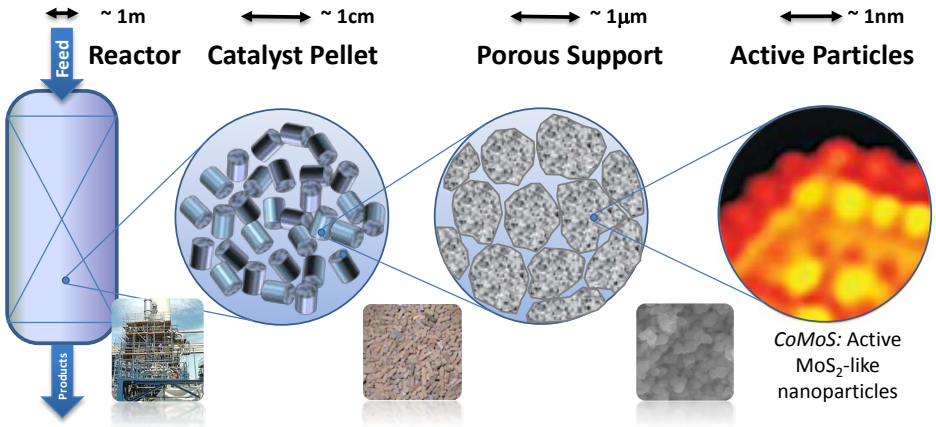
European Cluster on Catalysis

Strategy and Perspectives

March, 2015

Catalysis is a key technology for Europe

Catalysis is the most interdisciplinary and overarching technology in the chemical industry, because to perform a catalytic process requires controlling all the aspects over a multi-dimensional scale, from the molecular aspects of the reaction at the active site (nm scale) to the several meter scale of an industrial catalytic reactor (Scheme 1).



Scheme 1.

Furthermore, catalysis underpins several industrial strategic sectors (from energy to manufacture of materials and products), including its enabling role for environmental protection (from air/water industrial and municipal emissions, to the treatment of mobile emissions), recycling of waste and reduction of greenhouse gases (GHG). Catalysis represents thus a true key technology for European economy, industry, growth and sustainable future.

As a matter of fact, the production of 80% of the industrially relevant chemicals involves catalysis, and catalysis and catalytic processes account (directly and indirectly) for about 20-30% of world GDP.

Catalysis is of paramount importance in the chemical industry and discloses new routes to sustainable and environmentally friendly green chemistry and processes. As an example, of the 50 greatest volume commodities currently produced worldwide, 30 are produced via catalytic routes. Nevertheless, these 50 highest volume processes also account for more than 20 billion tons of carbon dioxide emitted to the atmosphere each year, an amount which could be reduced by innovative catalysis-based solutions. In this context, catalysis appears also as viable route to mitigate the environmental impact of commodities and chemicals production and processing.

In state-of-the-art and current literature, the term catalysis is typically closely associated and tightly intertwined with concepts such “green chemistry” and “sustainability”, since catalysis represents one of the most powerful methodological tool available to reduce the energy intensity of many industrial chemical processes as well as their environmental burden, at the same time fulfilling the economic constraints dictated by market and industrial production.

Therefore, green and sustainable future economy is dramatically dependent on breakthrough discoveries in the field of catalysis, which are either oriented to improve energy efficiency and/or to enhance and open up new pathways for energy storage, or to reduce or at least mitigate the environmental impact related to industrial production.

In the current “from sun to fossil fuels and back again” transition, catalysis may play a primary role in many of the solar-powered technical routes for the production of renewables.

It should also be highlighted that the valuable contribution of catalysis to environmental protection is not limited to chemical or refinery processes but extends well beyond, since catalysts are key tools in reducing, *inter alia*, air and water pollutant emissions from flue gas at power or other industrial plants, from car emissions (e.g. catalytic converters), in photocatalytic wastewater treatment and remediation.

Though, in the short to medium term (to 2025), progresses in implementing incremental improvements and deploying best practice technologies (BPT) could provide substantial energy savings and emissions reductions compared to business as usual, in order to face the energy challenges of the forthcoming decades, a radical step change in management of energy consumption and GHG emissions is a compelling requirement. This in turn requires the conception and development of "game changer" technologies, such as sustainable biomass feedstocks and hydrogen from renewable energy sources which have not yet reached commercial and technological maturity.
Therefore, the most challenging endeavor in this framework is to explore a radical paradigm shift in addressing innovation in catalysis, and only a longsighted and visionary strategy can efficiently cope with this relevant issue. Europe industrial leadership in manufacture has been critically dependent on the innovation capability in catalysis and chemistry, but the transition in progress to a new production cycle based on alternative raw materials from those currently used (mainly based on fossil-fuels) requires a new strategy in addressing research & development. This strategy should enable the acquisition of the knowledge necessary to maintain the front-end capability in research in catalysis, in order to open new sustainable paths of production, resulting in a true innovation capacity able to turn the progressive loss of chemical manufacturing production in Europe.
Therefore, incremental and even emerging technologies are not sufficient to address societal challenges (identified in the EU Horizon 2020 strategy), including GHG/energy targets and maintain competiveness of the EU chemical industry, In fact, though for many mature and established industrial processes approaching their thermodynamic limits, the opportunity of radical improvements diminishes and incremental and small changes across a large-volume chemical have a substantial global impact, incremental improvements are not enough to pursue the expected targets in terms of total energy consumption and GHG reduction neither to maintain competiveness of the European chemical industry.
It is necessary to push R&D on game changers, which essentially re-invent the way something is done by the following strategies:

- they follow an even more circuitous and difficult path to development than emerging technologies, often requiring advances on multiple technology fronts;
- catalysis can play a key role in enabling game changers to uncover alternative reaction pathways, as shown historically.
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In this regard, catalysis-focused *roadmaps* identify two potential game changers:

- use of hydrogen from renewable energy sources to produce NH_3 and CH_3OH
- use of biomass as feedstock

Modern catalysis presently faces five grand challenges:

1. Catalysis to address the evolving energy and chemical scenario

new raw materials (from natural gas to biomass and CO_2, including non-conventional fossil fuels); use of renewable energy in integration with catalysis; energy-saving processes through catalysis; process intensification by catalysis and integration of catalysis with other technologies as membrane to reduce the number of process steps; new catalytic technologies for energy storage and conversion (including fuel cells, H_2 production and storage); catalysis for novel polymers and intermediates;

2. Catalysis for a cleaner and sustainable future

catalysis for eco-technologies (from air to water and waste; stationary and mobile; including photocatalysis); towards 100% selectivity; catalysts in novel process design for resource and energy efficiency; cleaner fuels in refining ; novel catalytic processes to reduce eco-impact of fine and specialty chemicals production (including asymmetric catalysis, organocatalysis and enzymatic process, tandem process); eco-conception (LCA) of catalysts and processes;

3. Addressing catalysis complexity

catalyst design for multistep reactions, for bulky molecules; catalysis for materials with specific properties (electronic, photonic, magnetic); synthesis of advanced and hybrid catalytic systems with tailored reactivity: functional nanoarchitectures in catalysts, novel preparation methods, integrating homo-, hetero- an bio-catalysis, novel nanoparticles, organometallic complexes, organocatalysts, biomimetic catalysts and enzymes, catalysis with immobilized or single site complexes;

4. Understanding and design catalyst from molecular to material scale

from deductive to predictive catalysis; theory and modelling of catalysis; new approaches in catalysts and understanding of reactions mechanism (including in-situ and in-operando methods); model systems (including surface science approach); bridging molecular to reactor engineering aspects in design new processes; kinetics and reaction engineering;

5. Expanding catalysis concepts

catalysis with electrons, photons and other energy sources than heat; design catalysts to operate under non-conventional or extreme conditions; use of non-conventional solvents in catalytic processes; novel catalytic materials

To tackle these challenges, long-term investment and support for research and development (R&D) to enable innovation is required to ensure continue advances in new technologies in the field of catalysis, encompassing not only the design and tailor-made synthesis of new catalysts, but also their reliable testing, characterisation and multidimensional modelling, to move from a fit-for-use catalysis development to a catalyst and process coupled design, which accelerates the discovery of new paths and solutions for sustainable energy and chemistry.

The European Cluster on Catalysis initiative

Europe is a leading player in both academic research on catalysis as well in the industrial implementation of catalysts, but this leadership is being increasingly impaired by steeply growing economies such as China, or mature but still innovating economies such as US or Japan.

The European leadership in catalysis is progressively eroded from the still present fragmentation, the insufficient coordination between European and country-based activities, the sometime dramatic decrease of funds for fundamental research in many European countries, the lack of large-scale infrastructures dedicated to catalysis.

The key actions to be undertaken at European level in the next ten years in the field of catalysis are:

- Identify top catalyst/process-related opportunities; accelerate R&D that improve energy efficiency;
- Facilitate R&D on *game changers* with partners to lower barriers and operating costs;
- Undertake or stimulate academic and national laboratory research on large-volume/high-energy use processes;
- Promote synergies and cohesion between research groups on catalysis, with flagship initiatives;

The European strategy in this field is longsighted and comprehensive, and many of the strategic initiatives undertaken by the European Commission are closely intertwined with catalysis. In this regard it is worth to mention, *inter alia*:

- Energy Roadmap 2050
- Low-carbon economy: SET-Plan towards a Low Carbon future
- Materials Roadmap Enabling Low-Carbon Energy Technologies
- Roadmap to a Resource Efficient Europe
- SPIRE

Also considering the Societal challenges addressed by the European Union, most of them involve the rational use of catalysis:

• Food security, sustainable agriculture and forestry, water research, and the *bioeconomy;*
• Health, demographic change and wellbeing;
• Secure, *clean and efficient energy;*
• Smart, *green and integrated transport;*
• Climate action, *environment, resource efficiency and raw materials;*
• Europe in a changing world - inclusive, innovative and reflective societies;
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Nevertheless, weaknesses affecting the action of Europe in this strategic field are:

- segmented/fragmented and jeopardized research and technology efforts
- lack of a common vision and of coordination at EU level
- weak interaction/gap among national roadmaps and energy policies and H2020 vision
- often try-and-error approach to problem solving, not focused research
- strong competition from China, Russia, US, BRIC countries, Japan, Korea

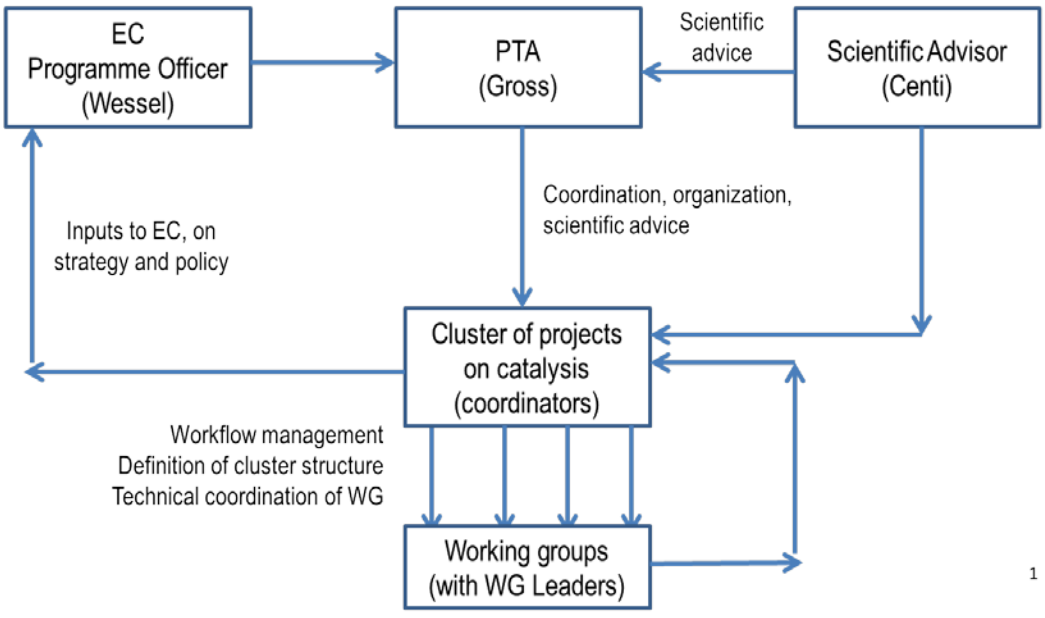
As a related consequence, EU programs to support research and innovation in this field provide only partial coverage of all technical/industrial issues related to catalysis.

To address these and further strategic challenges for Europe, the European Commission (NMP Research Programme) has launched several thematic clusters bringing together EU funded projects and other stakeholders. The main aim of this strategic cluster initiative is to better integrate fragmented activities in Europe, create synergies between EU funded projects and other stakeholders and provide inputs on potential future research needs to the European Commission.

The most recent cluster in this context is the European Cluster on Catalysis, gathering together EU-founded projects in the field of catalysis, organizations and institutions as well as industrial and other relevant stakeholders in catalysis at EU level.

The term catalysis encompasses in this particular framework different typologies and declinations of catalysis: heterogeneous, homogeneous, photocatalysis, electrocatalysis, biocatalysis and others as well as the corresponding technologies, such as CO_2 utilisation, artificial photosynthesis, biogenic materials, water technologies.

The Cluster will be organised by the European Commission (RTD/ Advanced Materials and Nanotechnology Unit), by the Project Technical Advisor (PTA) Dr. Silvia Gross and by Prof. Gabriele Centi as Scientific Advisor. Cluster activities shall be developed and implemented following a bottom up approach by the participants, as depicted in the flow chart (Scheme 2) below:



Scheme 2

To cope with the challenging issue of promoting a sustainable and competitive catalysis-supported economy, the Cluster has as ambitious primary goals to foster :

- coordinated, effective and rational approach to the Grand Challenges in catalysis
- synergy among stakeholders, research, academia, industry, initiatives at EU level
- integrated approach at EU level, this latter particularly important for areas of crosscutting activity linking key enabling technologies to their application in addressing societal challenges (e.g. *Competitive low-carbon energy)*

Related purposes of the Cluster are:

1. Identify and group projects according to application areas and technologies.
2. Identify European interests (scientific, technical and economic) regarding catalysis research.
3. Identify methods to support and strengthen common dissemination activities.
4. European roadmap on catalysis research.
5. Providing input on catalysis relevant aspects to the European Commission.

As practical outputs of the Cluster to be delivered to the European Commission, and to be accomplished in the short/medium term (Mid 2016) should be mentioned:

- coordinate, link together and integrate activities of EU founded projects on catalysis
- create networking and synergies among the existing networks
- edit a new roadmap for catalysis in Europe
- stimulate open-minded, interdisciplinary workshops and discussion forum on frontiers activities fostering new ideas, visions and directions in catalysis
- regulations/standardisation activity (e.g. test in photocatalysis)
- define policy for H2020 and themes/topics for future calls
- discuss and plan new joint proposals
- define coordinated and common actions to sensitize public, politicians and popularize the role and benefits of catalysis for the society

To accomplish these goals in a rational and fruitful way, coordination of the Cluster on Catalysis with similar initiatives would be beneficial, in particular with the Clusters on i) Raw materials, ii) Modelling (multiscale), iii) Engineering and up-scaling, iv) Environmental technologies and, less relevant, v) water treatment.

The Cluster is conceived as an open and dynamic platform accessible to all players and stakeholders, both from academia and industry, whose activity is focused on catalysis and applications thereof.
The idea is to launch the Cluster with the broadest aim, expecting that specialisation will follow later. The Cluster is always open to other future participants.

In order to pursue the different tasks in a smooth and rational fashion, the Cluster has been structured in three main Working Groups (WG), each one coordinated by a WG leader, and in further sub-WGs, each one committed with a specific task and involving 2-8 participants, according to the complexity of the task to be performed.

First Cluster meeting and next steps

The first meeting of the Cluster took place on 13th January 2015 at EC in Brussels, at the presence of different Programme Officers of the European Commission, of the PTA and Scientific Advisor and of the Coordinators of the involved projects as well as of representatives of different organizations and institutions.

During the one-day meeting, the future work of the Cluster has been planned, the schedule defined and the tasks assigned, as extensively reported in the Minutes of the Meeting. Further short/medium steps to be undertaken by the Cluster participants are, *inter alia*, i. the publication of the website (www.clustercatalysis.eu), presently in preparation, ii. the issue of a Newsletter and iii. of a Cluster Compendium, iv. the collection of relevant survey and information for the "European Roadmap on Catalysis", to be delivered to the European Commission by mid 2016.