European Cluster on Catalysis

"Catalysis towards FP9"

Position Paper of the European Cluster on Catalysis

A MOVE TO COORDINATE CATALYSIS RESEARCH IN EUROPE: THE EUROPEAN CLUSTER ON CATALYSIS

Europe is a leading player in both academic research on catalysis and the industrial implementation of catalysts, but this leadership is being increasingly challenged by rapidly growing economies (such as China and India) and mature but still innovating economies (such as the US or Japan). European leadership in catalysis is progressively eroded by still present **fragmentation, insufficient coordination** between European and National-based activities, the sometimes dramatic decrease of funds for fundamental research in many European countries, and the lack of large-scale infrastructures dedicated to catalysis.

To cope with these issues, and to address further strategic challenges for Europe, the European Commission (NMP Research Programme) launched, at the beginning of 2015, a thematic European Cluster on Catalysis (ECC), bringing together EU funded projects and other stakeholders in this field as well as closely related ones. The main aims of this strategic Cluster initiative are 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 EU.

The Cluster, to which more than 900 scientists from 20 countries all over Europe are affiliated, 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.

Besides compiling a comprehensive Compendium of all EU-financed projects in the field of catalysis, the Cluster also coordinates, links together and integrates activities of EU funded projects on catalysis, creates cooperation and synergies among the existing networks, and suggests policy for H2020 and themes/topics for future calls.

One of the main outputs of the Cluster was a "European Roadmap on Science and Technology of Catalysis. A path to create a sustainable future". The initial comprehensive draft was subject to an extensive public consultation involving many universities, research institutes, organisations, companies and individual scientists from all over Europe, committed to improve the Roadmap and pursue a shared European vision. The Roadmap is now published and it has been presented and discussed in various scientific major events (e.g. the 6th EuCheMs - the European Conference on Chemistry, Seville/Spain Sept. 2016 - and 16th ICC - the world conference on catalysis, Beijing/China July 2016). An overview on the Roadmap content is reported below.

EUROPEAN ROADMAP ON SCIENCE AND TECHNOLOGY OF CATALYSIS (PUBLISHED IN 2016)

The Roadmap is organised into three main sections, plus three thematic Annexes. The first part is dedicated to the vision and scenario analysis. Catalysis is an **enabling technology for chemical production and sustainable energy by leading to a carbon-neutral society**, therefore this first part of the Roadmap necessarily has a broader scope beyond catalysis itself, and addresses possible scenarios (from sustainability and competiveness perspectives) for the chemicals, transport and energy sectors. This includes aspects related to electrical to chemical energy conversion, which plays an important role in fostering the transition to renewable energy sources. The effort was to define the main paths for the transition and identify the critical elements that characterise the change. This section is thus of general interest for all chemistry and energy areas, and will be discussed in further detail below.

The second part of the Roadmap is dedicated to the identification of high-level goals for catalysis, and for this reason focussed on discussing of the "**grand challenges for catalysis**":

1. address the evolving energy and chemical scenario;
2. target a cleaner and a more sustainable future;
3. address catalysis complexity, which can be subdivided into four topics: (i) advanced design of novel catalysts, (ii) understanding catalysts from molecular to material scale and from model to realistic reaction conditions with novel upcoming tools, (iii) expanding catalysis concepts and (iv) theory, multiscale engineering concepts.

The third part is dedicated to the strategic research agenda and implementation plan for the grand-challenges for catalysis. This section is based on the previous existing roadmaps and documents on catalysis, notably the "Science and Technology Roadmap for Catalysis in the Netherlands" and the "Roadmap of Catalysis Research in Germany", but provides a new integrated approach based on the identified high-level goals.

This third part thus provides a general perspective for Europe, encompassing fundamental and applied research on catalysis, which should be shared by both companies and research Institutions. The Roadmap defines the priorities and objectives for research on catalysis, with emphasis on its impact on society and sustainable industrial production in Europe. A related objective is to maximise social and environmental impact through the development of improved catalytic materials and processes. To cope with these challenges, it is essential to foster and enhance the synergy between fundamental research and technological applications. Relevant aspects here include the integration of new catalytic materials, molecular chemistry and biosciences. Successful realisation of new catalytic solutions and technologies requires integration (in an inter- and multidisciplinary approach) of knowledge and expertise from fundamental areas (chemistry, physics, biology, mathematics, etc.), engineering (chemical and material engineering) and applied (industrial chemistry, etc.) aspects. Integration of *a priori* theoretical modelling with *in-situ/ operando* studies to understand the reaction mechanisms, science of catalyst preparation at the nanoscale level, advanced micro-kinetics and reactor modelling are examples of current trends in catalysis, which need to be raised to an enhanced level, along with eventual transferral into commercial catalyst manufacturing and operation. Another challenge is to pursue a unified approach for homogeneous, heterogeneous and bio-catalysis. All these aspects are elements of the generic challenge of "catalysis by design" that are supported by new large-scale facilities in Europe providing high-energy neutron and X-ray radiation.

THE ROLE OF CATALYSIS IN EUROPE GROWTH AND COMPETITIVENESS

Context. The production of chemicals and energy vectors in Europe is changing very rapidly with the goal to enhance competitiveness and to address societal challenges, the foremost being the effort to **transition to a clean and sustainable future**. Traditional raw materials and sometimes critical raw materials have to be substituted with more sustainable resources, cleaner and more intensified processes have to be developed, new production concepts should be implemented to combine high efficiency with changing and more variable feedstocks (waste for instance), flexible and modular production and new ways to use energy in chemical transformations have to be realised. There is thus an **evolving scenario** to move to a new economic cycle characterised by a seamless interconnection between energy and materials science, implemented with Green Chemistry principles. Many economic indicators confirm the reality of this transition and it is therefore critical to intensify research and development to enable the transition and exploit the **energy-chemistry nexus**.

Industrial and societal role. Catalysis plays a pivotal role in current chemicals and energy vector production. Catalysis is **the single most important and pervasive interdisciplinary technology in the chemical industry**, and perhaps one of the disciplines having the largest societal impact, although it is often hidden, poorly recognised or underestimated. For example, by enabling the production of fertilisers through the Bosch-Haber process, catalysis makes it possible to feed a world population of 7 billion humans. Catalysis allows the production of fuels from oil with the quality and scale that are necessary for the modern use of energy. Though the role of catalysis will be partially reshaped by the spread of reliable electrical mobility, catalysis can contribute to many of the missions of Innovation Europe and to the main societal challenges (reduced and zero emission, de-carbonising transport by for instance the production of neutral fuels by power to liquid concepts or from waste valorisation, carbon-neutral economy, circular economy).

In the production of many healthcare, pharmaceutical, and agrochemical products, catalysis is a **core technology**, thereby increasing our living standards.

Main core characteristics. Catalysis is a **key enabling technology** for most of the seven societal challenges in Horizon 2020.

In fact, as evidence for global climate change continues to grow, catalysis has moved to the front line of the struggle to obtain new, sustainable technologies for the future. Catalysis technology is intimately intertwined with new and emerging solutions for our current and future supply of energy.

Therefore, a green and sustainable future economy is critically dependent on continued advances in the field of catalysis, which are directed to improve energy efficiency, to enhance and open up new pathways for energy conversion and storage and to reduce the environmental impacts related to industrial production and transport. 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 renewable materials and energy vectors. This approach should also be extended to the wind-powered technical route. **Catalysis is the most interdisciplinary and overarching technology in the chemical industry**, as a successful catalytic process requires control over multiple scales, from the molecular aspects of the reaction at the active site (nm scale) to the multi-metre scale of an industrial catalytic reactor.

Catalysis and catalytic processes account directly or indirectly for 20-30 % of world Gross Domestic Product (GDP). Furthermore, the manufacture of catalysts in Europe has a large economic impact of 3-4 B€ (global market for catalysts: US$ 16.3 billion in 2012, chemical processing accounting ~ 75%, petroleum refining ~ 25%). Of the 50 largest volume chemicals currently produced, 30 are produced via catalytic routes, and most of the others are subsequently used in catalytic processes to manufacture derivatives. These 50 highest volume processes account for more than 20 billion tons of carbon dioxide emitted to the atmosphere each year. The manufacture of 18 products (among thousands) accounts for 80% of the energy demand and 75% of greenhouse gas (GHG) emissions in the chemical industry. Technical improvements in catalyst and related processes could **reduce energy intensity** for these products by 20% to 40% as a whole by 2050, combining all scenarios. In absolute terms, improvements could save as much as 13 EJ (exajoules) and 1 Gt of carbon dioxide equivalent (CO2-eq) per year by 2050 versus a "business-as-usual" scenario. Catalysis is thus crucial to reduce this environmental burden.

More than 85% of all today's chemical products are produced using catalytic processes, and catalytic processes enable the modern refining of fuels. Nevertheless, catalysis goes far beyond the chemical and pharmaceutical industries and petroleum refineries. It has a critical role in enabling a sustainable use of energy, for example in fuel cells and batteries, in the production of fossil- and bio-fuels, and in many consumer-orientated applications (for instance, washing powders), as well as protecting our environment and climate. Catalysis thus is at the core of the European process industry, one of the economic roots of the European economy (by transforming raw materials into intermediate and end-user products).

Catalysis must be placed among the core enabling sciences and technologies to achieve the strategic goals defined by the European Commission in the Europe 2020 strategy and across its various flagship initiatives, also beyond H2020.

Industrial potential. The **EU manufacturing sector** remains strong, but production of commodities is rapidly moving towards China, where manpower is much cheaper. Furthermore, manufacturing goods locally, where they are needed, helps to lower their carbon footprint. Additionally, traditional production of chemicals is moving towards countries where the feedstocks are cheaper. Therefore, progress in catalysis is required to support the redesign of the chemical industry and manufacturing in Europe. Many SMEs have their core-business in bioenergy or biomass, but highly specialised SMEs are not able to address the grand challenges in catalysis in these specific fields. Therefore, an effort at European level, able to support and structure research in the field of catalysis, is required.

In addition, and more importantly, catalysis underpins several European 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 GHGs (Green House Gases). **Catalysis thus represents a true key technology for Europe's economy, job creation, industry, growth and sustainable future**.

Due to on-going energy transition (*Energiewende*), the demand for catalysts will change radically since entirely new methods for storing electric energy and for replacing our feedstocks for chemical products, fuels and energy are being established. A further opportunity in this field arises from the use and application of unconventional feedstocks.

Sustainable energy is becoming competitive and, at the same time, fossil fuels will eventually be displaced by renewable energy as the most economic energy source. This will have severe consequences for the catalyst market, from refinery to treatment of emissions (stationary, mobile). At the same time, new opportunities are being offered, for example for chemical energy storage. It should be kept in mind that sustainable energy is harvested in a delocalised fashion and, since we may also use the products in a delocalised manner, entirely new processes may become competitive.

The role of catalysis in **Circular Economy** is also relevant, since, for instance, catalysis can solve the problem of waste (biogenic, fossil, municipal, industrial, etc.) by targeting either the recycling of high value building blocks or the degradation and rebuilding of molecules of interest. As such, the possibility of a unified energy and chemical production, based only on renewable sources for both energy and material production is emerging. Here, waste carbon sources (in integration and symbiosis with biomass-derived raw materials) will be the dominant, if not exclusive, source for the latter.

Threats and opportunities. Despite its outstanding relevance, the importance of catalysis in Europe is nevertheless often underestimated. In addition, it is often considered just a tool, rather than an enabling science. The fragmentation and lack of coordination in R&D efforts in catalysis exacerbates this situation. Efforts should be made to enhance the visibility of catalysis, which should be much higher than now.

Catalysis should be recognised as a **Key Enabling Technology** and therefore a suitable funding scheme, such as a **flagship focused on the global challenge of the energy transition or other large dedicated initiatives**, should be implemented by the European Commission in the forthcoming FP9, to support efforts through the whole spectrum, from fundamental to industrial research, to market. In order to meet the COP goals (see www.cop21paris.org/about/cop21), a much more substantial effort in terms of budget is needed to develop the energy technologies that will enable the clean energy transition. Catalysis will play the pivotal role of a Key Enabling Technology in many of the technological solutions to be developed in the context of the energy transition.

Thus, the impact of catalysis in terms of environmental sustainability and more generally in term of societal benefits should be much more highlighted since of even larger importance than the economic benefits.

In this regard, it should be highlighted that, whereas other Clusters established by the European Commission are focussed on methodologies (e.g. modelling, scale-up, pilot etc.) which can be envisioned as tools, catalysis is an enabling S&T, not merely a tool. The advent of **digitalisation** (big data analysis, data mining) and machine learning technologies combined to high-throughput, promises to revolutionise the rational design of catalysts, leading to unprecedented breakthrough technologies.

Besides investments in R&D, catalysis also deserves attention from the point of view of its economic impact. The market is changing fast and the embedded contribution of catalysis in many manufacturing-related sectors is often overlooked. Most of the catalyst producers (a market of over 12 B€) are located in Europe as headquarters, but the on-going transition may **decrease the current market by up to 70%** if new opportunities are not identified. This will have a large impact on employment, which can be estimated in over 200.000 **lost jobs**, often by highly qualified people (either directly or indirectly). In addition, the **overall**

economic value of catalysis should be fully recognised, encompassing not only the direct catalyst market, but also the relevant share of markets enabled by catalysis. In this regard, a **focussed Coordination and Support Action (CSA)** action to estimate the effective impact of catalysis on the European economy is recommended based on thorough data provided by market analysis and surveys. This study should determine the optimal strategies, with recommendations for companies, on how to reconvert the actual S&T capabilities in catalysis to new market opportunities and industrial needs. At the same time, academic research on catalysis in Europe should be aligned to these new directions. A CSA, combining academia and industry, could address this complex problem and provide indications, from academia and industry on one side and from EU and country/regional agencies on the other, on how to catalyse the transition by minimising the negative societal implications.

Concerning the involvement of the industry in large collaborative projects on catalysis, which is still scarce and for which better models are required, possible corrective actions can be outlined. There is a strong emphasis on demonstration scale/moving to higher Technology Readiness Level (TRL), which is partly driven by the chemical industry being less active at TRL5-7 themselves. Nevertheless, efforts to better coordinate innovative ERC-type (TRL1-3) research to the NMBP-type. research (TRL ≥ 5) should be undertaken, and development work at the interface of TRL3-5 should be safeguarded.

NEW VISIONS AND GRAND CHALLENGES FOR EUROPEAN CATALYSIS

Currently, the science of catalysis is moving **from description to prediction**, supported by ever more powerful **computational, analytical and *in situ/operando* techniques**. Each time new tools have become available, catalysis has made a significant step forward, hence this interplay needs to be tightened. Faster and more effective approaches to the development of innovative catalytic materials for new or evolving chemical processes (see societal, ecological and economic constraints analysed above) are in demand. However, translation into economic and societal benefits will require a continuum of connected activities from fundamental research to commercial catalyst manufacture and operation, with a thorough exchange of information, ideas and insights across this spectrum. International competitive advantage is likely to depend upon the effectiveness of this ecosystem for technology transfer.

Important elements of such new approaches include **computational modelling** of catalytic processes at various length- and time-scales (i.e. **multiscale modelling**), hierarchical understanding at all levels from the atomic to the macroscale and advanced or unconventional synthetic approaches, which have to be sustainable and scalable, aimed at delivering materials with improved catalytic performance, preferably starting from cheap, earth-abundant, easily accessible and low ecological impact-raw materials. Accelerating the development cycle for catalysts by computational methods is a viable approach, which could be pursued in tight synergy with the European Materials Modelling Council (https://emmc.info/), also established by the European Commission within the Cluster initiative. "**Catalyst intelligence**", e.g. the creation of smarter, faster and more effective ways to develop catalysts, is a further key concept in the multi-scale development of new and better performing catalysts. This will include computational modelling and in principle a digital twin.

Analogously, since the testing and the functional assessment of produced catalysts is very relevant to catalyst development, interactions and synergies can also be envisioned with the recently established European Materials Characterisation Council (EMCC) (www.characterisation.eu/).

The catalytic site economy, maximising the use of resources and atom economy, should become a research target. In this regard, **catalysis by design**, design of catalysts at the atomic level, and multifunctionality should be pursued by harnessing the creativity of the excellent European research landscape. Furthermore, new approaches are required to accelerate the transfer of 'catalysis by design' to practical commercial catalyst manufacture and industrial operation to support the above-mentioned transition. This also includes the transfer of tools available at large-scale facilities (synchrotron radiation sources, neutron sources, new electron microscopy centres) to the field of catalysis and lab infrastructures to those facilities. Completely new prospects will become possible with newly built, planned and upgraded sources.

The emerging opportunity for 'catalysis by design' created by advances in atomic scale understanding, analytical and in-*situ/operando* tools, computational methods is very exciting and represents a potential source of future competitive advantage. However, this still requires a much stronger linkage with practical and cost effective catalyst manufacturing and commercial operation in order to realise these potential economic, societal and competitive advantages.

In this framework, Life Cycle analysis (LCA) and Life Cycle Cost (LCC) researches initiated from scratch could aid exploration of innovative routes to more sustainable and efficient generations of catalysts. However, **dedicated methodologies and metrics** for catalysis studies should be developed.

In parallel with new paradigms for catalyst developments, there is a need to **redesign chemical processes to minimise the use of fossil fuels**, essentially by using renewable energy sources directly (eventually through the intermediate production of solar or wind fuels/chemicals) or indirectly via renewable carbon sources (see the previous analysis on renewable biogenic sources of energy), rather than heat produced from fossil fuels combustion, to drive the chemical conversion. This means development of novel processes driven by electrons, photons, electromagnetic radiation (e.g. microwaves), plasma-generated reactive species, etc. or adapted to new renewable feedstocks (biogenic types). This will require, for example, **conceptually new types of catalysts**, which are able to selectively control the reaction pathways in the presence of these highly-energetic inputs. Energy selectivity will be a sustainability factor reinforcing carbon-selectivity, and for this reason, new approaches to catalyst and process design are necessary. In the medium-term, new catalytic materials for efficient solar light harvesting and power-to-X conversion technologies are necessary, with biomass finding its niche as a source of biofuels (for transport, especially aviation and heavy trucks) and green materials. A complete Life Cycle Analysis of biofuels, attending mainly to their source, should be carried out to guarantee their sustainability.

Among the emerging fields in catalysis, **electro-catalysis** is challenging but could enable a more competitive and efficient production and use of renewable energy; therefore, efforts in this field would be justified.

Although **heterogeneous (solid) catalysis** will likely still dominate future industrial uses of catalysis, it is evident that many of the new challenges facing catalysis, from the use of solar energy to the use of bio-mass, require **integrating homogeneous, heterogeneous, enzymatic and bio-catalysis**. It is thus of critical relevance to foster this integration and develop a common vision between these scientific areas and overcome the remaining barriers.

Nowadays, catalysis is facing **further important challenges with respect to energy transition**, converting different forms of energy (electrical, light, thermal) to chemicals and *vice-versa*. This also leads to important questions with respect to the intermittent operation of catalysts, and the replacement of critical raw materials such as noble metals by earth-abundant, less polluting and cost effective materials. Additionally, challenges with respect to chemical reaction engineering (process intensification, electrochemical reaction engineering) have to be effectively addressed. Traditional interfaces with the chemical industry and manufacturing will remain important, but new approaches and synergies are required. In the process of redefining the future of catalysis, energy stakeholders (energy producers, network owners) should be involved, and connection to smart city initiatives are also needed. CO_2 capture will become more important leading to challenges in materials design and development of more efficient catalysts. Despite the general trend towards Electromobility, combustions engines will still be the prevailing technology for individual transport over the next decades. Recent discussions demonstrate that there are still significant issues to be solved by catalysis in the field of automotive exhaust gas cleaning in order to achieve clean air in urban areas

From a **strategic point of view**, open innovation models should be explored such as, but not limited to, innovation hubs and the Energy Lab 2.0 at KIT (https://www.elab2.kit.edu/english/index.php). Similar initiatives, as well as a better integration and coordination between Framework Program and the European Structural Funds (ESF) distributed at regional level, should also foster regional-wide cooperation schemes in which innovation hubs with specific focus should be established in the different EU Regions.

Educational and training efforts, devised and structured based on the current directions of catalysis, should be undertaken at the European level, training a new generation of scientists able to work in a highly interdisciplinary, pervasive and trans-sectoral field. In this regard, the support of public funding becomes mandatory to foster this cultural transition

Conclusions

Catalysis is highly comprehensive, pervasive, trans-sectoral and can be described as a Key Enabling Technology. As such, it should be supported at European level through dedicated financing tools and programs allowing in-depth pilot studies.

PROPOSAL FOR A CSA DEDICATED TO THE FIELD OF CATALYSIS TO BOOST THE EUROPEAN CATALYSIS CLUSTER ACTION

During the meeting, a specific action (requiring financial support from the EC) to promote the activities of the Cluster (also in terms of training, dissemination, regulations) and to extend its networking, was presented (by Claude Mirodatos) and discussed.

A CSA designed to support the Catalysis Cluster would mainly consist of support measures such as standardisation, dissemination, awareness and communication, networking, coordination and back-up services, policy exchanges, mutual learning and studies

In this sense, it would contribute to the complex process of decision-making leading to the launching of the future FP9 bi-annual work programmes. A CSA on catalysis would start from the existing Roadmap on catalysis, to define better in an integrated view with the other aspects indicated above and education/training, a new integrated view of actions to establish catalysis as the S&T enabling many societal challenges. As an example, a CSA could consider the generic topic of "Catalytic process and catalysts standardisation" and promote the development of a database on reference catalytic materials and processes to facilitate data transfer and performance benchmarking within the EU community. It might possibly focus on specific areas like biomass and waste conversion to chemical intermediates and/or transportation fuels: databases, analytical tools, circular economy concepts, among other domains to list as priorities. Due to the predominant role assigned to biomass as a source of energy and chemicals, the elaboration of a "White Book" on the sustainable use of biomass for these purposes will be one of the tasks to be carried out. This "White Book" will be used as reference guide to define sustainable strategies involving the use of biomass in broad sense.

The design of such a CSA would rely on the “EU cluster on catalysis” address book, would promote the development and use of tools and practices that follow findable, accessible, interoperable, reusable (FAIR) principles, and the validation of data quality measures. It would also integrate existing data/tools repositories and databases, including those from SETIS (Strategic Energy Technologies Information Systems) and from the IEA (International Energy Agency); https://setis.ec.europa.eu/about-setis, https://www.iea.org/

The last CSA concept, remarked above, is to use this instrument to define strategies and identify actions for a recovery plan for the catalysis industry, which has a relevant role in Europe and that will be significantly affected from the ongoing transition in energy and chemical production, should suitable solutions not be identified. This CSA should determine the optimal strategies, with recommendation for companies, about how reconvert the actual S&T capabilities in catalysis to new market opportunities and industrial needs.

Finally, a budget to set-up and run such a CSA would have to be defined in the proposal to be submitted to the EU H2020 portal (around 1 M€ could correspond to a typical funding of a CSA). Strong synergies between academy and industry in this CSA should be encouraged.

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