Science and technology for a sustainable world

The beauty and utility of science is recognized today more than ever. The fast reaction of science and technology to the challenge introduced by Covid-19 has shown the importance of fundamental research and knowledge acquisition to face present and future challenges within our society. Following this, I believe that, today, all critical boundaries between fundamental and applied science have to disappear. It is even clearer when considering the equations that are at the origin of the technological advances:

Science + Engineering = Technology
Technology + Marketing = Innovation

We can see that the fundamental knowledge (Science) acquired through basic research is at the origin of any technological breakthrough.
The above also applies to the research field I work in chemistry: heterogeneous catalysis and molecular sieve catalysts. This discipline has an extraordinary impact on our daily life for mobility, making molecules for polymers, healthcare, removal of contaminants, and, in general for improving chemical processes. Catalysts are able to increase the rate of chemical reactions, while directing them towards the formation of the desired products, avoiding the formation of undesired residues. We can see that catalysis is today a core discipline when considering sustainability and circular economy.
Furthermore, catalysis plays a very relevant role in the process of decarbonization. This involves the crucial tasks of designing and developing catalysts that are both highly active and stable, particularly in the electrochemical dissociation of water into oxygen and hydrogen and for the activation of carbon dioxide (CO_2). These processes can facilitate the production of chemical molecules using only renewable sources of carbon and hydrogen. These sources include carbon extracted directly from atmospheric CO_2 (and indirectly from biomass) and hydrogen derived from water. This emphasis on advancing catalyst technologies is a must for advancing in a sustainable and environmentally friendly chemical processes. Therefore, chemistry and catalysis are facing a new era in where the starting molecules to produce fuels and chemical products will shift from fossil hydrocarbons to CO_2 and H_2, as well as from biomass. We can see now the importance and relevance of the research carried out on CO_2 adsorption and separation, particularly in addressing emissions from stationary sources characterized by higher concentrations of CO_2. These sources include cement and steel manufacturing, the ceramic industry, power plants and refineries, among others.
One can say that net CO_2 emissions would not be produced in most of the above sectors, if fossil carbon was not used to produce energy by combustion. While, this is true and we know that real sustainability will require replacing fossil fuels, we also know that we still need time to develop alternative technologies. Thus, a dual strategy becomes imperative: on one side, efforts should be intensified to maximize energy saving, minimizing the environmental impact of today existing processes. Simultaneously, there is a need to booster the supply of renewable energies, together with recycling the CO_2 produced to obtain fuels and chemicals.

It should be pointed out, that many of the scientific and technological developments that were made when developing the oil refining a petrochemical and chemical industries will be key for the decarbonization program. There is no doubt that all the fundamental knowledge on chemistry and catalysis developed up to know will be at the bases for achieving the goals in the new scenarios. In fact, different solutions are contemplated for decarbonization, but none of them is seen yet as a clear unique solution. This forces researchers and inventors to keep the scenario open to all the potential solutions since more than one will probably be required to achieve the final objective. Even if we see today one of them more suitable as a final solution for a decarbonized society, the "kinetics" to reach that final state may be slow and, in the crossing of the dessert, several other "solutions" will also have to be used.
There is a tendency today to think that H_2 is the final word. While this may be true at a longer term, we have to take into account that we still have not the definitive solutions for storing and transporting H_2, provided, of course, that all the renewable energy for producing the H_2 required is available. Serious mass, and energy balances are required to know the requirements to substitute the ~$4.5x10^9$ metric tons per year of oil, plus ~$3x10^{12}$ m^3 of natural gas and ~$8x10^9$ Tm of carbon by renewal energy. Most of fossil carbon is used today to produce energy, but it is ~10% that is used for manufacturing chemicals. In other words, ~10% of the fossil carbon is used as a source of the carbon and hydrogen present in the chemical molecules that we produce. It appears that even in the case we can produce all the energy required from renewable sources, still we will have to obtain our chemicals containing carbon and hydrogen from renewable sources of carbon and H_2, i.e. CO_2, H_2O and biomass. We will need then to capture and activate CO_2, produce H_2 from water and to transform platform molecules from biomass into valuable chemical products.

In this commitment, catalysis is already playing a key role. Scientist working in catalysis are directing the efforts to achieve a nearly perfect design of catalysts by introducing the active sites that selectively will drive reactions to form the desired products. In the case of solid catalysts, to achieve a surface with well-defined and homogeneous active sites it is not trivial. This becomes even more challenging when considering the surface dynamics in the presence of reactants that have the potential to modify the nature of the initially synthesized catalysts. Then, to generate fundamental knowledge at the molecular level on the interactions and reactivity of the molecules on solid surfaces during the catalytic reactions it is important not only to understand how a given chemical process can be catalysed, but also to design new solid catalyst that can go beyond incremental improvements. Catalysis by being interdisciplinary will require advances in nanomaterials preparation, computational chemistry and operando spectroscopic characterization of realistic catalyst and under reaction conditions. We should also consider that microkinetic studies will help to understand the reaction mechanisms and the interaction of reactants and products with the active sites. We have attempted to follow the above methodology in our work on zeolites and zeolitic catalysis, by combining the synthesis work with characterization of the materials, computational chemistry and reactivity studies. Indeed, by controlling the synthesis conditions of zeolites and by introducing new concepts for directing the synthesis, we have achieved a plethora of new zeolite structures with a wide range of pore dimensions and pore topologies that have added new possibilities to these materials for molecular separations and for selective catalysis. Furthermore, by introducing machine-learning techniques we have added new possibilities for the synthesis of zeolite materials. Also, by locating the active sites selectively in pre-established positions in the structure, and by an "ab initio" synthesis of the zeolitic structure that better stabilizes the reaction transition state for a given reaction, we have approached the catalytic behaviour of zeolites to that of enzymes.

We have also attempted to achieve well defined single or multiple active sites in catalysis by supporting single metal atoms or clusters of 3-10 atoms on different solid structures with, sometimes, unique selectivities for different chemical reactions. Finally, the preparation of multifunctional solid catalysts show the benefit to perform multistep reactions in a cascade mode with the corresponding intensification of the process and their impact on sustainability.

I always felt that besides attempting to increase the general knowledge in my discipline, I should try to transfer that knowledge into applications for improving the living standards of humankind. Following this, besides reporting our results in scientific publications, we have published a number of patents that have found applications in several industrial process. These processes are in the frame of sustainability. I am proud that the concept of doing good science while transferring this science to the production system, has been successfully transmitted and it is now in the DNA of my students and collaborators, being this a key characteristic of the Instituto de Tecnología Química (ITQ) that we found in 1990.

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Patents:

- Process for the obtainment of a light paraffin isomerization catalyst.
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- Structure material of the zeolite type with ultralarge pores and a lattice comprised of silicone and titanium oxides: its synthesis and utilization for the selective oxidation of organic products.
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Authors: Valencia Valencia S.; Canos Corma A.
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- Oxidation of ketones to esters using a tin substituted zeolite beta.
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- Microporous acidic oxide with catalytic properties itq-18
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