasingly been applied in industrial R&D centres as well as in academia. However, as of today, a comprehensive workflow for the application of modelling, data mining and validation in a catalyst application has not been developed;
- There is a need to improve in-situ characterisation techniques for catalysts under typical working conditions and to link these techniques with the calculations and modelling mentioned above.

7.4 R&D objectives

- Deeper understanding of catalytic mechanisms and materials by a computational approach combined with catalyst characterisation techniques;
- Development of analytical tools capable of analysis of catalysts under real working conditions;
- Design of new catalytic materials for NO_x reduction down to 50% of the EURO 6 target value;
- Synthesis of model catalytic materials;
- Laboratory testing of model catalysts;
- Full scale validation by end-users.

7.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects or a call for large projects ranging from basic materials research to application oriented testing and system integration to address the challenges of the topic. A "large" projects call would offer the chance to establish a 'European Task-force for $DeNO_x$ after-treatment' with wide-scale cooperation between the most experienced academic and industrial labs. For cooperation along the value chain a link with the Green Cars PPP should be established.

8 Theme: Smart and resistant materials

Topic: Smart coatings for robust building exterior

The exterior of a building has to fulfil a multitude of different functions. It has to protect the building's structure as well as the inhabitants from heat, cold, humidity, pollution, noise, and dust. At the same time the exterior façade could provide functionalities for the building, like energy gains or water collection.

Since the façade is an integral part of the building it must be considered by the static and the building procedures. Lightweight, multifunctional and highly energy efficient building skins could result in a multitude of energy gains during the building life-cycle, during construction, during operation and finally during demolition. Easy application and exchange in case of damage or redesign reduces building costs, while high insulation and sound absorption parameters produce a good living condition for inhabitants, and lightweight textile structures result in a significant reduction of building loads which increases construction speed and helps to reduce costs.

The materials of these membranes as well as their coating are of special interest to the chemical industry. The insulation properties must be achieved with ultra lightweight and high efficient new materials, such as aerogels or nanofoams. Switchable new materials could result in an energy gain during winter seasons due to solar radiation, and an insulating effect during summer seasons.

8.1 Relation to SusChem IAP

This topic is an extension of the themes sustainable quality of life: the home as an eco-efficient environment in the IAP, and of SusChem's visionary project on the Smart Energy Home (SEH).

8.2 FP7 Uptake of this topic

The topics of heat and energy storage were addressed in EeB.NMP-2010-2 *"New technologies for energy efficiency at district level"*. Switchable systems are part of call EeB – NMP – 2010 - 1 *"New nanotechnology…"*. Nanostructures for textile facades and membranes were part of topic 4 of the NMP call in FP7. However, a coherent systems approach is lacking. Projects that were actually funded in FP7 did not cover the overall system improvement approach.

8.3 Gaps

In terms of science and research in general the following gaps have been identified:

- ➔ Pigments with high UV absorption and a switch point where absorption gets reduced;
- ➔ Long-term stable textiles, sustainable in harsh environmental conditions;
- ➔ Switchable insulation and absorption behaviour of a façade. A new generation of absorbing and temperature controlled pigments could show the way to such a solution;
- ➔ Cyclic stable and cheap heat storing devices;
- ➔ Computer models that can predict performance within standard calculation software like Trnsys.

In terms of earlier calls:

- ➔ There is a need to not just concentrate on the improvement or development of a single material but rather to orientate efforts on the system performance.

8.4 R&D objectives

- ➔ New material combinations and innovative technologies for better system performance to address the gaps identified above.

8.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects or a call for large projects ranging from basic materials research to application oriented testing and system integration addressing the challenges of the topic. A link with the Energy efficient Buildings PPP should be established.