Catalysis Today 138 (2008) 69–76

Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Catalysis, a driver for sustainability and societal challenges[☆]

Gabriele Centi [*], Siglinda Perathoner

Department of Industrial Chemistry and Engineering of Materials and ELCASS (European Associated Laboratory for Catalysis and Surface Science), Salita Sperone 31, 98166 Messina, Italy

ARTICLE INFO

Article history:
Available online 11 June 2008

Keywords:
Catalysis challenge
Renewable
Catalyst nano-architecture
Nanoreactor
Catalytic nanofactories

ABSTRACT

Catalysis is an enabling technology to promote sustainability, environment, energy, health and quality of life. This contribution discusses the role of catalysis in achieving these objectives and some of the factors which will drive the changes in catalysis research in the next years, in particular the need to go to more sustainable and modular-design of the chemical processes (F^3-factory), the use of biomass and of renewables, including solar energy, and the challenges offered from electrocatalysis. It is also emphasized the need to strength research on catalysis, and some examples of how to overcome fragmentation barriers, particularly in catalysis areas (homo-, hetero- and bio-) and in academy–industry interactions. The need to create a longer term vision and strong collaborations in order to develop a knowledge platform, in order to accelerate the innovation path. Finally, the need to develop new catalytic materials, particularly of tailoring catalyst nano-architectures and develop new catalysts based on the concepts of nanoreactors and catalytic nanofactories are discussed.

1. Introduction

The original concept of sustainability [1] emphasized the needs to combine social objectives (health, quality of life, employment) to the management of the scarce resources (energy and raw materials) and the preservation of the natural bases for life, e.g. the need to adopt all actions such as cleaner processes, recycle waste, reduce pollutant emissions necessary to preserve biodiversification. The actual concept of sustainability is broader and takes into account that sustainability is also the engine for innovation. The fast modifying socio-economic and geo-strategic context requires a societal change and adaptation to put the capacity of innovation at the core of competitiveness and economics.

In addition to the role of catalysis in promoting feasibility, eco-efficiency and economics of over 90% of the chemical processes, catalysis was one of the critical enabling factors for sustainability also out of the specific field of chemical processes in the last two decades. In the mobility sector, without the introduction of catalytic converters starting from the 60s, it was not possible to counterbalance the increasing level of emissions of pollutants such as NO_x, CO and hydrocarbons associated to the worldwide expansion of the car market. This is demonstrated in Fig. 1 which reports the contribution of various aspects in the reduction of the NO_x emissions from vehicles. Without the introduction of catalytic converters it was not possible to reduce the total NO_x emissions below values sustainable for the society, e.g. to limit issues such as smog formation, acid rain and increase of diseases and allergy due to pollutants.

Achieve a sustainable mobility was thus linked to the capacity to develop and consecutively further improve the catalytic converters for emissions from cars, buses and trucks. There are still several challenges in this area, particularly related to the need to find more effective catalysts for the reduction of NO_x in the presence of oxygen (very relevant problem to address the increasing share of diesel engines), better catalytic filters for particulate and catalysts more active at low temperature (to reduce cold start emissions). Catalysis was thus one of the enabling factors for a critical societal need such as mobility, but will continue to play a critical role in this area, because further R&D is needed. The regulations on CO_2 emissions from vehicles under discussion currently (a limit of 120 g CO_2/km has been proposed in EU) poses new challenges also for catalysis, because new requirements also for catalytic converters derive from the necessary changes in engines to meet these limits.

The introduction of catalytic converters and their progressive improvement was always dictated from regulations in vehicle emissions and essentially never used as a factor demonstrating the capacity of car manufacture company to be innovative and environmental friendly. More recently, however, the introduction of catalytic filters for diesel particulate anticipated regulations and was used also in advertisements to demonstrate the innovative profile of some car manufacture companies. Catalysis is thus not

---

[☆] Opening speech at Paul Sabatier 5th European Conference on Catalysis, Ottrott (France), September 12–16th, 2007.

[*] Corresponding author. Fax: +39 090 391518.
E-mail address: centi@unime.it (G. Centi).

0920-5861/$ – see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.cattod.2008.04.037

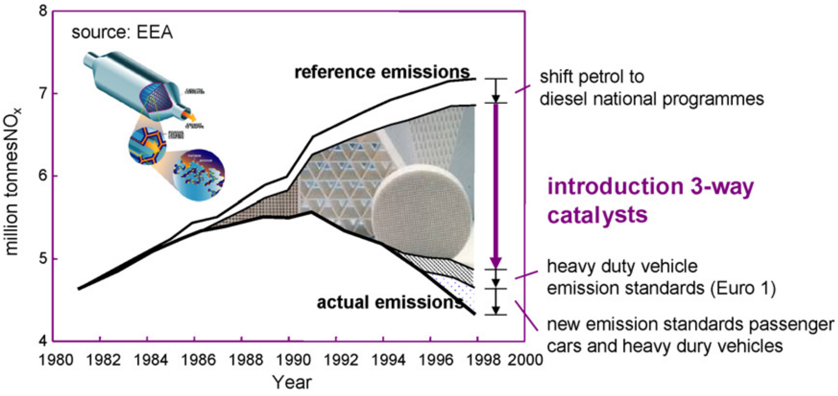

Fig. 1. NO$_x$ emissions from road transport showing the different contributions in the reduction of NO$_x$ emissions and the role of the introduction of 3-way catalyst cars (adapted from European Environmental Agency – EEA, 2001).

considered only as a tool to meet regulations, but part of the factors determining car appealing of the customers.

Also in chemical and refinery production something similar was happening. Catalysts were the components functional to the process economy and thus their performances were mainly associated to the ability to improve yields/productivity, and reduce process costs (longer catalyst life, milder reaction conditions, reduction of separation and environmental costs). Today, there is an increasing attention, at least in some companies, to consider catalysis as a part of the company's image and marketing strategy. A new catalytic process is an opportunity to gain market shares or to enter into new markets. New regulations (REACH in Europe, in particular) which impose to take record of the production process of the chemicals will further change the use of catalysis from being a tool to achieve process targets to be part of the strategic vision of the companies. Not only the quality of a chemical product will be important in the future, but also the quality of their production chain. It will be thus not more possible to produce in remote areas where the environmental criteria or controls are less severe. The environmental performance indexes, from energy efficiency to greenhouse gases and pollution emission factors (and other factors which may be estimated from life cycle assessments), will be the key parameters for evaluation in a society which should include in the production cost also the use of the limited natural resources. The actual dramatic lack in some raw materials is already a clear signal of the need to progress in this direction. The increasing concerns on greenhouse gas emissions is another signal.

2. Factors driving the changes in catalysis research

Foster innovation in chemical industry, through integration of different elements, but having catalysis as the core component, is a key factor to meet sustainability, as pointed out for example from the European Technology Platform on Sustainable Chemistry (ETP SusChem) [2] promoted by Cefic (European Chemical Industry Council) and EuropaBio (European Association for Bioindustries). To implement this vision, however, it is necessary not only a concerted strategy of the stakeholders of the sector (objective of the cited platform), but also the progressively introduction of radically new approaches to chemical industrial production. A part of this vision is the need to breakdown the scale economy, at least in some chemical processes.

This concept was earlier introduced [3], but it is now an integral part of the strategy for the future F^3-Factory (Future, Fast, Flexible), the visionary idea for the future of chemical production. Future sustainable F^3 chemicals production will combine a much broader range of production scales with interlinking technologies and logistics. An important strategy to meet the F^3 challenge is process intensification. This is a strategic and interdisciplinary approach employing different tools (such as micro reaction technology and modularization) to improve processes holistically. However, a core technology to achieve process intensification is a new design of catalysts (for example, to develop catalysts suitable for microreactor technology), evidencing how advances in catalysis are strictly related to innovation and sustainability in chemical production.

The idea is directed in order to develop efficient modular design of chemical processes. There are several conceptual advantages of this processing design. First, a single efficient module can be designed, while later increase in the production can be achieved simply by parallel modules. This gives a very high production flexibility (also in terms of time response), a critical factor in several productions (high fluctuations in the chemical trade is a major current limit for planning of new investments in the chemistry area), and limits the costs of scale-up (the unit can be the pilot plant and a module of the final process at the same time).

Second, the investment costs can be reduced to a single module and only in a later stage the production could be increased. This fact greatly facilitates the introduction of new processes often hindered from the large investment costs which are necessary. Third, the production capacity can be limited to the self-depuration capacity of the environment. A sustainable production requires that the impact on the environment is below the critical threshold of local self-depuration of the environment. This is typically not achieved in large refinery and/or petrochemical sites. A modular design of the chemical processes allows to delocalize chemical production and avoid the concentration in few sites. A small modular design would imply also a reduction in the risks (transport and management of chemicals, storage hazard products, fugitive emissions) and process complexity (large number of equipments and process sections).

However, a modular design cannot be implemented using the actual process design. It is necessary to implement new solutions for process intensification, integration of reaction-separation and handling energy. More efficient solutions to provide energy for the process (alternative to thermal energy) are needed. Clearly, these changes in process design require also a different catalyst design (the same catalyst in a conventional and microreactor cannot be used), where a better control of the nanostructure allows to maximize catalyst efficiency in relation to the new operational and fluidodynamic conditions imposed by the new reactor design.

Therefore, the critical elements for sustainability and innovation in chemical processing, such as to (i) down-size and integrate the (chemical) production to minimize transport and storage, and avoid large plants and concentration, (ii) develop a smart use of resources, materials and energy (reduce materials and energy intensity of goods and services, increase durability), (iii) maximize recycle and minimize utilities, and (iv) integrate processes (catalysts for multi-step reactions, reaction and separation), all pointed out the need for a new catalysts design.

The progressive revolution in chemical and fuel area deriving from the socio-political need of new uses in biomass resources [4] is another factor which determines the need to intensify the research on new catalyst solutions. Biomass is far more complex than oil and convert biomass to a concentrated and easy transportable form of energy equivalent to those deriving from oil requires a very intense research. There are many process steps which require the development of novel catalysts, starting from the need of efficient and stable solid catalysts for vegetable oil transesterification, to solid catalysts for cracking, hydrolysis or selective depolymerization of (hemi)cellulose and lignin, and to new enzymes for fermentation to products different from ethanol. The passage from the first to the second generation of biofuels requires an intensified research on new catalysts.

In general terms, products which could be obtained from biomasses contain more oxygen than the analogous derived from oil. While the chemistry based on oil was essentially based on search of selective catalysts able to insert hetero-atoms, whereas starting from biomass-derived chemicals (extracted from biomass, or platform molecules obtained from biomass conversion) it is necessary to develop novel catalysts able to selectively deoxygenate the organic substrate. Typically the catalyst should have also multi-functional behavior to perform in one-step the transformations to useful chemicals of platform molecules. Process conditions are typically milder with respect to the equivalent oil-based processes. As a consequence, low temperature activity is a requirement which determines the need of new catalytic approaches.

Biomasses are very different each from the others. Oil is a complex mixture, but the various components can be lumped in relatively small number of homogeneous classes of chemicals having similar reactivities. In addition, they are all in the same liquid phase. The biomass composition is more complex, is heterogeneous and it is not possible a similar lumping mechanism. A biomass-based society needs thus to develop multi-purpose catalytic solutions which can handle different feedstocks. On the other hand, going to a biomass-based society the problem is determined from motivations out from economy-driven analyses. It is thus not correct to evaluate the transition from this perspective, but it is instead better to ask themselves which catalyst's design is needed to improve sustainability of this transitions.

Catalysis for fuel cells is another relevant area which needs an intensified effort of research. There are many relevant challenges for catalysis (increase the efficiency of the chemical to electrical energy conversion and the stability of operations, reduce costs of electrocatalyst) which are necessary to contribute in making a step forward in the application of fuel cells out of niche areas. This objective requires also to develop efficient fuel cells fuelled directly with non-toxic liquid chemicals (ethanol, in particular, but also other chemicals such as ethylene glycol are possible). Together with improvement in other fuel cell components (membranes, in particular), ethanol direct fuel cells require to develop new more active and stable electrocatalysts.

But fuel cells should be considered also as an element of a broader area where catalysis is used in combination to electrons to perform selective reactions. For example, it is possible to feed waste streams from agro-food production to an electrochemical device essentially analogous to a fuel cell to produce at the same time electrical energy and chemicals. Fig. 2 shows this novel concept of combined production of chemicals and energy. This approach is interesting in SMEs for using wastewater or byproduct solutions derived from agro-food production. A limiting factor is the need to develop new nanostructured electrocatalysts, because conventional fuel cell electrodes have limited effectiveness and they are tailored for total oxidation. The challenge is to develop new electrocatalysts which do not break the C–C bond, have a high activity to make industrially feasible the process (e.g. have close to 100% Faradaic efficiency, and current densities of about 100–150 mW/cm^2 at temperatures lower than 90 °C) and to be stable in the strong basic medium required to use anion-exchange membranes. Target products are low-molecular weight oxygenates of industrial valuable interest. Recent results [5] showed that it is possible to oxidize selectively ethanol, glycerol, 1,2- and 1,3-propanediol and ethylene glycol to the corresponding (di)carboxylic acids, hydroxy- or cheto-acids, in DAFC-type cells (polymeric membrane fuel cells fed with alcohols).

Catalytic chemistry with fuel cells may be thus considered part of the general effort towards new delocalized chemical productions, because this approach is suited especially for SMEs.

Electrocatalysis could be combined with photocatalysis for interesting opportunities, starting from the possibility to increase current density in fuel cells. It was shown [6] that a hybrid carbon fiber electrode consisting of a TiO_2 semiconductor photocatalyst and a Pt-Ru catalyst boosts the performance of direct methanol fuel cells (DMFC) and increases current generation under UV-light irradiation. However, the challenge is to combine the two concepts for a next step in the use of renewables, e.g. use solar energy to convert biomass products to fuels. It was shown recently [7] that it is possible to produce H_2 by photoreforming in liquid phase of products derived from biomasses (bioethanol, or directly sugars obtained from cellulose). A remarkable increase (approximately two orders of magnitude) in the production of H_2 (with respect to the photocatalytic splitting of pure water) was observed by irradiation with a medium power Xe-arc lamp an aqueous solution of glucose using 0.5% Pt/TiO_2 as the photocatalyst. Fig. 3 shows this concept and the difference in the scheme of reaction between water splitting, photo-oxidation of organic substances in solution and photoreforming. In particular, the results of Patsoura et al. [7] demonstrate that H_2 derives both from water and the organic substance, and that the organic substance is fully oxidized to CO_2. It is still necessary to demonstrate the explitability of this approach (in particular, stability of the operations and production rates) and the possibility to develop new nanostructured titania-based catalysts active in this reaction using visible light. However, this direction shows interesting perspectives, better than the well

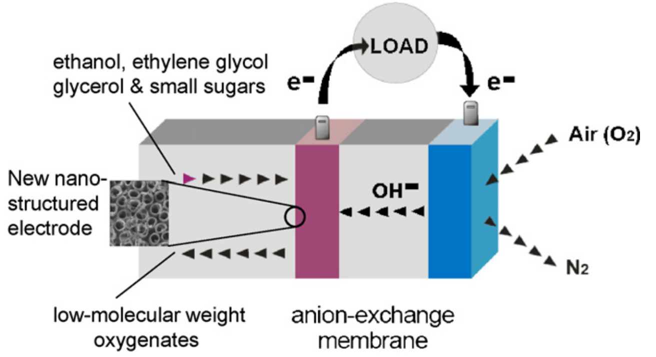

Fig. 2. Advanced electrocatalytic approach (direct alcohol fuel cell, DAFC) for combined chemical and energy production.

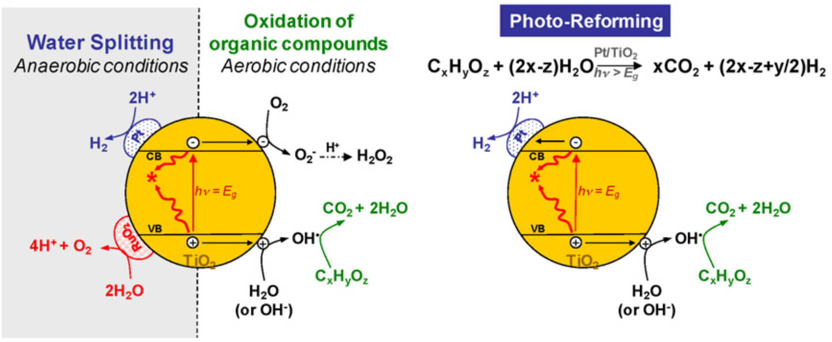

Fig. 3. Simplified scheme of the photocatalytic processes on TiO_2 during anaerobic water splitting, oxidation of organic compounds and photo-reforming processes.

advertised production of H_2 by catalytic reforming in aqueous solution [8,9].

A further challenge is to combine photocatalysts and electrocatalysts in a single photoelectrocatalytic (PEC) device. Classical PEC devices operate in liquid phase, but new possibilities are offered using a different configuration based on a modified PEM fuel cell (Fig. 4) where the electrocatalyst operates in gas phase and is substantially based on nanostructured carbon [10], instead of that operating in the liquid phase which is made of flat electrodes (conventional PEC devices). By combining this configuration with new nanostructured titania thin films [11] it is possible to convert CO_2 back to liquid fuels using solar energy and water [12]. Only the proof of the concept has been made, and actually there is the need of an intense research to solve a number or problems, starting from productivity and stability of operations. However, also in this case new opportunities are offered for catalytic research in a key area for societal challenges. Worth to note, the same device can be used also for the production of physically separated flows of H_2 and O_2 during water photosplitting, as shown in Fig. 4.

These are only few examples, clearly not exhaustive of the wide range of possibilities offered by new research directions in catalysis to address societal challenges, but evidencing how the new requests of sustainability together with a fast changing energetic scenario drive the need to find new catalytic solutions. Up to few years ago several peoples especially in companies argued about the need of further research in catalysis, but the same persons are now concerning about the time lost due to low incentives in developing new catalytic solutions. In all the field of research an S-shaped curve (technology pervasiveness vs. R&D effort) describes the degree of maturity of a technology. For catalysis many factors, some of which discussed above, are driving a significant change in the area, posing new problems and requiring new approaches. This means we are in the fast raising part of the S-shaped curve. There is thus a revitalization of the research in catalysis (catalysts market is projected to increase at a rate of 3–4% up to 2010), but it is necessary at the same time also to enlarge the fundamental knowledge to address more efficiently the new needs.

Some of the critical areas in which it is necessary to intensify the research in catalysis are the need to (i) better integrate hetero-, homo- and bio-catalysis, (ii) make a significant step forward in bridging the gap between surface science and theory and applied catalysis, (iii) better understand the catalytic chemistry and dynamics in operand conditions, (iv) explore catalysis in combination to sources of energy alternative to thermal, (v) develop more solid bases for the control of selectivity in multi-step reactions, and (vi) integrate catalyst and reactor design, especially taking into consideration the advances from advances in microreactor technology and in combined reaction-separation devices.

3. How to strength research on catalysis

There are many societal challenges which stimulate new research on catalysis, but this requires also to make more efficient the research on catalysis. One of the actual factors limiting often research on catalysis is the fragmentation of the research groups, while at the same time there is the need of a highly multidisciplinary approach to address the complex problems outlined

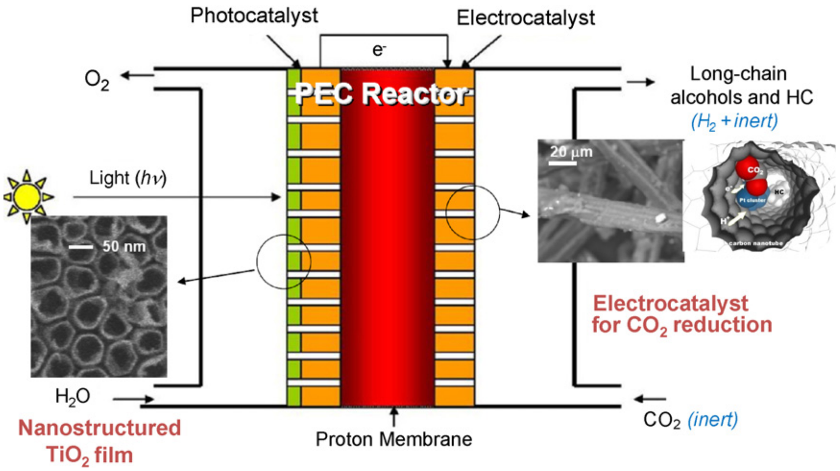

Fig. 4. Scheme of photoelectrochemical (PEC) reactor for the conversion of CO_2 to long-chain alcohols and hydrocarbons using solar light and water. The same PEC reactor could be used also for the physically separate production of H_2 and O_2 in anaerobic water splitting.

before. It is thus necessary to find efficient mechanisms to create and maintain a critical mass, fostering long-term collaboration and providing the incentives to joint efforts for collaboration in challenging long-term objectives. This requires the creation and sharing of a long-term vision and an intensified activity to develop research roadmaps (shared between companies and academy) which could also shift the financial support from short to medium-long terms. The output could be the creation of a platform of knowledge which anticipate industrial and societal needs.

There are examples of effort in this direction. EU is financing a specific Network of Excellence on catalysis (IDECAT, Integrated Design of Catalytic Nanomaterials for Sustainable Production, http://www.idecat.org) to reach above objectives, and in particular strength catalysis by reducing fragmentation, improve long-term joint effort on challenging areas, and define research roadmaps. Over 40 research groups belong to the network which cover a wide range of aspects in terms of scientific (homo-, hetero- and bio-catalysis) and disciplinary areas (surface science, theory and modeling, applied and industrial catalysis, reaction and catalyst engineering, material science, etc.). A lasting objective is the creation of a Virtual Institute with permanent structuring effect in the area and aimed to become a reference centre for catalysis, academy–industry relationships, public dissemination activities and also to be a single voice for promotion of catalysis at political and governmental levels. This Virtual Institute called ERIC (European Research Institute on Catalysis) is expected to start operations in Spring 2008. It could be a model also out of Europe for not-traditional overstructures, e.g. out of the classical model of a research centre, necessary to promote catalysis research and facilitate the process in going from idea to application through innovation.

An illustrative alternative example on how to realize an efficient company–academy interaction to realize above objectives is offered from the analysis of the progresses in photocatalysis in Japan [13,14]. In 1972 Fujishima and Honda [15] showed photo-oxidation of water using TiO_2 under UV illumination, e.g. the possibility of production of H_2 from water with a titanium dioxide electrode exposed to UV radiation. However, only about 10 years later research on the photocatalytic properties of TiO_2 started to attract a larger interest, following the discovery that polycrystalline TiO_2 electrodes show a high activity for the photo-oxidation of organic's (to reduce smell in the University bathrooms) [16]. Later, starting from about 1995, an exponentially raising number of papers on the photo-oxidation of organic pollutants including pesticides and hormone analogues were observed. Most of the papers regarded degradation of pollutants in water and using TiO_2 in the form of powders, while most of the Japan patents regarded titania catalysts in the form of thin films and applications for air purification. Only in late 90s started to be published several papers on the photocatalytic destruction of pathogenic organisms and cancer cells. An interesting aspect regards the number of publication and patents of Japan's researchers on photocatalysis with respect to those of the rest of the world. Japan's researchers published in 2002 about 25% of the total papers in the sector, while the percentage increased to nearly 90% considering the patents in the area of photocatalysis. In terms of market share, Japan's companies hold about 75% of the total market of photocatalysts (about 400 M$ in 2002).

Looking more in detail at the motivations of the leading role of Japan in photocatalysis it is possible to note a strong collaborative network between University/Public Institute and Industry, in particular centered around the Fujishima-Hashimoto group which anticipated in patents the results reported in open literature by several years, including for example anti-bacterial tile (1993), self-cleaning glasses (1995), anti-fogging mirrors (1996), removal of endocrine disrupters (1999) and anti-bacterial medical tubes (2000). Nearly all the patents were on thin titania films, while the majority of publications were on powders.

The following steps could be observed in the analysis of the collaboration between university–industry in Japan on photocatalysis [13,14]:

1. Initially, leading university scientists operate as a hub of networks of the S&T community and promote growth in the number and variety of participants in the community (open university/public institute ↔ private company). The function was necessary to maintain the innovative edge of the research. Following the first breakthrough results on H_2 photocatalytic production, a series of typically bilateral university–industry research collaborations started, using an academic virtual network to exchange ideas and results.
2. In a second stage, companies working closely with University succeeded in the development and commercialization of products. Note that in this specific example, the application of TiO_2 photocatalysts was in a different area from the initial discovery, e.g. oxidation of organics instead of that of production of H_2 from water using solar light. This step allowed to create an innovation–application link and to demonstrate the benefits for society, e.g. to enlarge interest on the results of R&D. Following this step, together with an increase of the nucleation sites for academy–industry collaborations, a significant increase in the number of companies interacting with each academic center was observed.
3. Then, other companies with previous experiences in commercialization of products moved into applications for environmental protection. This further step opened new market opportunities. A change in the pattern of academy–industry relationships is noted at this stage, with the creation of strong network links also between academic groups.
4. Finally, public sectors worked as a bridge in developing technologies for environmental protection. For example, patent applications on photocatalysis by Fujishima-Hashimoto groups reached a peak of around 40 patents in 1996 with core and other firms, in parallel with the discovery of self-cleaning glass and anti-fogging mirror behavior of titania thin films – superhydrophilicity. The number of patents with companies strongly declines in the consecutive years, but counterbalanced by a fast increase in the number of patents with the public sector in parallel to the discovery of the behavior of titania in the removal of endocrine disrupters and for preparing anti-bacterial medical tubes. This further step was necessary to strength innovation.

This successful story on TiO_2 shows that starting from a curiosity-driven research it is possible to develop a significant market only by creating the right academy–industry network. It is thus necessary not only a good science, but also to create the scientific infrastructure which allows the effective transfer of ideas to innovation and business. It is also shown that original breakthrough results may find applications in a different area from the original discovery, but several years later may come back to the original field (Section 2) when advances in fundamental research can put original results in a different perspective.

4. The need to develop novel catalytic materials

The above discussion on titania as photocatalyst, although concise, showed that a critical factor to extend the role of catalysis for sustainable production and energy is the need to develop novel materials and concepts. This allows also to extend catalysis to the general area of functional materials, e.g. extending knowledge on the synthesis, control and mastering of catalytic nano-objects to advanced materials (sensors, smart and tunable materials, functional coatings, advanced storage, photonics, high-temperature resistant materials).

A very novel, but highly challenging area is that of introducing smart (catalytic) functionalities in materials for controlled drug release, cancer detection, new diagnostic methods, enhanced biosensing, and bio-compatible materials. For example, developing nanosized mesoporous materials in which the pore mouth is blocked by light-switchable molecular gates (for example, a molecule which can isomerize by light irradiation). The nanosized drug vehicle can also host functionalities for a preferential anchoring to target cells (to favor a selective recognition) and to enhance in-situ monitoring (fluorescent molecules, for example). The knowledge developed in the preparation of nano-tech catalysts is very important to design these smart systems for target drug release. However, it can also inspire new concepts for catalysis, for example in the design of smart catalysts hosted in a nanosized inorganic shell. A similar concept was used to stabilize metal nanoparticles by hosting in a porous silica shell (core–shell nanostructures) [17,18]. However, it may be also used to develop novel catalytic elements to improve performances of nanocomposite or control polymerization processes during forming or extrusion.

An enabling factor for all these applications, but also critical for the design of new advanced catalysts, is the possibility of control of the nano-architecture. The control, tuning and design of nano-architecture is a main priority for research in advanced materials and catalysis [19], and the key to develop a quite broad range of applications, in going from health protection, to advanced coatings and new catalysts. New synthesis methods offer new possibilities in this direction.

A critical aspect to develop catalysts for new sustainable processes is the possibility to realize in one-step complex multi-step reactions, possibly avoiding the presence of solvents. This will reduce waste, process complexity and risks, and improve process economics as well. However, it is necessary to develop multi-functional catalysts able to perform selectively complex multi-step reactions and/or design new efficient materials able to host in a single nanoreactor different catalytic components to perform efficiently cascade reactions.

A challenge is to nanostructure metal oxides to realize this suitable architecture. In fact, a key aspect of metal oxides is that they possess multiple functional properties: acid–base, redox, electron transfer and transport, chemisorption by σ and π-bonding of hydrocarbons, O-insertion and H-abstraction, etc. The control of the catalyst multi-functionality requires the ability to control their nano-architecture, e.g. the 3D spatial arrangement around the sites of adsorption. The active site is not the only relevant aspect for catalysis. The surrounding around the active site orients or assists the coordination of the reactants, may induce sterical constrains on the transition state, and influences short-range transport (nano-scale level). Therefore, it plays a critical role in determining the reactivity and selectivity in multiple pathways of transformation. In addition, there are indications pointing out that the dynamics of adsorbed species, e.g. their mobility during the catalytic processes, which is also an important factor determining the catalytic performances in complex surface reactions [20] is influenced from the nano-architecture.

Most of the studies on “nanostructured” oxides are based on materials not having a well-defined 3D structure (both on short- and long-range), being composed of irregularly shaped nano-crystals. These materials are polycrystalline, and show several nano-interfaces, which stabilize microstrains, oxygen vacancies or metal ions in unusual coordination states. A 3D environment for adsorption/transformation may significantly modify the adsorption of reactants and stabilization of transition state complexes, a well-known concept for enzymes, but typically not considered for solid catalysts.

In zeolite and mesoporous materials there are ample demonstrations of the relevance of these aspects on the catalytic behavior, thanks to the fine control of their pore structure. But the challenge is to develop a tailored 3D nano-architecture also for transition metal oxides. The advantages of a controlled 3D nano-architecture of transition metal oxides are the following: (i) a better control of the exposed crystalline faces, (ii) tuning of the supra-molecular effects around the active sites, (iii) improved mass- and heat-transfer, (iv) a better control of the spatial arrangement of active sites in cascade reactions, for example, (v) a possible vectorial-type electron and oxygen mobility which limit side reactions and (vi) the creation of new functional properties. It is known, for example, that V_2O_5 is not selective in *n*-butane oxidation, but become selective when vanadium oxide nanorods are formed by template preparation in carbon nanotubes [21]. Similarly, very small V_2O_5 nanoparticles (below 1 nm) supported on silicalite [22] are selective and more active (higher turnover number) in the oxidative dehydrogenation of propane, but larger particles only oxidize to carbon oxides, due to easier lattice oxygen removal and easier reconstruction to avoid surface oxygen vacancies which increase Lewis acidity of surface vanadium sites. However, sintering of these nano-oxides is an issue. The challenge is thus to create a nano-architecture which combines the advantages of nanosized oxides with a controlled nano-architecture allowing their stabilization and a fast mass- and heat-transfer.

Novel nano-fabrication techniques allow to synthesize metal oxides with defined nanostructure. An example of such materials is given by ordered arrays of vertically aligned 1D nanostructures (nanotubes, rods, coils, etc.) prepared by anodic oxidation [23–25]. These materials represent an interesting opportunity to develop improved catalysts. Some of the possibilities include (i) nanostructuring the surface in the form of catalytic nanoreactors, (ii) nanoconfinement and 3D geometrical architectures of active sites, (iii) nano-building of catalytic components, (iv) integration of homogeneous, heterogeneous and bio-catalytic elements, and (v) heterogenization of liquid phase reactions in surface-confined nano-drops.

Fig. 5 shows a conceptual example of the possibilities offered from structuring the surface of oxides in terms of nanoreactors. The SEM image in the inset of Fig. 5 shown an example of the TiO_2 nanostructures obtained in the case of anodic oxidation of titanium foils. Although there are several problems to overcome the difficulties in the preparation of practical catalysts based on this concept of nanostructured engineering of the surface of oxide catalysts (in particular, how to realize macro-structured catalysts with high surface area based on this nanostructuring concept), Fig. 5 shows that there are several challenging possibilities offered from this novel catalyst design.

It is possible to further extend this concept in terms of catalytic nanofactories which is schematically shown in Fig. 6. Similarly to a production chain in a factory, it is possible to consider that the future design of catalysts can be based on the possibility of tailored sequential introduction of active centres in a nanotube (all then assembled in an ordered array to form a membrane) to perform selectively the conversion of molecules passing through this porous film.

This imply the ability to understand the microkinetics of the aimed reactions, how to design optimal active catalytic elements for each of these steps, how to introduce these catalytic centers in the right sequence, etc. In other words, next generation catalysts should be based not on the testing of a number of materials to find

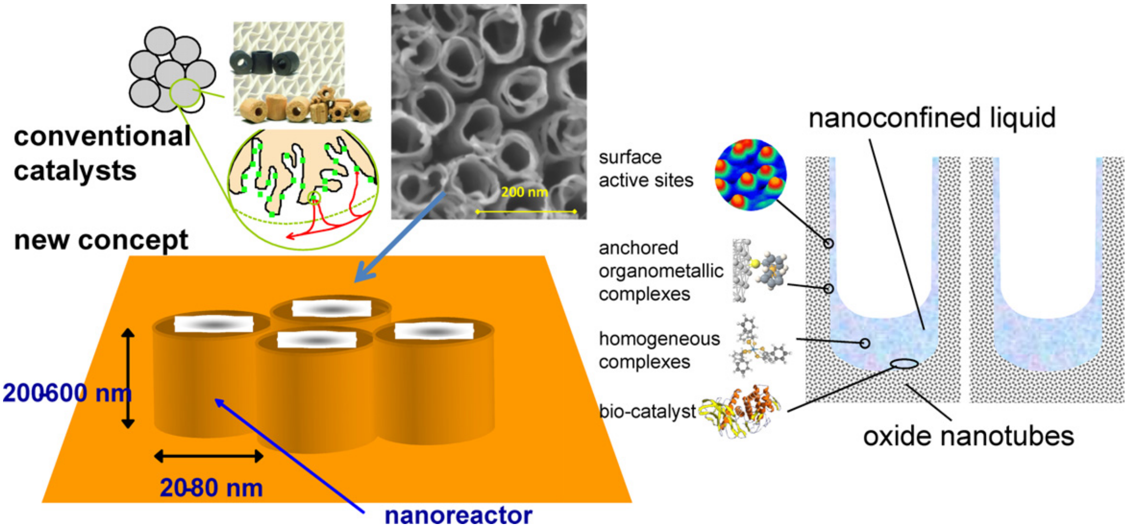

Fig. 5. Concept of nanoengineering of oxide catalytic surface in terms of nanoreactor array, some of the possibilities offered by this concept (in particular in terms of realizing multi-functional catalysts for cascade reactions in nanoconfined liquids) and a SEM image of an array of TiO_2 nanotubes produced by anodic oxidation of Ti foils.

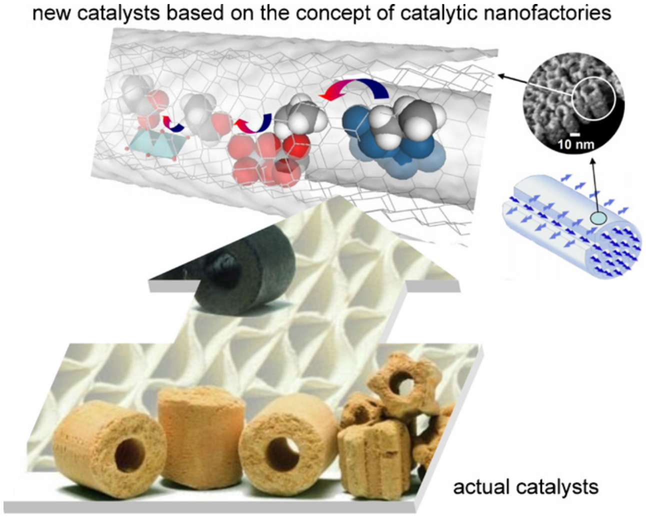

Fig. 6. Concept of change from actual catalysts to new generation of catalysts based on the concept of catalytic nanofactories.

the better ones for the target reaction, but on the ability to plan the sequence of active sites able to realize selectively the target reaction. The realization of this objective requires to create a platform of knowledge on catalysis, but at the same time allows to anticipate the need of a sustainable society.

5. Conclusions

Catalysis in an enabling technology to promote sustainability, environment, energy, health and quality of life. There is an increase of interest on catalysis, but at the same time a fast evolution of this area. Various factors driving the changes in catalysis research were discussed above, such as the need to go to more sustainable and modular-design of the chemical processes, the use of biomasses and renewables, the use of solar energy and/or electrocatalysis.

However, to fully implement catalysis as a enabling technology for societal challenges, not only an excellent research is necessary, but it is also need to overcome fragmentation barriers, particularly in catalysis areas (homo-, hetero- and bio-) and in academy–industry interactions. This requires to create a longer term vision and strong collaborations to develop a knowledge platform, in order to accelerate the innovation path. The realization of catalysis–society interactions, e.g. the creation of interfaces and structures to promote dissemination and spreading to society, is another relevant component for this objective.

Finally, the need to develop new catalytic materials, extend the use of catalysts to other areas, and address key societal issues (for example CO_2 conversion, sustainable energy) were emphasized.

Acknowledgements

This contribution was realized in the frame of the activities of the Network of Excellence IDECAT (NMP3-CT-2005-011730, Integrated Design of Catalytic Nanomaterials for a Sustainable Production) supported from the European Commission.

References

[1] UN World Commission On Environment, Development (headed by, G.H. Brundtland), Our Common, Future, Oxford University Press, Oxford, 1987.
[2] The European Technology Platform for Sustainable Chemistry, http://www.suschem.org.
[3] G. Centi, S. Perathoner, Catal. Today 77 (2003) 287.
[4] G. Centi, R.A. van Santen (Eds.), Catalysis for Renewables,, Wiley VCH Pub, Weinheim (Germany), 2007.
[5] P. Bert, C. Bianchini, G. Giambastiani, A. Marchionni, A. Tampucci, F. Vizza, It Patent. FI2007A000078 (2007).
[6] K. Drew, G. Girishkumar, K. Vinodgopal, P.V. Kamat, J. Phys. Chem. B 109 (2005) 11851.
[7] A. Patsoura, D.I. Kondarides, X.E. Verykios (University of Patras), Production Of Hydrogen By Photo-Induced Reforming At Room Temperature, EUROPACAT-VIII 26–31 August 2007, Turku/Åbo, Finland.
[8] G.W. Huber, J.W. Shabaker, J.A. Dumesic, Science 300 (2003) 2075.
[9] G.W. Huber, R.D. Cortright, J.A. Dumesic (Eds.), Angewandte Chemie, Intl. Ed. 43 (2004) 1549.
[10] S. Perathoner, G. Centi, M. Gangeri, Chimica e l'Industria (Milan Italy) 88 (2006) 28.
[11] G. Centi, R. Passalacqua, S. Perathoner, D.S. Su, G. Weinberg, R. Schlögl, Phys. Chem. Chem. Phys. 9 (2007) 4930.
[12] G. Centi, S. Perathoner, G. Winè, M. Gangeri, Green Chem. 9 (2007) 671.
[13] M. Yarime, University-Industry Collaboration for New Materials Innovation: The Case of Titanium Dioxide Photocatalyst in Japan, Presentation at the Workshop on Sustainable Materials Annual Meeting of the Alliance for Global Sustainability, Chalmers University of Technology, Gothenburg, Sweden, 2004, March 21–24.
[14] Y. Baba, M. Yarime, Science-technology-commercialization interaction networks: the case of titanium dioxide photocatalyst, in: Presentation at the International Symposium on Consolidation of Technology Management with Science Policy Research, Tokyo, January 30, 2003.

[15] A. Fujishima, K. Honda, Nature 238 (1972) 37.
[16] M. Fujihira, Y. Satoh, T. Osa, Nature 293 (1981) 206.
[17] J.D. MacKenzie, E.P. Bescher, Acc. Chem. Res. 40 (2007) 810.
[18] H. Hofmeister, P.-T. Miclea, W. Mörke, Part. Part. Syst. Char. 19 (2002) 359.
[19] G. Centi, S. Perathoner, Studies in Surface Science and Catal. 172 Science and Technology in Catalysis 2006, Kodansha/Elsevier, 2007,, p. 79.
[20] G. Centi, F. Cavani, F. Trifirò, Selective oxidation by heterogeneous catalysis, in: M.V. Twigg, M.S. Spencer (Eds.), Series: Fundamental and Applied Catalysis, Recent Developments, Kluwer/Plenum Publishing Corporation, New York & London, 2001.
[21] X.-W. Chen, Z. Zhu, M. Haevecker, D. Su, R. Schloegl, Mater. Res. Bull. 42 (2007) 354.
[22] G. Bellussi, G. Centi, S. Perathoner, F. Trifiro, ACS Symposium Series (1993), 523 (Catalytic Selective Oxidation), 281
[23] G.K. Mor, O.K. Varghese, M. Paulose, K. Shankar, C.A. Grimes, Sol. Energy Mater. Sol. Cells 90 (2006) 2011.
[24] S.P. Albu, A. Ghicov, J.M. Macak, R. Hahn, P. Schmuki, Nano Lett. 7 (2007) 1286.
[25] G. Centi, S. Perathoner, in: J.J. Spivey (Ed.), Nano-architecture and Reactivity of Titania Catalytic Materials. Quasi-1D Nanostructures, in Catalysis, 20, Royal Society of Chemistry Pub, Cambridge, 2007, p. 367.